Lecture Notes on Solid State Physics

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Chapter 1 Lattice Vibration

1.1 Lattice vibration of monoatomic linear chain and phonon 1
1.2 Fluctuation of energy and position and coherent state 7
1.3 Lattice vibration of one-dimensional diatomic lattice 11
1.4 Lattice vibration of three-dimensional lattice 14
1.5 Sum rule and Coulomb lattice 18
1.6 Long wavelength vibrations of optical branches 21
1.7 Electron-longitudinal optical phonon interaction 28

Chapter 2 Electron-Lattice Interaction (Monovalent Metal Case)

2.1. Separation of the electronic and nuclear motions 36
2.2 Electron-phonon interaction 40
2.3 Rigid Ion Approximation 43
2.4 Pseudopotential Methods and Electron-Phonon Interaction 44
2.5 Electron-Phonon Interaction and Screening Effect 50

Chapter 3 Deformation Potential

3.1 Bardeen-Shockley Theory 56
3.2 Deformation Potentials in Silicon and Germanium 60

Chapter 4 Motion of Wave Packet and the Boltzmann Equation

4.1 Motion of Wave Packet 64
4.2 Concept of Holes 71

Chapter 5 Slowly Varying Fields

5.1 Wannier Function and Slater's Theory 76
5.2 Effect of the Magnetic Field on an Electron moving in the Periodic Potential 80

Chapter 6 Transport Phenomena

6.1 Bloch Equation 85
6.2 Relaxation Time Approximation 88
6.3 Electrical and Thermal Conductivities 90
6.4 Thermoelectric Effects, Kelvin Relation and Onsager Relations 95
6.5 Phonon Drag Effect 107
6.6 Transport Coefficients of Semiconductors 113

6.7 General Theory of the Transport Phenomena in Magnetic Fields 115

Chapter 7 Mechanism of Scattering Processes

7.1 Acoustic Phonon Scattering 145
7.2 Phon Cloud 152
7.3 Scattering Processes in Many Valley Semiconductors 154
7.4 Herring-Vogt’s Theory 155
7.5 Piezoresistance and Deformation Potential 158
7.6 Scattering due to Non-Polar Optical Phonon 164
7.7 Intervalley Scattering and Mobilities of *n*-Ge and *n*-Si 166
7.8 Ionized Impurity Scattering 172
7.9 Coulomb Scattering and Validity of the Born Approximation 180
7.10 Piezoelectric Scattering 184
7.11 Polar Optical Phonon Scattering 192
7.12 Neutral Impurity Scattering 197
7.13 Dipole Scattering due to the Ion Pairs in Compensated Semiconductors 201

Chapter 8 Band Structures of Semiconductors and Fermi Surface of Semimetals

8.1 Kane model 204
8.2 Band Structures and Mobilities of P-type Germanium and Silicon 209
8.3 Fermi Surfaces of Bismuth, Antimony, and Arsenic 219
8.4 Band Structure and Fermi Surface of Graphite 229

Chapter 9 Boltzmann-Bloch Equation

9.1 Conductivity of Monovalent Metals with an Isotropic Effective Mass 235
9.2 Thermal Conductivity of Metals, 250
9.3 Application of Variation Principle to Conduction Phenomena 253
9.4 Calculation of the Transport Coefficients due to the Variation Principle 261
9.5 Electrical conductivity of polar Semiconductors, Application of Variation Principle 268
9.6 T^2 dependence of the electrical resistivity in the Semimetals with elongated Fermi Surface 278
9.7 Validity of the Boltzmann-Bloch Equation 286

Chapter 10 Interaction with Localized Spins

10.1 Magnetic Semiconductors 290
10.2 *s*-*d* Interaction 291
10.3 Spin Disorder Scattering due to Localized Spins 295
10.4 Magnetoresistance of the Ferromagnetic Semiconductors 303

10.5 Critical Scattering around the Curie Temperature 307
10.6 Example of the Magnetic Semiconductors 310
10.7 Kondo Theory of the Resistance Minimum 320

Chapter 11 Conduction in Strong Magnetic Field (I)

11.1 Wave Function in Magnetic Field, Landau Level 335
11.2 Theory of Transverse Conductivity (Adams-Holstein Theory) 343
11.3 Tileica Theory on the Transverse Conductivity in Strong Magnetic Field 349
11.4 Kubo formula 352
11.5 Quantum Theory of the Electrical Conduction in Strong Magnetic Field 356
11.6 Impurity Scattering in Strong Magnetic Field 363
11.7 Phonon Scattering in Strong Magnetic Field 380
11.8 Acoustic Phonon Scattering 384
11.9 de Haas-van Alphen Effect 390

Chapter 12 Conduction in Strong Magnetic Field (II)

12.1 Conduction with Non-equilibrium Phonon Distribution 398
12.2 Thermomagnetic Coefficients in Strong Magnetic Field and the Onsager Relation 402
12.3 A Note on the Diffusion Term of the Thermopower in Strong Magnetic Field 411
12.4 Negative Longitudinal Magnetoresistance in the Quantum Limit 414
12.5 Esaki Kink Effect 421
12.6 Magnetic Breakdown 423

Chapter 13 Surface and Size Effects. Electron-Sound Wave Interaction 430
13.1 Chamber’s Theory 431
13.2 Normal Skin Effect 436
13.3 Anomalous Skin Effect 438
13.4 Azbel-Kaner Cyclotron Resonance 446
13.5 Surface State induced by Magnetic Field 453
13.6 Electron-Sound Wave Interaction 461
13.7 Weinreich Relation 477
13.8 Conduction Electron Spin Resonance (CESR) 479

Chapter 14 Transport Phenomena related to the Nonequilibrium Phonon Distribution.

14.1 Phonon Drag Effect in Semiconductors. Herring Theory 493
14.2 Theory of the Phonon Drag Effect based on the Boltzmann Equation 513
14.3 Two-Stage Drag Effect 529

Chapter 15 Theory of the Galvanomagnetic Effects with Magnetic Breakdown

15.1 Application of the Chamber's Theory to the Case with Magnetic Breakdown 532
15.2 Magnetoresistance for the Electron Orbit with a One-dimensional Periodic Potential 536
15.3 Transition Matrix for the Hexagonal Orbit 538

APPENDIX

Appendix 1 541
Appendix 2 547
Appendix 3 548
Appendix 4 553
Appendix 5 555
Appendix 6 557
Appendix 7 559
Appendix 8 564
Appendix 9 569
Appendix 10 571
Appendix 11 573
Appendix 12 574
Appendix 13 575
Appendix 14 578

REFERENCES 583

Chapter 1 Lattice Vibration

1.1 Lattice vibration of monoatomic linear chain and phonon

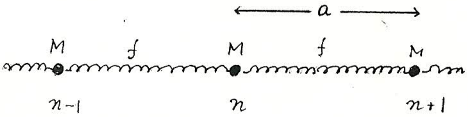

Fig. 1.1 Monoatomic linear chain

Consider a linear chain of equivalent atoms of mass M with an equilibrium lattice constant a and assume the harmonic forces between neighboring atoms. Hamiltonian of the system is

$$\mathcal{H} = \sum_n \left\{ \frac{p_n^2}{2M} + \frac{f}{2}(x_n - x_{n+1})^2 \right\}, \tag{1.1}$$

where p_n is the momentum of the n-th atom and x_n is the displacement from the equilibrium position. The equation of motion of the n-th atom is

$$\dot{x}_n = \frac{\partial \mathcal{H}}{\partial p_n} = \frac{p_n}{M}, \quad \dot{p}_n = -\frac{\partial \mathcal{H}}{\partial x_n} = f(x_{n+1} + x_{n-1} - 2x_n). \tag{1.2}$$

To find solutions of (1.2), we employ the periodic boundary condition $x_{n+N} = x_N$ which was introduced by Born and von Karman.

We transform x_n and p_n to normal coordinates Q_q and P_q:

$$x_n = \frac{1}{\sqrt{NM}} \sum_q e^{iqna} Q_q , \quad p_n = \sqrt{\frac{M}{N}} \sum_q e^{-iqna} P_q \tag{1.3}$$

The allowed values of q are obtained by the periodic boundary condition $x_{n+N} = x_n$ as follows :

$$qa = \frac{2\pi l}{N} , \quad -N/2 < l < N/2 . \tag{1.4}$$

The coordinates x_n and p_n are real variables, so that

$$Q_{-q} = Q_q^+ , \quad P_{-q} = P_q^+ . \tag{1.5}$$

By making use of the relation

$$\sum_{n=1}^{N} e^{ina(q-q')} = N \delta_{q,q'} . \tag{1.6}$$

we get

$$Q_q = \sqrt{\frac{M}{N}} \sum_{n=1}^{N} e^{-iqna} x_n , \; P_q = \frac{1}{\sqrt{NM}} \sum_{n=1}^{N} e^{iqna} p_n , \tag{1.7}$$

Thus the Hamiltonian (1.1) is written as

$$H = \sum_q \left\{ \frac{1}{2} P_q^+ P_q + \frac{f}{M} (1 - \cos qa) Q_q^+ Q_q \right\} . \tag{1.8}$$

Using (1.2) and (1.7),

$$\ddot{Q}_q = - \frac{2f}{M} (1 - \cos qa) Q_q = - \omega_q^2 Q_q . \tag{1.9}$$

Then,

$$H = \sum_q \left(\frac{1}{2} P_q^+ P_q + \frac{1}{2} \omega_q^2 Q_q^+ Q_q \right) . \tag{1.10}$$

(1.10) indicates that the Hamiltonian is an assembly of N independent harmonic oscillators.

In the long wave length limit $q \to 0$, ω_q becomes

$$\omega_q = \sqrt{\frac{fa}{M/a}}\, q. \qquad (1.11)$$

(1.11) is equal to the classical circular frequency of the vibration of string with tension fa and linear density M/a.

Above results correspond to the classical mechanics. The extension to quantum mechanics is straightforward.

The commutation relation $[p_n, x_{n'}] = (\hbar/i)\,\delta_{nn'}$ leads to

$$[P_q, Q_{q'}] = \frac{\hbar}{i}\,\delta_{qq'}. \qquad (1.12)$$

Let introduce the linear transformation:

$$b_q = \frac{\omega_q Q_q + i P_q^+}{(2\hbar\omega_q)^{1/2}}, \quad b_q^+ = \frac{\omega_q Q_q^+ - i P_q}{(2\hbar\omega_q)^{1/2}}. \qquad (1.13)$$

b^+, b obey the Boson commutation relation

$$\begin{cases} [b_q, b_{q'}^+] = \delta_{q,q'} \\ [b_q, b_{q'}] = [b_q^+, b_{q'}^+] = 0 \end{cases} \qquad (1.14)$$

The inverse transformation to (1.13) is

$$Q_q = \sqrt{\frac{\hbar}{2\omega_q}}\,(b_q + b_{-q}^+), \qquad P_q = -i\sqrt{\frac{\hbar\omega_q}{2}}\,(b_{-q} - b_q^+). \qquad (1.15)$$

Inserting (1.15) into (1.10), we obtain

$$\mathcal{H} = \sum_q \hbar\omega_q \left(b_q^+ b_q + \frac{1}{2}\right) = \sum_q \mathcal{H}_q .$$

In deriving (1.16), (1.14) is employed. From (1.14) and (

one finds

$$[b_q^+, \mathcal{H}] = -\hbar\omega_q b_q^+ , \quad [b_q, \mathcal{H}] = \hbar\omega_q b_q . \qquad ($$

If $|n\rangle$ is an eigenvector of $n = b^+ b$, and E_n the corre
eigenvalue, then

$$\begin{cases} \langle n' | b^+ | n \rangle (E_n - E_{n'} + \hbar\omega) = 0, \\ \langle n' | b | n \rangle (E_n - E_{n'} - \hbar\omega) = 0. \end{cases} \qquad ($$

Namely, b^+ is an operator inducing the transition $E \rightarrow E +$
and on the contrary b induces the transition $E \rightarrow E - \hbar\omega$
b^+ and b are called creation and annihilation (or destru
operators. (1.18) indicates that the energy level arranges wi
equidistance $\hbar\omega$.

The ground state ψ_0 satisfying the condition of $b\psi_0 = 0$
certainly exists. If it does not so, by operating b
repeatedly on an arbitrary eigenfunction ψ we get
state with negative energy.

Therefore,

$$\hbar\omega_q b_q^+ b_q \psi_0 = (H_q - \tfrac{1}{2}\hbar\omega_q)\psi_0 = 0, \qquad (1.19$$

ψ_0 is the state with eigenvalue $\frac{1}{2}\hbar\omega_q$ which is the zero po energy. The zero point energy is characteristic in the quantu mechanics.

From (1.18) we obtain $\langle n|b^+b|n\rangle = \langle n|b^+|n-1\rangle\langle n-1|b|n\rangle$ $= |\lambda_n|^2 = n$ and (1.16) becomes

$$H = \sum_q \hbar\omega_q (n_q + 1/2), \quad b_q^+ b_q = n_q = 0, 1, 2, \cdots. \qquad (1.2$$

The system composed of the classical harmonic oscillators is quantized and normal modes are replaced by an equival corpuscular description, so called "phonon". Its occupation number in thermal equilibrium is given by the Planck distribution :

$$n_q^\circ = 1/(e^{\hbar\omega_q/k_0T} - 1), \quad k_0: \text{Boltzmann constant.} \qquad (1.$$

Nonvanishing matrix elements of b_q and b_q^+ are

$$\langle n_q - 1|b_q|n_q\rangle = \langle n_q|b_q^+|n_q - 1\rangle = \sqrt{n_q}. \qquad (1.$$

Inserting (1.15) into (1.3), one gets

$$x_n(t) = \sum_q \sqrt{\frac{\hbar}{2NM\omega_q}} \left\{ e^{i(qna - \omega_q t)} b_q(0) + e^{-i(qna - \omega_q t)} b_q^+(0) \right\}. \qquad (1.$$

(1.23) denotes that n_q is proportional to the square of the q-th normal mode of $x_n(t)$.

In the language of wave mechanics the Hamiltonian of a harmonic oscillator is

$$H = -\frac{\hbar^2}{2M}\frac{d^2}{dx^2} + \frac{1}{2}M\omega^2 x^2, \qquad (1.24)$$

and the ground state eigenfunction is

$$\psi_0 = (M\omega/\pi\hbar)^{1/4} \exp\left(-\frac{M\omega}{2\hbar}x^2\right). \qquad (1.25)$$

Normalized excited wave function is given by

$$\left\{\begin{aligned} &\psi_n = (n!)^{-1/2}(b^+)^n\psi_0 = \left\{\left(\frac{\alpha}{\pi}\right)^{1/2}\frac{1}{2^n n!}\right\}^{1/2} e^{-\alpha x^2/2} H_n(\sqrt{\alpha}\, x), \\ &\alpha = \frac{M\omega}{\hbar}, \quad H_n: \text{ n-th order Hermite function.} \end{aligned}\right. \qquad (1.26)$$

It should be noted that behavior of $|\psi_0|^2$ is entirely different from that of the classical oscillator. In the classical case the probability distribution in the vicinity of $x=0$, where the velocity takes a maximum value, should be minimum, while $|\psi_0|^2$ becomes maximum at $x=0$. However, with increasing n $|\psi_0|^2$ asymptotically approaches to the classical distribution.$^{1)}$

1.2 Fluctuation of energy and position and Coherent state

After quantizing procedure of the classical wave equation (1.2), quantum mechanical corpuscule "phonon" is introduced.

Such a wave-corpuscule duality is clearly revealed by inspection of energy fluctuation of the harmonic oscillator.

For simplicity, a dispersion relation $\omega_q = v_s q$ is assumed.

The number of modes in a frequency range $\Delta\omega$ is

$$f = \frac{L}{2\pi}\Delta q = \frac{L\Delta\omega}{2\pi v_s}, \quad (L : \text{length of the linear chain}). \qquad (1.27)$$

From (1.21) and (1.27) the mean energy becomes

$$\langle E\rangle = f\hbar\omega n_q^{\circ} = L\,U(\omega)\Delta\omega = \frac{L\hbar\omega}{2\pi v_s}\,\frac{\Delta\omega}{e^{\hbar\omega/k_oT}-1}. \qquad (1.28)$$

Since f modes are independent each other,

$$L\,U(\omega)\Delta\omega = \sum_{s=1}^{f}\langle E_s\rangle = \langle E\rangle. \qquad (1.29)$$

Assuming E_s being dependent on a variable λ,

$$\langle E_s\rangle = \sum_{\lambda} E_s(\lambda)\, e^{-E_s(\lambda)/k_oT} \Big/ \sum_{\lambda} e^{-E_s(\lambda)/k_oT}. \qquad (1.30)$$

Similarly, $\langle E_s^2\rangle$ is obtained from (1.30). Thus, we have

$$\langle \Delta E^2\rangle = \left\langle \left(\sum_s E_s - \sum_s \langle E_s\rangle\right)^2\right\rangle = \sum_{s=1}^{f}\langle (E_s - \langle E_s\rangle)^2\rangle$$

$$= \sum_{s=1}^{f}\left(\langle E_s^2\rangle - \langle E_s\rangle^2\right). \qquad (1.31)$$

(1.30) and (1.31) lead to

$$\langle \Delta E^2 \rangle = \frac{\partial \langle E \rangle}{\partial(-1/k_0T)} = \frac{L\, U(\omega)}{\partial(-1/k_0T)} \Delta\omega. \tag{1.32}$$

Then,

$$\langle \Delta E^2 \rangle = \frac{L\,(\hbar\omega)^2 \Delta\omega}{2\pi v_s} \left\{ \frac{1}{e^{\hbar\omega/k_0T}-1} + \frac{1}{(e^{\hbar\omega/k_0T}-1)^2} \right\}, \tag{1.33}$$

$$\left\{ \begin{aligned} &\langle \Delta E^2 \rangle = \hbar\omega \langle E \rangle + \frac{2\pi v_s \langle E \rangle^2}{L\Delta\omega}, \\ &\frac{\langle \Delta E^2 \rangle}{\langle E \rangle^2} = \frac{1}{\langle E \rangle/\hbar\omega} + \frac{1}{L\Delta\omega/2\pi v_s} \end{aligned} \right. \tag{1.34}$$

(1.34) is the same formula to the one derived by Einstein in the photon system. The first term in the right hand side corresponds to the particle fluctuation and the second term denotes the coherent effect of the elastic wave. This indicates that the Planck distribution includes the wave-corpuscule duality.

Fluctuation of the position at absolute zero temperature is calculated from (1.22) and (1.23)

$$\langle (\Delta x_n)^2 \rangle = \langle 0 | x_n^2 | 0 \rangle = \sum_q \left(\frac{\hbar}{2NM\omega_q} \right) \left(b_q b_q^+ + b_q^+ b_q \right) = \frac{\hbar}{2NM} \sum_q \frac{1}{\omega_q}, \tag{1.35}$$

where $\langle 0 | x_n | 0 \rangle = 0$ is employed.

(1.35) is roughly proportional to $1/M\Theta_D$, where Θ_D is the Debye temperature.

According to Dirac, we can introduce the phase operator ϕ of the wave, putting

$$b_q = e^{i\phi_q}\sqrt{n_q}\,, \quad b_q^+ = \sqrt{n_q}\, e^{-i\phi_q}. \tag{1.36}$$

For ϕ we then get the equation from (1.14)

$$e^{i\phi_q} n_q - n_q e^{i\phi_q} = e^{i\phi_q} \tag{1.37}$$

(1.37) is satisfied if ϕ_q and n_q obey the commutation relation

$$[\phi_q, n_q] = -i\,. \tag{1.38}$$

This can be easily verified. By repeated application of (1.38) we obtain $[\phi^k, n] = -ik\phi^{k-1}$. Multiplying $i^k/k!$ and summing over k, one obtains (1.37). From (1.38) we might conclude the uncertainty relation

$$\Delta n_q \Delta\phi_q \geq 1. \tag{1.39}$$

However, this is not correct. ϕ is not a well-defined Hermite operator.[2)] But in the case of the particle number N being enough large, namely $N \gg \sqrt{N} \gg 1$, we can construct the state where the particle number and the phase are simultaneously determined. This state is termed as the coherent state.

The wave packet defined by

$$\left\{\begin{array}{l} \Phi(\phi) = \sum_{n=0}^{\infty} e^{in\phi} \sqrt{w_n}\, \psi_n , \\ \\ \psi_n = (n!)^{-1/2} (b^+)^n \psi_0 , \quad w_n = N^n e^{-N}/n! , \end{array}\right. \tag{1.40}$$

is introduced. $\Phi(\phi)$ is an eigenstate of the operator b, because

$$b\,\Phi(\phi) = \sqrt{N}\, e^{i\phi}\, \Phi(\phi). \tag{1.41}$$

The particle fluctuation ΔN for (1.40) satisfies $\Delta N = \sqrt{N} \ll N$. The state of the total system is represented by

$$\Phi = \prod_q \Phi(\phi_q). \tag{1.42}$$

The mean value of x_n is given by

$$\langle \Phi | x_n | \Phi \rangle = \sum_q \sqrt{\frac{\hbar}{2NM\omega_q}} \sqrt{n_q} \left\{ e^{i(qna - \omega_q t + \phi_q)} + e^{-i(qna - \omega_q t + \phi_q)} \right\}. \tag{1.43}$$

(1.43) represents a classical vibration with amplitude $\sqrt{\hbar n_q / 2NM\omega_q}$ and phase ϕ_q.

The coherent state is very useful to present a quantum mechanical description of the coherent light source,[3)] and superconducting and superfluid states.

1.3 Lattice vibration of one-dimensional diatomic lattice

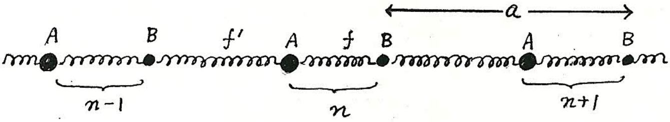

Fig. 1.2 One-dimensional diatomic lattice

Consider a linear chain with lattice constant a, with two atoms in each unit cell, the masses of the atoms being m_A and m_B. Force constants are f and f'. Equilibrium positions are denoted by X_{An}, X_{Bn}. The equation of motion can be written as

$$\begin{cases} m_A \ddot{x}_{An} = f(x_{Bn} - x_{An}) + f'(x_{Bn-1} - x_{An}), \\ m_B \ddot{x}_{Bn} = f'(x_{An+1} - x_{Bn}) + f(x_{An} - x_{Bn}). \end{cases} \tag{1.44}$$

Assuming

$$\begin{cases} x_{An} = \dfrac{1}{\sqrt{Nm_A}} \sum\limits_q C(q)\, e_A(q)\, e^{i(qX_{An} - \omega(q)t)}, \\[2ex] x_{Bn} = \dfrac{1}{\sqrt{Nm_B}} \sum\limits_q C(q)\, e_B(q)\, e^{i(qX_{Bn} - \omega(q)t)}, \end{cases} \tag{1.45}$$

and inserting (1.45) into (1.44), one obtains

$$\begin{cases} \omega^2(q)\, e_A(q) = M_{AA}\, e_A(q) + M_{AB}\, e_B(q), \\ \omega^2(q)\, e_B(q) = M_{BA}\, e_A(q) + M_{BB}\, e_B(q), \end{cases} \tag{1.46}$$

where

$$\left\{\begin{aligned} M_{AA} &= \frac{f+f'}{m_A}, \quad M_{BB} = \frac{f+f'}{m_B}, \\ -M_{AB} &= \frac{f}{\sqrt{m_A m_B}} e^{iq(X_{Bn}-X_{An})} + \frac{f'}{\sqrt{m_A m_B}} e^{iq(X_{Bn-1}-X_{An})}, \\ -M_{BA} &= \frac{f}{\sqrt{m_A m_B}} e^{iq(X_{An}-X_{Bn})} + \frac{f'}{\sqrt{m_A m_B}} e^{iq(X_{An+1}-X_{Bn})}. \end{aligned}\right. \tag{1.47}$$

$M_{AB} = M_{BA}^{+}$, since $X_{An+1} - X_{Bn} = X_{An} - X_{Bn-1}$ (See Fig. 1.2).

Rewriting (1.46) in the matrix form

$$\omega^2(q)\,\mathbf{e}(q) = \mathbf{M}(q)\,\mathbf{e}(q),$$

$$\mathbf{e}(q) = \begin{pmatrix} e_A(q) \\ e_B(q) \end{pmatrix}, \quad \mathbf{M}(q) = \begin{pmatrix} M_{AA} & M_{AB} \\ M_{BA} & M_{BB} \end{pmatrix}. \tag{1.48}$$

(1.48) is only compatible if

$$\begin{vmatrix} M_{AA}-\omega^2 & M_{AB} \\ M_{BA} & M_{BB}-\omega^2 \end{vmatrix} = 0. \tag{1.49}$$

The roots of this are

$$\omega^2(q) = \frac{f+f'}{2}\left(\frac{1}{m_A}+\frac{1}{m_B}\right) \pm \frac{1}{2}\sqrt{(f+f')^2\left(\frac{1}{m_A}+\frac{1}{m_B}\right)^2 - \frac{16ff'}{m_A m_B}\sin^2\left(\frac{qa}{2}\right)}. \tag{1.50}$$

ω_q - q curve consists of two branches. The branch relating to the minus sign before the square root is called the acoustic branch, and for this branch $\omega(q) \to 0$ as $q \to 0$. The other branch is called the optical branch, and as $q \to 0$ $\omega^2(q) \to (f+f')(1/m_A + 1/m_B)$.

To get qualitative feature of (1.50), we put $m_A = m_B = m$. (1.50) becomes

$$\begin{cases} \omega_1^2(q) = \dfrac{f+f'}{m} - \dfrac{1}{m}\sqrt{(f+f')^2 - 4ff'\sin^2\left(\dfrac{qa}{2}\right)}, \\ \omega_2^2(q) = \dfrac{f+f'}{m} + \dfrac{1}{m}\sqrt{(f+f')^2 - 4ff'\sin^2\left(\dfrac{qa}{2}\right)}. \end{cases} \qquad (1.51)$$

In Fig. (1.3) ω_1, ω_2 versus q curves are shown, where $f > f'$ is assumed.

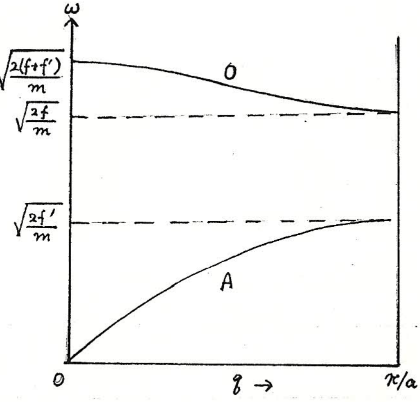

Fig. 1.3 Dispersion curves of one-dimensional diatomic lattice. A : acoustic mode; O: optical mode.

For the acoustic mode

$$\frac{e_B(q)}{e_A(q)} = \frac{\Gamma(q)}{|\Gamma(q)|},$$

and for the optical mode

$$\frac{e_B(q)}{e_A(q)} = -\frac{\Gamma(q)}{|\Gamma(q)|},$$

where

$$\Gamma(q) = e^{iq(X_A - X_B)}(f + f' e^{iqa}). \qquad (1.52$$

X_A and X_B are the equilibrium positions in a unit cell.

As $q \to 0$, two atoms A and B move in phase in the acoustic branch, and out of phase in the optical branch.

1.4 Lattice vibration of three-dimensional lattice

The procedures in treating the three-dimensional lattice vibration are in principle the same as for the one-dimensional case. The Hamiltonian is

$$H = \sum_i \frac{P_i^2}{2M} + \frac{1}{2}\sum_{i \neq j} V(R_i - R_j). \qquad (1.53)$$

Putting $R_i = R_i^0 + \xi_i$ and developing $V(R_i - R_j)$ around the equilibrium position R_0 up to the second order in ξ_i, we get

$$\sum_{i \neq j} V(R_i - R_j) = \sum_{i \neq j} \Big\{ V(R_i^0 - R_j^0) + \big[(\xi_i \cdot \nabla_i)(\xi_i \cdot \nabla_i) + (\xi_i \cdot \nabla_i)(\xi_j \cdot \nabla_j)\big]$$
$$\times V(R_i^0 - R_j^0) \Big\} = \text{constant} + \sum_{ij} \xi_i \cdot \Gamma_{ij} \cdot \xi_j. \qquad (1.54)$$

To get the explicit expression of Γ_{ij}, we decompose $V(R_i^0 - R_j^0)$ into the Fourier series:

$$V(R_i^0 - R_j^0) = \sum_q V_q e^{iq \cdot R_{ij}^0}, \quad (R_{ij}^0 = R_i^0 - R_j^0), \qquad (1.55)$$

where $\sum_q$ is taken over all q including reciprocal vectors.

Then,

$$\begin{cases} \Gamma_{ij} = \sum_{q} qq\, V_q\, e^{iq\cdot R_{ij}^0} \quad (i \neq j) \\ \Gamma_{ii} = -\sum_{q}\sum_{j(\neq i)} qq\, V_q\, e^{iqR_{ij}^0}. \end{cases} \tag{1.56}$$

Since V is real, $V_q^+ = V_{-q}$ and ~~accordingly~~ Consequently $\Gamma_{ij} = \Gamma_{ij}^+$ are concluded.

Introducing the normal coordinates

$$\xi_i = \frac{1}{\sqrt{NM}} \sum_{q} Q_q \mathbf{e}_q e^{i(q\cdot R_i^0 - \omega_q t)}; \tag{1.57}$$

By use of (1.54) and (1.57) the equation of motion $M\ddot{\xi}_i = -\partial \mathcal{H}/\partial \xi_i$ becomes

$$M\omega_q^2 \mathbf{e}_q = \sum_{j} \Gamma_{ij} \mathbf{e}_q e^{iq\cdot R_{ji}^0}. \tag{1.58}$$

By solving (1.58) three polarization vectors $\mathbf{e}_q$ and three frequencies ω_q are obtained for a given q vector.

(1.58) is a Hermitian eigenvalue problem, then the three polarization vectors $\mathbf{e}_q$ are orthogonal each other.

As was done in Section 1.1, ξ_i and $\mathbf{p}_i$ are expanded by use of the normal coordinates Q and P:

$$\xi_i = \frac{1}{\sqrt{NM}} \sum_{q\lambda} Q_{q\lambda} \mathbf{e}_{q\lambda} e^{iq\cdot R_i^0}, \quad \mathbf{p}_i = \sqrt{\frac{M}{N}} \sum_{q\lambda} P_{q\lambda} \mathbf{e}_{q\lambda} e^{-iq\cdot R_i^0}, \tag{1.59}$$

where λ specifies polarization and the values of q are restricted to the first Brillouin zone.

In general $e_{q\lambda}$ has no simple relation to the crystal axes or to the propagation vector q, but for long waves the crystal behaves like an isotropic solid. Then one of the vibrations is longitudinal wave, while the other two are transverse and have equal frequencies.

$Q_{q\lambda}$ in (1.59) corresponds to $Q_{q\lambda}e^{-i\omega_q t}$ in (1.57).

Since ξ_i, p_i are real,

$$Q_{q\lambda}^{+} = Q_{-q\lambda}\,,\quad P_{q\lambda}^{+} = P_{-q\lambda}\,,\quad e_{q\lambda} = e_{-q\lambda}. \tag{1.60}$$

From the Hermitian property, we have

$$(e_{q\lambda}\cdot e_{q\lambda'}) = \delta_{\lambda\lambda'}. \tag{1.61}$$

Aside from the constant term, the Hamiltonian (1.53) becomes

$$\mathcal{H} = \frac{1}{2}\sum_{\lambda}\sum_{q}\left(P_{q\lambda}^{+}P_{q\lambda} + \omega_{q\lambda}^{2}Q_{q\lambda}^{+}Q_{q\lambda}\right). \tag{1.62}$$

In deriving (1.62) the relation

$$\sum_{i} e^{i(q-q')\cdot R_i^0} = N\delta_{q,q'+G} = N\delta_{q,q'}. \tag{1.63}$$

is employed. Since the values of q are restricted to the first Brillouin zone, the reciprocal vector G should be put to zero.

The commutation relation is imposed on P_i and ξ_j:

$$[P_{i\alpha}, \xi_{j\beta}] = \frac{\hbar}{i}\,\delta_{ij}\,\delta_{\alpha\beta}, \quad (\alpha, \beta = 1.2.3),$$

then

$$[P_{q\lambda}, Q_{q\lambda'}] = \frac{\hbar}{i}\,\delta_{qq'}\,\delta_{\lambda\lambda'}. \tag{1.64}$$

The phonon creation and annihilation operators are introduced by

$$b_{q\lambda} = \frac{\omega_{q\lambda} Q_{q\lambda} + i P^{+}_{q\lambda}}{(2\hbar\omega_{q\lambda})^{1/2}}, \quad b^{+}_{q\lambda} = \frac{\omega_{q\lambda} Q^{+}_{q\lambda} - i P_{q\lambda}}{(2\hbar\omega_{q\lambda})^{1/2}}. \tag{1.65}$$

The inverse transformations to (1.65) are

$$Q_{q\lambda} = \left(\frac{\hbar}{2\omega_{q\lambda}}\right)^{1/2}(b_{q\lambda} + b^{+}_{-q\lambda}), \quad P_{q\lambda} = i\left(\frac{\hbar\omega_{q\lambda}}{2}\right)^{1/2}(b^{+}_{q\lambda} - b_{-q\lambda}), \tag{1.66}$$

and the (1.62) is expressed by

$$H = \sum_{q\lambda} \hbar\omega_{q\lambda}\left(b^{+}_{q\lambda} b_{q\lambda} + \frac{1}{2}\right). \tag{1.67}$$

1.5 Sum rule and Coulomb lattice

Substituting (1.56) into (1.58) we obtain

$$M\omega_{q\lambda}^2 \mathbf{e}_{q\lambda} = -\sum_j \sum_{q'} \mathbf{q}'(\mathbf{q}'\cdot \mathbf{e}_{q\lambda}) V_{q'} e^{i\mathbf{q}'\cdot \mathbf{R}_{ij}^0}$$
$$+ \sum_j \sum_{q'} \mathbf{q}'(\mathbf{q}'\cdot \mathbf{e}_{q\lambda}) V_{q'} e^{i(\mathbf{q}-\mathbf{q}')\cdot \mathbf{R}_{ij}^0} .$$

$\sum_{q'}$ is carried out over the q values including all reciprocal lattice vectors. Using (1.63),

$$M\omega_{q\lambda}^2 \mathbf{e}_{q\lambda} = -N\sum_{G_n} \mathbf{G}_n(\mathbf{G}_n\cdot \mathbf{e}_{q\lambda}) V_{G_n} + N\sum_{G_n}(\mathbf{q}+\mathbf{G}_n)(\mathbf{q}+\mathbf{G}_n)\cdot \mathbf{e}_{q\lambda} V_{q+G_n}$$

$$= NV_q \mathbf{q}(\mathbf{q}\cdot \mathbf{e}_{q\lambda}) + N\sum_{G_n\neq 0}\left\{(\mathbf{q}+\mathbf{G}_n)(\mathbf{q}+\mathbf{G}_n)\cdot \mathbf{e}_{q\lambda} V_{q+G_n} - \mathbf{G}_n(\mathbf{G}_n\cdot \mathbf{e}_{q\lambda}) V_{G_n}\right\}. \quad (1.68)$$

The first term in the last expression corresponds to the longitudinal wave and the second one to the transverse wave.

Multiplying $\mathbf{e}_{q\lambda}$ and summing up over λ,

$$\sum_\lambda M\omega_{q\lambda}^2 = NV_q \sum_\lambda (\mathbf{q}\cdot \mathbf{e}_{q\lambda})^2 + N\sum_\lambda \sum_{G_n\neq 0}\left[\{(\mathbf{q}+\mathbf{G}_n)\cdot \mathbf{e}_{q\lambda}\}^2 V_{q+G_n}\right.$$
$$\left. - (\mathbf{G}_n\cdot \mathbf{e}_{q\lambda})^2 V_{G_n}\right]. \quad (1.69)$$

The polarization vectors can be chosen to satisfy the following orthogonality relations :

$$\sum_{\lambda} (\mathbb{e}_{q\lambda})_{\alpha} \, (\mathbb{e}_{q\lambda})_{\beta} = \delta_{\alpha\beta} \quad (\alpha, \beta = x, y, z). \tag{1.70}$$

Consequently, we obtain the sum rule:

$$M \sum_{\lambda} \omega_{q\lambda}^{2} = N V_{q}\, q^{2} + N \sum_{G_n \neq 0} \left\{ V_{q+G_n} (\mathbb{q} + \mathbb{G}_n)^{2} - V_{G_n} G_n^{2} \right\}. \tag{1.71}$$

Consider the ions immersed in a uniform negative charge sea. The "bare" Coulomb interaction between ions provides

$$V_{q} = \frac{4\pi (Ze)^{2}}{\Omega\, q^{2}}, \quad \left(\begin{array}{l} \Omega : \text{volume of the sample}, \\ Ze : \text{nuclear charge}. \end{array} \right) \tag{1.72}$$

Combining with (1.71),

$$\sum_{\lambda} \omega_{q\lambda}^{2} = \frac{4\pi N (Ze)^{2}}{\Omega M} = \omega_{p}^{2}. \tag{1.73}$$

ω_p is the ionic plasma frequency. ω_p can be simply obtained as follows. Consider the ions between parallel plates. Polarization $\mathbb{P}$ induced by a displacement $\mathbb{r}$ of the ions as a whole, is

$$\mathbb{P} = z \left(\frac{N}{\Omega} \right) e\, \mathbb{r} \tag{1.74}$$

This polarization field creates an electric field $\mathcal{E}$ in the parallel plates

$$\mathcal{E} = -4\pi \mathbb{P}. \tag{1.75}$$

The equation of motion of an ion in the electric field $\mathcal{E}$ is

$$M\ddot{\mathbf{r}} = ze\,\mathcal{E} = -4\pi (ze)^2 \left(\frac{N}{\Omega}\right) \mathbf{r}. \tag{1.76}$$

Then,

$$\mathbf{r} \propto e^{i\omega_p t}, \quad \omega_p^{\,2} = \frac{4\pi N (ze)^2}{\Omega M}. \tag{1.77}$$

In the limit of $q \to 0$ the transverse frequency ω_T becomes zero, and the longitudinal wave frequency ω_L remains finite.

$\omega_L (q \to 0) = \omega_p$ contradicts with the conclusion obtained in the previous Sections that the long wave length acoustic mode frequencies should vanish linearly with q.

When considering ionic motion, it is essential to take the screening effect of the conduction electrons into account

We should replace (1.75) by

$$\mathcal{E} = -\frac{4\pi P}{\varepsilon}, \tag{1.78}$$

where ε is the electron gas dielectric constant. Therefore, ω_q changes into

$$\omega_q \to \frac{\omega_q}{\sqrt{\varepsilon_q}}. \tag{1.79}$$

As $q \to 0$, the dielectric constant is given by the Thomas-Fermi form (See Section 2.5):

$$\varepsilon_q = 1 + \frac{q_s^2}{q^2} \cong \frac{q_s^2}{q^2}, \quad q_s^2 = \frac{6\pi n e^2}{E_F}, \tag{1.80}$$

where $n = ZN/\Omega$ and $E_F \left(= \frac{1}{2} m v_F^2\right)$ is the Fermi energy.

Therefore, as $q \to 0$

$$\omega_q^2 \cong \frac{Z}{3} \frac{m}{M} v_F^2 q^2, \tag{1.81}$$

and the velocity of the longitudinal sound is given by

$$v_e = \left(\frac{Z}{3} \frac{m}{M}\right)^{1/2} v_F, \tag{1.82}$$

which is known as the Bohm-Staver relation.[4)]

1.6 Long wavelength vibrations of optical branches[5)]

If a primitive cell contains two atoms which are crystallographically non-equivalent, there is a vibration mode called optical branch. The frequency of the optical branch becomes finite as $q \to 0$ and the two atoms move out of phase (see section 1.3).

Therefore, the polarization field P induced by the transverse optical vibration, in ionic crystals interacts with the electromagnetic field. While, we expect the longitudinal optical phonons to interact strongly with electrons through the electric field of the polarization wave. This is a long-range Coulomb interaction. Since we are interested in the long wave vibration, the macroscopic treatment is available.[5)] For simplicity, we consider the isotropic ionic crystal with + and − ions in a unit cell.

A quantity w which is proportional to the relative displacement of + and − ions, is introduced:

$$w = \sqrt{\frac{M_{red}}{v_0}}\,(\xi_+ - \xi_-)\,, \quad \xi_\pm : \text{displacement of ions,}$$

$$M_{red} = M_+M_-/(M_+ + M_-), \quad v_0 : \text{volume of the unit cell.} \qquad (1.83)$$

The macroscopic theory is fully embodied in the following equations:

$$\ddot{w} = b_{11}\,w + b_{12}\,\mathcal{E}, \quad P = b_{21}\,w + b_{22}\,\mathcal{E}, \qquad (1.84)$$

where P and $\mathcal{E}$ are the polarization and electric field in the Maxwell equations. The linear relationship in (1.84) corresponds to the usual approximation employed in considering lattice vibrations where the higher order terms than $O(\xi^2)$ are disregarded.

We can show the following relation:

$$b_{12} = b_{21}. \qquad (1.85)$$

The effective field $\mathcal{E}_{eff}$ at the equilibrium position of the ions is

$$\mathcal{E}_{eff} = \mathcal{E} + \frac{4\pi}{3}P, \tag{1.86}$$

The dipole moments of ± ions are

$$p_{\pm} = \pm ze\xi_{\pm} + \alpha_{\pm}\mathcal{E}_{eff}, \tag{1.87}$$

where $\alpha_{\pm}$ are their electronic polarizabilities. Then the total polarization is

$$P = \frac{1}{v_0}(p_+ + p_-) = \frac{1}{v_0}\{ze(\xi_+ - \xi_-) + (\alpha_+ + \alpha_-)\mathcal{E}_{eff}\}. \tag{1.88}$$

In deriving (1.87) and (1.88), we have made the following assumption. In the displacement of the ions, they are considered as rigid entities. It seems to be a rough approximation, since their outer electronic shells are in contact (and even overlap).

In considering this situation, (1.88) is generalized into the form:

$$P = \frac{1}{v_0}\{ze^*(\xi_+ - \xi_-) + \alpha\,\mathcal{E}_{eff}\}. \tag{1.89}$$

There is no guarantee that the total polarizability is equal to the simple addition $\alpha_+ + \alpha_-$, then it is replaced by α.

Since $\mathcal{E}_{eff}$ is not a macroscopic field, but depends on the microscopic crystal structure, it is desirable to eliminate $\mathcal{E}_{eff}$ by making use of the relation $\mathcal{E}_{eff} = \mathcal{E} + \frac{4\pi}{3} P$.

Then,

$$P = \frac{1}{v_0}\left(1 - \frac{4\pi}{3}\frac{\alpha}{v_0}\right)^{-1}\left\{ ze^*(\xi_+ - \xi_-) + \alpha\mathcal{E} \right\}. \qquad (1.90)$$

The value of $4\pi/3$ for the Lorentz factor appears, since we consider a cubic crystal. To calculate the effective field in less symmetric crystal structures is not so easy.

The overlap potential between the positive and negative ions due to the relative displacement $\xi_+ - \xi_-$, induces the short range restoring force. The force acting on the positive ion is given by

$$f_s = -K(\xi_+ - \xi_-), \qquad (1.91)$$

and the corresponding force acting on the negative ion is $-f_s$.

Beside the overlap forces, there is the long range force due to $\mathcal{E}_{eff}$. On the positive and negative ions it is

$$f_e = \pm ze^* \mathcal{E}_{eff} = \pm ze^*\left(\mathcal{E} + \frac{4\pi}{3} P\right). \qquad (1.92)$$

The equations of motion for + and − ion are given by

$$\begin{cases} M_+ \ddot{\xi}_+ = -K(\xi_+ - \xi_-) + ze^*\left(\mathcal{E} + \frac{4\pi}{3}P\right), \\ M_- \ddot{\xi}_- = K(\xi_+ - \xi_-) - ze^*\left(\mathcal{E} + \frac{4\pi}{3}P\right). \end{cases} \qquad (1.93)$$

In consideration of w defined by (1.83) and (1.90), we get

$$M_{red}\,\ddot{w} = -K w + z e^* \sqrt{M_{red}/v_0}\,\left(\mathcal{E} + \frac{4\pi}{3}P\right). \qquad (1.94)$$

$$P = \frac{1}{v_0}\left(1 - \frac{4\pi}{3}\frac{\alpha}{v_0}\right)^{-1}\left(ze^*\sqrt{v_0/M_{red}}\,w + \alpha\mathcal{E}\right). \qquad (1.95)$$

Eliminating P from (1.94), one obtains

$$\ddot{w} = \left\{-\frac{K}{M_{red}} + \frac{4\pi}{3}(M_{red}v_0)^{-1/2}\left(1 - \frac{4\pi}{3}\frac{\alpha}{v_0}\right)^{-1} z^2 e^{*2}\right\} w$$

$$+ z e^* \{M_{red} v_0\}^{-1/2}\left(1 - \frac{4\pi}{3}\frac{\alpha}{v_0}\right)^{-1}\mathcal{E}. \qquad (1.96)$$

From (1.95), (1.96) and (1.84)

$$b_{12} = b_{21}. \qquad (\text{Q.E.D.})$$

b_{11} corresponds to the short range restoring force and then it is related to the transverse optical mode frequency ω_t by

$$-b_{11} = \omega_t^2, \qquad (1.97)$$

because the transverse wave can not induce the electric field $\mathcal{E}$. To relate the b-coefficients to measurable quantities, let us consider the response of the system to the periodic field. Then, we put

$$\mathcal{E},\ w,\ P \propto e^{-i\omega t} . \tag{1.98}$$

(1.84) becomes

$$\begin{cases} -\omega^2 w = b_{11} w + b_{12}\mathcal{E} \\ P = b_{21} w + b_{22}\mathcal{E} . \end{cases} \tag{1.99}$$

Eliminating w from (1.99)

$$P = \left(b_{22} + \frac{b_{12} b_{21}}{-b_{11} - \omega^2}\right)\mathcal{E} . \tag{1.100}$$

Combining with $\mathbb{D} = \mathcal{E} + 4\pi \mathbb{P} = \varepsilon\mathcal{E}$

$$\varepsilon = 1 + 4\pi b_{22} + \frac{4\pi b_{12} b_{21}}{-b_{11} - \omega^2} . \tag{1.101}$$

(1.101) can be rewritten

$$\varepsilon = \varepsilon_\infty + \frac{\varepsilon_0 - \varepsilon_\infty}{1 - (\omega/\omega_t)^2} , \tag{1.102}$$

where ε_∞ is the high frequency dielectric constant ($\omega \gg \omega_t$), and ε_0 the static dielectric constant. ε_∞ remains constant as far as it is measured in the frequency range where ω is enough smaller than the electronic motion. This range corresponds to the infrared frequency. Since the frequency of electronic motion is much larger than ω_t, the above limitation on ω provides no difficulty in the measurement of ε_∞.

Thus,

$$b_{11} = -\omega_t^2;\quad b_{12} = b_{21} = \left(\frac{\varepsilon_0 - \varepsilon_\infty}{4\pi}\right)^{1/2}\omega_t,\quad b_{22} = \frac{\varepsilon_\infty - 1}{4\pi}. \tag{1.103}$$

Eliminating div $\mathbb{P}$ from div $\mathbb{D}$ = div $(\mathcal{E} + 4\pi\mathbb{P}) = 0$ and the equation operating div on (1.99), we obtain

$$\operatorname{div}\mathcal{E} = -\frac{4\pi b_{21}}{1 + 4\pi b_{22}}\operatorname{div}\mathbf{w}, \tag{1.104}$$

$\mathbf{w}$ can be decomposed into the two components – the transverse component $\mathbf{w}_t$ and longitudinal component $\mathbf{w}_l$:

$$\begin{cases} \mathbf{w} = \mathbf{w}_t + \mathbf{w}_l \\ \operatorname{div}\mathbf{w}_t = 0, \quad \operatorname{curl}\mathbf{w}_l = 0. \end{cases} \tag{1.105}$$

(1.104) leads to

$$\operatorname{div}\mathcal{E} = -\frac{4\pi b_{21}}{1 + 4\pi b_{22}}\operatorname{div}\mathbf{w}_l. \tag{1.106}$$

Solution of (1.106) is simply given by

$$\mathcal{E} = -\frac{4\pi b_{21}}{1 + 4\pi b_{22}}\mathbf{w}_l, \tag{1.107}$$

because it satisfies curl $\mathcal{E} = 0$. Substituting (1.107) into (1.84), we get

$$\ddot{w}_e + \ddot{\mathbf{w}}_t = \left(b_{11} - \frac{4\pi b_{12} b_{21}}{1+4\pi b_{22}} \right) \mathbf{w}_e + b_{11} \mathbf{w}_t . \qquad (1.108)$$

This equation is separated into the two equations:

$$\begin{cases} \ddot{\mathbf{w}}_t = b_{11} \mathbf{w}_t = -\omega_t^2 \mathbf{w}_t , \\ \ddot{\mathbf{w}}_e = \left(b_{11} - \dfrac{4\pi b_{12} b_{21}}{1+4\pi b_{22}} \right) \mathbf{w}_e = - \left(\dfrac{\varepsilon_0}{\varepsilon_\infty} \right) \omega_t^2 \mathbf{w}_e . \end{cases} \qquad (1.109)$$

Patting

$$\begin{cases} \mathbf{w}_l = \mathbf{w}_l(\mathbf{r}) e^{i\omega_l t} + \mathrm{c.c.}, \\ \mathbf{w}_t = \mathbf{w}_t(\mathbf{r}) e^{i\omega_t t} + \mathrm{c.c}, \end{cases} \qquad (1.110)$$

we obtain the Lyddane-Sachs-Teller's relation:

$$\omega_l = \left(\frac{\varepsilon_0}{\varepsilon_\infty} \right)^{1/2} \omega_t \quad (\omega_l > \omega_t). \qquad (1.111)$$

1.7 Electron-longitudinal optical phonon interaction

In ionic crystals electrons are strongly interacting with the longitudinal optical phonons (LO-phonon). In the following we derive the expression of the interaction.

In the presence of the free charges $\rho(\mathbf{r}) = \sum_i e_i \, \delta(\mathbf{r} - \mathbf{r}_i)$, the Poisson equation $\mathrm{div}\,(\mathcal{E} + 4\pi \mathbb{P}) = 4\pi\rho$ becomes

$$\operatorname{div}\mathcal{E} = \frac{4\pi(-b_{21}\operatorname{div}\mathbf{w}_l + \rho)}{1+4\pi b_{22}}, \tag{1.112}$$

where $\mathbf{w} = \mathbf{w}_t + \mathbf{w}_l$, $\operatorname{div}\mathbf{w}_t = 0$ and (1.84) are employed. The electric field induced in the vacuum by ρ is

$$\mathcal{E}_{vac}(\mathbf{r}) = -\operatorname{grad}\int\frac{\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}''|}\,d\mathbf{r}'. \tag{1.113}$$

If the time variation of the electromagnetic field is slow, it is permissible to put $\operatorname{curl}\mathcal{E} = -\dot{\mathbb{H}}/c \doteqdot 0$. Then,

$$\mathcal{E} = -\frac{4\pi b_{21}}{1+4\pi b_{22}}\mathbf{w}_l + \frac{\mathcal{E}_{vac}}{1+4\pi b_{22}}. \tag{1.114}$$

is the solution of (1.112). Rewriting (1.114) by making use of (1.103) and (1.111), we get

$$\mathcal{E} = -\omega_l\left\{4\pi\left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0}\right)\right\}^{1/2}\mathbf{w}_l + \frac{1}{\varepsilon_\infty}\mathcal{E}_{vac}. \tag{1.115}$$

The presence of the term $\mathcal{E}_{vac}/\varepsilon_\infty$ modifies (1.109) and we have

$$\begin{cases} \ddot{\mathbf{w}}_t = -\omega_t^2\,\mathbf{w}_t, \\ \ddot{\mathbf{w}}_l = -\omega_l^2\,\mathbf{w}_l + \omega_l\left\{\dfrac{1}{4\pi}\left(\dfrac{1}{\varepsilon_\infty} - \dfrac{1}{\varepsilon_0}\right)\right\}^{1/2}\mathcal{E}_{vac}. \end{cases} \tag{1.116}$$

The equations of the electromagnetic field are

$$\left\{\begin{aligned} &\mathrm{div}\,(\mathcal{E}+4\pi\mathbf{P}) = 4\pi\sum_i e_i\,\delta(\mathbf{r}-\mathbf{r}_i),\\ &\mathrm{div}\,\mathbf{H} = 0\,,\\ &\mathrm{curl}\,\mathcal{E} = -\frac{1}{c}\dot{\mathbf{H}}\\ &\mathrm{curl}\,\mathbf{H} = \frac{1}{c}\left\{\dot{\mathcal{E}}+4\pi\dot{\mathbf{P}}+4\pi\sum_i e_i\,\dot{\mathbf{r}}_i\,\delta(\mathbf{r}-\mathbf{r}_i)\right\}. \end{aligned}\right. \qquad (1.117)$$

From the last two equations in (1.117) div $\mathbf{S}$, where $\mathbf{S}$ denotes the Poynting vector, $\frac{c}{4\pi}(\mathcal{E}\times\mathbf{H})$; is given by

$$\frac{c}{4\pi}\,\mathrm{div}\,\mathbf{S} = \frac{c}{4\pi}(\mathbf{H}\cdot\mathrm{curl}\,\mathcal{E}-\mathcal{E}\cdot\mathrm{curl}\,\mathbf{H})$$

$$= -\left\{\frac{1}{4\pi}(\mathcal{E}\cdot\dot{\mathcal{E}}+\mathbf{H}\cdot\dot{\mathbf{H}})+\mathcal{E}\cdot\dot{\mathbf{P}}+\sum_i e_i\,\dot{\mathbf{r}}_i\,\mathcal{E}(\mathbf{r})\,\delta(\mathbf{r}-\mathbf{r}_i)\right\}. \qquad (1.118)$$

From the Green's theorem,

$$\frac{c}{4\pi}\int_\Omega \mathrm{div}\,\mathbf{S}\,d\tau = \frac{c}{4\pi}\int_f \mathbf{S}\cdot d\mathbf{f}$$

$$= -\int_\Omega\left\{\frac{1}{4\pi}(\mathcal{E}\cdot\dot{\mathcal{E}}+\mathbf{H}\cdot\dot{\mathbf{H}})+\mathcal{E}\cdot\dot{\mathbf{P}}+\sum_i e_i\,\dot{\mathbf{r}}_i\,\mathcal{E}(\mathbf{r})\,\delta(\mathbf{r}-\mathbf{r}_i)\right\}d\tau. \qquad (1.119)$$

This indicates the rate of energy decrease in the volume Ω.

The last term $-\sum_i e_i\,\dot{\mathbf{r}}_i\,\mathcal{E}(\mathbf{r}_i)$ represents the decreasing rate of the kinetic energy. From the equation of motion $m_i \ddot{\mathbf{r}}_i = e_i \mathcal{E}(\mathbf{r}_i)$, we get

$$-\sum_i \frac{d}{dt}\left(\frac{1}{2} m_i \dot{\mathbf{r}}_i^2\right) = -\sum_i e_i \dot{\mathbf{r}}_i \mathcal{E}(\mathbf{r}_i). \qquad (1.120)$$

Accordingly, the quantity

$$\frac{1}{4\pi}\left(\mathcal{E}\cdot\dot{\mathcal{E}} + H\cdot\dot{H}\right) + \mathcal{E}\cdot\dot{P}, \qquad (1.121)$$

denotes the time variation of the energy density of the lattice vibrations and the electromagnetic field.

(1.121) is composed of the three terms — the potential energy of the system, the electromagnetic field energy and the kinetic energy of the lattice system.

Now, we introduce the quantity

$$U = \frac{1}{2}\dot{w}^2 - \frac{1}{2} b_{11} w^2 - b_{12} w\cdot\mathcal{E} - \frac{1}{2} b_{22}\mathcal{E}^2 + \mathcal{E}\cdot P + \frac{1}{8\pi}\left(\mathcal{E}^2 + H^2\right), \qquad (1.122)$$

Then, dU/dt becomes

$$\frac{dU}{dt} = \dot{w}\left(\ddot{w} - b_{11} w - b_{12}\mathcal{E}\right) + \dot{\mathcal{E}}\left(P - b_{12} w - b_{22}\mathcal{E}\right) + \mathcal{E}\cdot\dot{P} + \frac{1}{4\pi}\left(\mathcal{E}\cdot\dot{\mathcal{E}} + H\cdot\dot{H}\right). \qquad (1.123)$$

From (1.84) the first and second terms in (1.123) are zero.

Therefore, dU/dt is equal to (1.121). This indicates that U represents the energy density.

Total Hamiltonian is given by

$$\mathcal{H} = \frac{1}{2}\sum_i m_i \dot{\mathbf{r}}_i^2 + \int d\tau \left\{ \frac{1}{2}(\dot{\mathbf{W}}^2 + \omega_t^2 \mathbf{W}^2) + \frac{1}{8\pi}(\varepsilon_\infty \boldsymbol{\mathcal{E}}^2 + \mathbf{H}^2) \right\}, \tag{1.124}$$

where

$$U = \frac{1}{2}(\dot{\mathbf{W}}^2 + \omega_t^2 \mathbf{W}^2) + \frac{1}{8\pi}(\varepsilon_\infty \boldsymbol{\mathcal{E}}^2 + H^2). \tag{1.125}$$

Assuming the time variation of the electromagnetic field being enough slow and putting $\mathbf{H} \to 0$, curl $\boldsymbol{\mathcal{E}} = -\frac{1}{c}\dot{\mathbf{H}} = 0$ (electrostatic approximation), we have from (1.124)

$$\begin{aligned} \mathcal{H} = \frac{1}{2}\sum_i m_i \dot{\mathbf{r}}_i^2 + \int d\tau \Big[\Big\{ & \frac{1}{2}(\dot{\mathbf{W}}_l^2 + \omega_t^2 \mathbf{W}_l^2) + \frac{1}{2}(\dot{\mathbf{W}}_t^2 + \omega_t^2 \mathbf{W}_t^2) \\ & + \frac{1}{2}\left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0}\right)\varepsilon_\infty \omega_l^2 \mathbf{W}_l^2 - \omega_l \left\{ \frac{1}{4\pi}\left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0}\right) \right\}^{1/2} \mathbf{W}_l \cdot \boldsymbol{\mathcal{E}}_{vac} \\ & + \frac{1}{8\pi\varepsilon_\infty} \boldsymbol{\mathcal{E}}_{vac}^2 \Big]. \end{aligned} \tag{1.126}$$

Since $\boldsymbol{\mathcal{E}}_{vac}$ is the electric field resulting from charges in vacuum,

$$\frac{1}{8\pi}\int d\tau\, \boldsymbol{\mathcal{E}}_{vac}^2 = \frac{1}{2}\sum_{i \neq j} \frac{e_i e_j}{|\mathbf{r}_i - \mathbf{r}_j|}. \tag{1.127}$$

Moreover, combining the relation $\omega_\ell^2 = (\varepsilon_0/\varepsilon_\infty)\,\omega_t^2$ and (1.127), we arrive at

$$\mathcal{H} = \frac{1}{2}\sum_i m_i \dot{\mathbf{r}}_i^{\,2} + \frac{1}{2\varepsilon_\infty}\sum_{i\neq j}\frac{e_i e_j}{|\mathbf{r}_i-\mathbf{r}_j|} + \int d\tau\left\{\frac{1}{2}\left(\dot{\mathbf{W}}_\ell^{\,2}+\omega_\ell^2\mathbf{W}_\ell^2\right)\right.$$

$$\left.+\frac{1}{2}\left(\dot{\mathbf{W}}_t^{\,2}+\omega_t^2\mathbf{W}_t^2\right)\right\} - \omega_\ell\left\{\frac{1}{4\pi}\left(\frac{1}{\varepsilon_\infty}-\frac{1}{\varepsilon_0}\right)\right\}^{1/2}\int \mathbf{W}_\ell\cdot\mathcal{E}_{vac}\,d\tau. \qquad (1.128)$$

The last term in (1.128) corresponds to the electron-LO phonon interaction. This interaction is transformed into a more convenient form in terms of the phonon operators. We are interested in the longitudinal phonons which can interact with carriers. Relative displacement $\mathbf{W}_\ell$ is expressed by the phonon operators:

$$\left\{\begin{array}{l} \mathbf{W}_\ell = \displaystyle\sum_q \sqrt{\frac{\hbar}{2\Omega\,\omega_\ell}}\;\mathbf{e}_q\left(b_q e^{i\mathbf{q}\mathbf{r}} + b_q^+ e^{-i\mathbf{q}\mathbf{r}}\right), \\ b_q \propto e^{-i\omega_\ell t}, \quad b_q^+ \propto e^{i\omega_\ell t}, \quad \mathbf{e}_q = \mathbf{q}/q, \end{array}\right. \qquad (1.129)$$

here b and b^+ obey

$$[b_q, b_{q'}] = [b_q^+, b_{q'}^+] = 0, \quad [b_q, b_{q'}^+] = \delta_{q,q'}. \qquad (1.130)$$

Thus, the LO-phonon energy becomes

$$\int\frac{1}{2}\left\{\dot{\mathbf{W}}_\ell^{\,2} + \omega_\ell^2\mathbf{W}_\ell^2\right\}d\tau = \sum_\ell \hbar\omega_\ell\left(b_q^+ b_q + \tfrac{1}{2}\right)$$

$$= \sum_\ell \hbar\omega_\ell\left(n_q + \frac{1}{2}\right). \qquad (1.131)$$

By making use of the relations

$$\begin{cases} \mathbf{W}_l = \mathrm{grad}\,\varphi_l\,, \quad \varphi_l = -i\sum_q \sqrt{\dfrac{\hbar}{2\Omega\omega_l}}\;\dfrac{1}{q}\left(b_q e^{iqr} - b_q^{+} e^{-iqr}\right), \\ \mathrm{div}\,\mathcal{E}_{vac} = 4\pi \sum_i e_i\,\delta(\mathbf{r}-\mathbf{r}_i), \quad (e_i = -e) \end{cases} \tag{1.132}$$

LO-phonon - electron interaction Hamiltonian takes the form

$$H_{e\text{-}LO} = ie\sqrt{\frac{2\pi\hbar\omega_l}{\Omega}\left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0}\right)}\;\sum_q \frac{1}{q}\left(b_q e^{iqr} - b_q^{+} e^{-iqr}\right). \tag{1.133}$$

Dispersion of ω_l is disregarded. (1.133) is called the Fröhlich Hamiltonian.⁶⁾ By introducing a dimensionless parameter α (Fröhlich parameter). (1.133) is rewritten in the form

$$\begin{cases} H_{e\text{-}LO} = 2i\sqrt{\dfrac{\pi\alpha}{\Omega}}\;\hbar\omega_l\left(\dfrac{\hbar}{2m^*\omega_l}\right)^{1/4}\sum_q \dfrac{1}{q}\left(b_q e^{iqr} - b_q^{+} e^{-iqr}\right), \\ \alpha = \dfrac{1}{2}\left(\dfrac{1}{\varepsilon_\infty} - \dfrac{1}{\varepsilon_0}\right)\dfrac{e^2}{\hbar\omega_l}\left(\dfrac{2m^*\omega_l}{\hbar}\right)^{1/2}. \end{cases} \tag{1.134}$$

$\alpha/2$ gives an expectation value of the virtual phonons around each electron. (See Section 7.2)

Values of ε_∞, ε_0, $\hbar\omega_l$, α and m^* are listed for several ionic crystals and semiconductors:

	KCl	AgBr	CdS	CdTe	ZnS	InSb	InP	GaSb	GaAs
ε_0	4.49	10.6	9.0	10.9	8.3	17.64	14	15	12.5
ε_∞	2.20	4.68	5.20	7.2	5.13	15.75	10.7	14	10.9
ω_e (meV)	26.3	16.4	3.8	21.34	44	24.4	42.0	29	35.2
α	3.60	1.60	0.71	0.38	0.68	0.019	0.08	0.02	0.06
m^*/m	0.47	0.215	0.20	0.096	0.27	0.014	0.07	0.047	0.072

Table 1.1 Values of ε_0, ε_∞, $\hbar\omega_e$, α and m^* for several ionic crystals and semiconductors.[7)]

Chapter 2 Electron-Lattice Interaction (Monovalent Metal Case)

2.1 Separation of the electronic and the nuclear motions

In the monovalent metals, negative charge of the conduction electrons, whose density is $\sim 10^{22}\ \mathrm{cm}^{-3}$, is neutralized by the positive ions. Besides the mutual Coulomb interactions electrons move in a strong potential field due to the nuclear system. At first sight one might consider that it is impossible to separate the motion of the conduction electrons from that of the ions. However, as is shown in the following the motions of the two systems can be approximately separated. It is the adiabatic principle 8) proposed by Born-Oppenheimer that provides a theoretical basis for it.

This principle is based on the situation that the conduction electrons adjust themselves adiabatically to the instantaneous positions of the ions in the vibrating lattice, since the electronic motion is much faster than the nuclear motion.

The electron-ion Hamiltonian is

$$\left\{\begin{aligned} \mathcal{H} &= \mathcal{H}_e + \mathcal{H}_I, \\ \mathcal{H}_e &= -\sum_i \frac{\hbar^2}{2m}\frac{\partial^2}{\partial \mathbf{r}_i^2} + \sum_{i>j}\frac{e^2}{|\mathbf{r}_i-\mathbf{r}_j|} + \sum_{i,l} V_b(\mathbf{r}_i - \mathbf{R}_l), \\ \mathcal{H}_I &= -\sum_l \frac{\hbar^2}{2M}\frac{\partial^2}{\partial \mathbf{R}_l^2} + \sum_{l>l'} W_b(\mathbf{R}_l - \mathbf{R}_{l'}) \end{aligned}\right. \qquad (2.1)$$

Here r_i and R_l are, respectively, the coordinates of the i-th electron and the l-th ion. The third term in H_e is the "bare" Coulomb interaction between the electrons and the ions. The second term in H_I is the "bare" interaction between the ions. (The word "bare" is used here to denote the interaction between two particles in the absence of all the other particles of the system.)

Here the inner core electrons strongly bound to nucleus are included in ion and assumed to move with nucleus.

According to the adiabatic principle the eigenstates of the electrons are determined from the Hamiltonian H_e in a fixed configuration of the ions:

$$H_e \psi_k(r,R) = E_k(R)\psi_k(r,R). \tag{2.2}$$

We expand the total wave function Ψ_q in terms of the complete orthonormal set $\{\psi_k\}$ as follows:

$$\Psi_q(r,R) = \sum_k \varphi_{q,k}(R)\psi_k(r,R), \tag{2.3}$$

and Ψ_q obeys the equation

$$H \Psi_q = E_q \Psi_q. \tag{2.4}$$

Substituting (2.3) into (2.4), multiplying both sides by ψ_k^* and integrating over all the electron coordinates, we get the following equation for φ_{qk}'s :

$$\left(H_I + E_k(R) + A_{kk} + B_{kk}\right)\varphi_{gk} + \sum_{k\neq k'} \left(A_{kk'} + B_{kk'}\right)\varphi_{gk'} = E_g \varphi_{gk}, \qquad (2.5)$$

where

$$A_{kk'} = -\frac{\hbar^2}{M}\sum_l \int d\mathbf{r}\, \psi_k^* \frac{\partial}{\partial R_l}\psi_{k'} \frac{\partial}{\partial R_l},$$

and

$$B_{kk'} = -\frac{\hbar^2}{2M}\sum_l \int d\mathbf{r}\, \psi_k^* \frac{\partial^2 \psi_{k'}}{\partial R_l^2}.$$

In the spirit of the adiabatic approximation the nondiagonal terms $(k\neq k')$ are neglected. Then, we have

$$\left(H_I + E_k(R) + A_{kk} + B_{kk}\right)\varphi_{gk} = E_g \varphi_{gk}. \qquad (2.6)$$

It is verified that $\langle gk | A_{kk} | gk \rangle \cong 0$. Major contribution to $(\partial/\partial R_l)\psi_k$ comes from the cell around R_l. In this region $\psi_k(r,R)$ is approximated in the form $\psi_k(r-R_l)$. Then,

$$\int d\mathbf{r}\, \psi_k^* \frac{\partial}{\partial R_l}\psi_k \cong -\int_{cell} d\mathbf{r}\, \psi_k^* \frac{\partial}{\partial r}\psi_k. \qquad (2.7)$$

(2.7) does not depend on the ion coordinate R_l. ~~accordingly~~ Therefore, in the stationary states $\langle gk | A_{kk} | gk \rangle \propto \sum_l \langle gk | \frac{\partial}{\partial R_l} | gk \rangle = 0$. Similary, since $(\partial^2/\partial R_l^2)\psi_k \cong (\partial^2/\partial r^2)\psi_k$ in the l-th cell, B_{kk} is given by

$$B_{kk} \cong \frac{m}{M}\int d\mathbf{r}\, \psi_k^* \left(-\frac{\hbar^2}{2m}\Delta\right)\psi_k. \qquad (2.8)$$

Since (2.8) is independent of the ion coordinates, B_{kk} only gives a small constant energy shift, which is equal to (m/M) times the electron kinetic energy. The motions of the ions is thus determined by the "effective" Hamiltonian:

$$\tilde{H}_I = -\frac{\hbar^2}{2M}\sum_l \frac{\partial^2}{\partial R_l^2} + \sum_{l>l'} W_b(R_l - R_{l'}) + E_k(R). \tag{2.9}$$

The last term $E_k(R)$ is called the adiabatic potential.

It should be noted that we do not assume the interaction between the two systems being small.

The ions will vibrate about some mean position, and these vibrations are small in amplitude. The last two terms in (2.9) correspond to the potential energy of the ion system. Expanding the potential energy $E_n(R)$ around the equilibrium position R_0, one gets

$$E_n(R) \cong E_n(R_0) + \frac{1}{2}\left(\frac{d^2 E_n}{dR^2}\right)_0 (R-R_0)^2 + \cdots . \tag{2.10}$$

The second term is related to the vibration frequency of the ions by

$$\frac{1}{2} M \omega_0^2 (R-R_0)^2 = \frac{1}{2}\left(\frac{d^2 E_n}{dR^2}\right)_0 (R-R_0)^2 . \tag{2.11}$$

Namely, $\omega_0 = \sqrt{(d^2 E_n/dR^2)_0/M}$. On the other hand, $E_n \cong E_e \cong \hbar^2/2ma^2$, where a denotes the lattice constant and E_e represents a typical electronic energy (see (2.9)). Then $(d^2E_n/dR^2)_0 \approx E_e/a^2$. Comparing E_e with the lattice vibrational energy $E_v \simeq \hbar\omega_0$, we obtain

$$\frac{E_v}{E_e} \longleftarrow \frac{E_e}{E_v} \approx \sqrt{\frac{m}{M}} . \qquad (2.12)$$

2.2. Electron - Phonon Interaction

The terms $B_{kk'}$ are diagonal with the eigenstates of the ionic motion. Therefore, only $A_{kk'}$ gives rise to the electron-phonon interaction. It is inconvenient to use the expression of $A_{kk'}$ in (2.5). Here, we introduce a more easier procedure instead of using (2.5). Momentum of the l-th ion is

$$P_l = \frac{\hbar}{i}\frac{\partial}{\partial R_l} = M\dot{\xi}_l , \quad \xi_l = R_l - R_{l0}, \qquad (2.13)$$

where ξ_l is already given in Section 1.4::

$$\xi_l = \sum_{q\lambda}\sqrt{\frac{\hbar}{2NM\omega_{q\lambda}}}\, e_{q\lambda}\left(b_{q\lambda}e^{iqR_{l0}} + b^{+}_{q\lambda}e^{-iqR_{l0}}\right). \qquad (2.14)$$

(2.13) and (2.14) provide

$$A_{kk'} = -\hbar\sum_{l}\sum_{q\lambda}\sqrt{\frac{\hbar\omega_{q\lambda}}{2NM}}\, e_{q\lambda}\left(b_{q\lambda}e^{iqR_{l0}} - b^{+}_{q\lambda}e^{-iqR_{l0}}\right)\int dr\, \psi^{*}_{k'}\frac{\partial}{\partial R_l}\psi_k . \qquad (2.15)$$

Ψ_k is the wave function of the total electronic system satisfying (2.2). Let consider Ψ_k, which is expressed by the Slater determinant composed of the Bloch functions $\phi_{k_1}, \phi_{k_2}, \cdots, \phi_{k_n}$. In this case the quantum number k is given by an assembly $k = \{k_1, k_2, \cdots, k_n\}$. n-electron wave function also satisfies the Bloch condition:

$$\Psi_k(r+R_0) = e^{ik \cdot R_0} \Psi_k(r), \quad r+R_0 \equiv \{r_1+R_0, r_2+R_0, \cdots, r_n+R_0\}, \qquad (2.16)$$

where R_0 is an arbitrary lattice vector.

Potential $V(r,R)$ exerted on the electrons is expdanded around the equilibrium position R_0:

$$V(r,R) = V(r,R_0) + \sum_l \xi_l \cdot B_l + \cdots, \quad B_l = \left(\frac{\partial V}{\partial R_l}\right)_0. \qquad (2.17)$$

The corresponding wave function $\Psi_k(r,R)$ is approximated by

$$\Psi_k(r,R) \cong \Psi_k(r,R_0) + \sum_{k'} \frac{\langle k' | \sum_l \xi_l \cdot B_l | k \rangle}{E_k - E_{k'}} \Psi_{k'}(r,R_0). \qquad (2.18)$$

We are interested in the real transitions - phonon absorption or emission processes, then $E_k - E_{k'} \neq 0$. From (2.18) we get

$$\int dr\, \Psi_{k'}^* \frac{\partial \Psi_k(r,R)}{\partial R_l} \cong \frac{\langle k' | B_l | k \rangle}{E_k - E_{k'}}. \qquad (2.19)$$

In the absorption or the emission processes of the phonon $q\lambda$, $E_k - E_{k'} = \pm \hbar\omega_{q\lambda}$

On making use of (1.22), we obtain

$$A_{kk'} = -\sqrt{\frac{\hbar}{2NM\omega_{q\lambda}}} \times \begin{cases} \langle n_{q\lambda}-1 | b_{q\lambda} | n_{q\lambda} \rangle \langle k' | \sum_{l} e^{iq.R_l} e_{q\lambda} \cdot B_l | k \rangle , \\ \\ \langle n_{q\lambda}+1 | b^{+}_{q\lambda} | n_{q\lambda} \rangle \langle k' | \sum_{l} e^{-iq.R_l} e_{q\lambda} B_l | k \rangle , \end{cases} \tag{2.20}$$

where R_{l0} is expressed by R_l.

Let define the quantity

$$B_q(r) = \frac{1}{N} \sum_{l} e^{iq.R_l} B_l . \tag{2.21}$$

Since B_l has the lattice periodicity, for an arbitrary lattice vector R, B_q satisfies

$$B_q(r+R) = e^{iq.R} B_q(r). \tag{2.22}$$

From (2.16) and (2.22) we have

$$\begin{aligned} \langle k' | B_q | k \rangle &= \frac{1}{N} \sum_{l} \int \psi^{*}_{k'}(r+R_l) B_q(r+R_l) \psi_k(r+R_l) \, dr \\ &= \frac{1}{N} \sum_{l} e^{i(-k'+q+k).R_l} \int \psi^{*}_{k'}(r) B_q(r) \psi_k(r) \, dr , \end{aligned} \tag{2.23}$$

so that

$$k' = q + k + G , \quad G : \text{reciprocal lattice vector.} \tag{2.24}$$

G is introduced so as to obtain q in the first Brillouin zone. Accordingly, (2.20) becomes

$$A_{kk'} = -\sqrt{\frac{\hbar}{2NM\omega_q}} \times \begin{cases} \sqrt{n_q} \, \langle k' | e_q . B_q | k \rangle , \\ \sqrt{n_q+1} \, \langle k' | e_q . B_{-q} | k \rangle , \end{cases} \tag{2.25}$$

where the suffix λ is omitted. Since (2.25) is the matrix element of the electron-phonon interaction corresponding to the n-electron system, it is not convenient to get a concrete expression. In the following, (2.25) is transformed into the formula in the one-electron system.

2.3 Rigid Ion Approximation

To get the explicit expression of (2.25), the n-electron wave function is approximated by the product of the Hartree-Fock one electron wave function $\psi_k(r_i)$. $\psi_k(r_i)$ and the corresponding potential $V(r_i, R)$ are determined self-consistently.

Thus,

$$V(r,R) = V(r_1, r_2, \cdots, r_n, R) \cong \sum_i V(r_i, R), \tag{2.26}$$

and assuming

$$V(r,R) = \sum_l U(r - R_l), \tag{2.27}$$

we obtain

$$\xi_l \cdot B_l = \xi_l \cdot \nabla_l U(r - R_l) = -\xi_l \cdot \nabla U(r - R_l), \tag{2.28}$$

and

$$\langle k' | \sum_l e^{iq \cdot R_l} e_q \cdot B_l | k \rangle = \overset{1/\Omega)}{\sum_l} \int dr\, e^{-ik'r} e^{iqR_l} e_q \cdot \nabla U(r - R_l)\, e^{ikr}$$

$$= \sum_l e^{i(-k'+k+q)\cdot R_l} \int dr\, e^{i(k-k')r} e_q \cdot \nabla U(r) = -i\,\delta_{k', k+q+G}\, e_q \cdot (k - k')\, U(k - k'), \tag{2.29}$$

where
$$U(k) = N\int d\mathbf{r}\, e^{ikr}\, U(r).$$

In deriving (2.29) the wave function is taken to be e^{ikr}. From (2.29), (2.25) becomes

$$A_{kk'} = -i\sqrt{\frac{\hbar}{2NM\omega_q}}\begin{cases}\sqrt{n_q}\; e_q\cdot(k-k')\,U(k-k')\,\delta_{k',k+q+G} \\ \sqrt{n_q+1}\; e_q\cdot(k-k')\,U(k-k')\,\delta_{k',k-q+G}\end{cases} \qquad (2.30)$$

As is shown in (2.27), (2.30) is obtained on the assumption that each ion can diplace independently. In this sence, it is called the rigid ion approximation. The weakest point in (2.30) is that the matrix element is unreasonably overestimated due to the introduction of the plane wave function. Improvement on this point will be discussed in the next Section.

2.4 Pseudo-potential Methods and Electron-Phonon Interaction

In calculating the electron-phonon interaction there are two important problems to be considered. The first is that in the vicinity of the nucleus the Born approximation loses its validity due to the strong potential field exerted on the electrons. The second problem is as follows. The electric field induced by the ionic motions is screened by the conduction electrons. This problem will be treated in the next Section, and in the present Section we pay attention to the first problem.

The conduction electrons in the alkaline metals can be considered to be nearly free and their wave functions are well described by the orthogonalized plane wave method (OPW method).[9]

The eigenstates of the inner-electrons strongly bound to nucleus are the solutions of the following Schrödinger equation:

$$\left\{-\frac{\hbar^2}{2m}\Delta + U(r)\right\}\phi_t = E_t\,\phi_t, \qquad (2.31)$$

and the Bloch function in the tight binding approximation is given by

$$\psi_{tk}(r) = \frac{1}{\sqrt{N}}\sum_{l} e^{ik.R_l}\,\phi_t(r-R_l). \qquad (2.32)$$

The spirit of the OPW method is to make the state which is orthogonal to ψ_{tk} and behaves like free electrons around the midway between nuclei. This can be done as follows..

We define

$$\chi_{k+g}(r) = \frac{1}{\sqrt{\Omega}}e^{i(k+g).r} - \sum_t b_{t,k+g}\,\psi_{tk}, \qquad (2.33)$$

where Ω is the crystal volume and g is a reciprocal vector.

Putting $\langle \psi_{tk} | \chi_{k+g} \rangle = 0$, one obtains

$$b_{t,k+g} = \frac{1}{\sqrt{\Omega}} \int \psi_{tk}^{*} e^{i(k+g)r} dr. \qquad (2.34)$$

Inserting

$$\psi_k(r) = \sum_g C_{k+g} \chi_{k+g}(r), \qquad (2.35)$$

into the Schrödinger equation, we can determine the coefficients C_{k+g}. Thus, (2.29) becomes

$$\langle k' | \sum_l e^{iqR_l} e_q \cdot B_l | k \rangle = N \sum_{g,g'} C^{*}_{k'+g'} C_{k+g} \int dr\, \chi^{*}_{k'+g'} e_q \cdot \nabla U(r) \chi_{k+g}(r)$$

$$\times\, \delta_{k',k+q+G}. \qquad (2.36)$$

After a lengthy calculations,10) $A_{kk'}$ takes the form:

$$\begin{cases} A_{kk'} = -i\alpha_q^{(\pm)} \sum_{g,g'} C^{*}_{k'+g'} C_{k+g}\, e_q \cdot (k+g-k'-g') U_{eff}(k+g-k'-g') \delta_{k',k\pm q+G}, \\ \alpha_q^{(+)} = \sqrt{\frac{\hbar}{2NM\omega_q}} \sqrt{n_q}, \quad \alpha_q^{(-)} = \sqrt{\frac{\hbar}{2NM\omega_q}} \sqrt{n_q+1}, \\ U_{eff}(k+g-k'-g') = U(k+g-k'-g') + \sum_t (E_k - E_t) b^{*}_{t,k'+g'} b_{t,k+g}. \end{cases} \qquad (2.37)$$

In the simple metals like sodium or potassium, we often encounter with the case where only one OPW function provides a good approximation. In this case, putting $g = g' = 0$, we get

$$U_{eff}(k-k') = U(k-k') + \sum_t (E_k - E_t) b^{*}_{tk'} b_{tk}. \qquad (2.38)$$

The first term in the right hand side of (2.38) is negative, since it is due to the attractive potentials of the ions. On the other hand, the second term is positive because of $E_k > E_t$, then both terms cancell each other. As the result U_{eff} becomes much smaller than U. Electrons are accerlated through the strong electric field in the vicinity of the nuclei, and rapidly pass over the region near the nuclei. Then, the conduction electrons spend major part of time in the weak potential region. This is the physical meaning of (2.38).

The Fourier component of the pseudo potential, which plays an important role in the band calculation, is given by

$$\sum_t (E_k - E_t)\, b^*_{t,k+g'}\, b_{t,k+g}. \tag{2.39}$$

Let consider for a little about the pseudo potential. Matrix element of $H - E\mathbb{1}$ between the OPW $\chi_{k+g'}$ and χ_{k+g}, where H is the total Hamiltonian and $\mathbb{1}$ denotes the unit matrix, is given by

$$\langle \chi_{k+g'} | H - E\mathbb{1} | \chi_{k+g} \rangle = \left\{ \frac{\hbar^2}{2m}(k+g)^2 - E \right\} \delta_{gg'} + V(g-g')$$
$$+ \sum_t (E_k - E_t)\, b^*_{t,k+g'}\, b_{t,k+g}, \tag{2.40}$$

where $$V(K) = \frac{1}{\Omega} \int d\mathbf{r}\, e^{iK\mathbf{r}}\, V(\mathbf{r}).$$

The secular equation for C_{k+g} is

$$\sum_{g} \langle \chi_{k+g'} | H - E\mathbf{1} | \chi_{k+g} \rangle C_{k+g} = 0. \qquad (2.41)$$

The third term in the right hand side of (2.40) is equal to (2.39). Now, we define the localized pseudopotential $U_{ps}(r-R_\ell)$, whose Fourier component is given by (2.39)::

$$\begin{cases} U_{ps}(g-g') = \sum_{t} (E - E_t)\, b_{t,k+g'}^{*}\, b_{t,k+g}, \\ V_{ps}(r) = \sum_{\ell} U_{ps}(r - R_\ell). \end{cases} \qquad (2.42)$$

In the space of the plane-wave function instead of OPW, the effective Hamiltonian becomes

$$H_{eff} = H + V_{ps}. \qquad (2.43)$$

Therefore, we have

$$\langle \chi_{k+g'} | H - E\mathbf{1} | \chi_{k+g} \rangle = \langle e^{i(k+g')r} | H + V_{ps} - E\mathbf{1} | e^{i(k+g)r} \rangle, \qquad (2.44)$$

and the corresponding wave function is

$$\phi_k = \sum_{g} C_{k+g}\, e^{i(k+g)\cdot r}. \qquad (2.45)$$

(2.45) is called the pseudowave function. The third formula in (2.37) and (2.38) are written in terms of U_{ps} as follows:

$$\begin{cases} U_{eff}(K) = U(K) + U_{ps}(K), \\ U_{eff}(r) = U(r) + U_{ps}(r). \end{cases} \qquad (2.46)$$

On making use of the following simple model for $U_{eff}(r)$, we calculate $A_{kk'}$.

Consider the crystal which can be filled compactly by the Wigner-Seitz cell. Next, this cell is approximated by the sphere with equal volume and we choose the model:

$$U_{eff}(r) = \begin{cases} U_0 & : r < r_s , \\ 0 & : r > r_s , \end{cases} \tag{2.47}$$

where r_s is the radius of the sphere. (2.47) indicates that the cancellation is nearly complete and the deep negative potential near the nucleus is removed. Moreover, we confine our discussion to the simple case where a single OPW provides a good approximation to the wave function. In this case, from (2.37) we obtain

$$\begin{aligned} A_{kk'} &= -i\alpha_q^{(\pm)} C_{k'}^{*} C_k \, e_q \cdot (k - k') \, \delta_{k';k\pm q+G} \, 4\pi N U_0 \int_0^{r_s} dr \, r^2 \frac{\sin|k-k'|r}{|k-k'|r} \\ &= -i\alpha_q^{(\pm)} C_{k'}^{*} C_k \, (e_q \cdot K) \, \delta_{k',k\pm q+G} \, U_0 F(K r_s) , \end{aligned} \tag{2.48}$$

$$\begin{cases} K = k' - k , \quad F(x) = 3 \left(\dfrac{x \cos x - \sin x}{x^3} \right) , \\ C_K = \left(1 - \sum\limits_t |b_{t,K}|^2 \right)^{-1/2} . \end{cases} \tag{2.49}$$

Besides $C_{k'}^{*} C_k$ the above expression was derived by Mott-Jones.[11)] It should be noted that the small potential U_0 due to the cancellation effect appears instead of the large potential $U(k-k')$ in (2.30).

In the next Section we consider the screening effect due to the conduction electrons.

2.5 Electron-Phonon Interaction and Screening Effect

We assume that the bare ion potential V_b is given by the simple sum of each ion contribution $U(r-R_l)$ and behaves rigidly in the displacement process (see (2.27)):

$$V_b(r, R) = \sum_l U(r-R_l) = V_b(r) + \sum_l \overset{\delta R_l}{\xi_l} \cdot B_l = V_b(r) + \delta V_b(r). \qquad (2.50)$$

Apperance of δV_b enables the conduction electrons to screen δV_b through their rearrangement. Change of the electron charge density $\delta\rho$ accompanies the induced potential δV_i. Then, the resultant potential change becomes

$$\delta V_{scr} = \delta V_b + \delta V_i. \qquad (2.51)$$

Since all events occur consistenlly, change of the wave function $\delta\psi$ should be determined by δV_{scr}. The charge density corresponding to $\psi + \delta\psi$ is

$$\begin{aligned} \rho(r, R) &= \frac{1}{\Omega}\left\{ \sum_k \psi_k^* \psi_k + \sum_k \left(\psi_k^* \delta\psi_k + \delta\psi_k^* \psi_k \right) + \cdots \right\} \\ &= \rho(r) + \delta\rho(r). \end{aligned} \qquad (2.52)$$

Poisson's equation gives

$$\Delta \delta V_i = -4\pi e^2 \delta \rho = -\frac{4\pi e^2}{\Omega} \sum_k f_k \left(\psi_k^* \delta \psi_k + \delta \psi_k^* \psi_k \right), \tag{2.53}$$

where f_k is the Fermi distribution.

$\delta \psi_k$ is related to δV_{scr}.

$$\delta \psi_k = \sum_{k'} \frac{\langle k' | \delta V_{scr} | k \rangle}{E_k - E_{k'}} \psi_{k'} . \tag{2.54}$$

Substituting (2.54) into (2.53), we obtain

$$\Delta \delta V_i = -\frac{4\pi e^2}{\Omega} \sum_k f_k \sum_{k'} \left\{ \frac{\langle k' | \delta V_b + \delta V_i | k \rangle}{E_k - E_{k'}} \psi_k^* \psi_{k'} + \frac{\langle k | \delta V_b + \delta V_i | k' \rangle}{E_k - E_{k'}} \psi_{k'}^* \psi_k \right\}$$

$$= -\frac{4\pi e^2}{\Omega} \sum_{k, k'} \frac{f_k - f_{k'}}{E_k - E_{k'}} \langle k' | \delta V_b + \delta V_i | k \rangle \psi_k^* \psi_{k'} . \tag{2.55}$$

Consider that δV_b is induced by a displacement with wave vector $\mathbf{q}$. Then,

$$\delta V_b = \sum_{\mathbf{G}} \delta V_b(\mathbf{q} + \mathbf{G}) e^{i(\mathbf{q} + \mathbf{G}) \cdot \mathbf{r}} . \tag{2.56}$$

Similarly,

$$\delta V_i = \sum_{\mathbf{G}} \delta V_i(\mathbf{q} + \mathbf{G}) e^{i(\mathbf{q} + \mathbf{G}) \cdot \mathbf{r}} , \tag{2.57}$$

where $\mathbf{G}$ is the reciprocal lattice vector.

From (2.55), (2.56) and (2.57), we get

$$(q+G)^2\,\delta V_i(q+G) = \frac{4\pi e^2}{\Omega}\sum_{k,g,G'}\frac{f_k - f_{k+q+g}}{E_k - E_{k+q+g}}\langle k|e^{-i(q+G)r}|k+q+g\rangle$$

$$\times\langle k+q+g|e^{i(q+G')r}|k\rangle\{\delta V_b(q+G') + \delta V_i(q+G')\}. \qquad (2.58)$$

Introducing the dielectric function ε by the following relation:

$$\delta V_{scr}(q+G) = \delta V_b(q+G) + \delta V_i(q+G)$$

$$= \sum_{G'}\varepsilon^{-1}(q+G, q+G')\,\delta V_b(q+G'), \qquad (2.59)$$

we find

$$\varepsilon(q+G, q+G') = \delta_{GG'} - \frac{4\pi e^2}{\Omega(q+G)^2}\sum_{k,g}\frac{f_k - f_{k+q+g}}{\underset{\uparrow}{E_k} - E_{k+q+g}}\langle k|e^{-i(q+G)r}|k+q+g\rangle$$

$$\times\langle k+q+g|e^{i(q+G')r}|k\rangle. \qquad (2.60)$$

これは一般式であって wave function は Bloch function である。

If the wave function is represented by a plane wave, putting $g = G = G' = 0$ we obtain the scalar dielectric constant

$$\varepsilon(q) = 1 - \frac{4\pi e^2}{\Omega q^2}\sum_k\frac{f_k - f_{k+q}}{E_k - E_{k+q}}. \qquad (2.61)$$

This is called the Lindhard formula. Due to the electron screening U_{eff}, which is defined by (2.38), is reduced to

$$U_{scr}(q) = U_{eff}(q)/\varepsilon(q). \quad (\varepsilon(q) > 1) \qquad (2.62)$$

On making use of the relation

$$-\frac{1}{\Omega}\sum_{k}\frac{\partial f_k}{\partial E_k}=\frac{1}{\Omega}\sum_{k}\delta(E_k-E_F)=N(E_F), \qquad (2.63)$$

where $N(E_F)$ is the density of states at E_F, we obtain the $\varepsilon(q)$ for $q\to 0$ (Thomas - Fermi formula):

$$\varepsilon(q)=1+\frac{4\pi e^2}{q^2}N(E_F). \qquad (2.64)$$

To get a value of $\varepsilon(q)$ for large q, it is necessary to know the explicit expression of E_k. In the case of free electrons, we have

$$\left\{\begin{aligned} &\varepsilon(q)=1+\frac{4\pi e^2}{q^2}\,\frac{n}{\frac{2}{3}E_F}\,G(q/2k_F),\\ &G(x)=\frac{1}{2}+\frac{1-x^2}{4x}\ln\left|\frac{1+x}{1-x}\right|, \end{aligned}\right. \qquad (2.65)$$

where k_F is the Fermi momentum and n is the electron density. Here, n and $N(E_F)$ are related by

$$N(E_F)=\frac{3}{2}\,\frac{n}{E_F}. \qquad (2.66)$$

$G(x)$ is called the Kohn function and its dependence on x is shown in Fig. 2.1. $G'(x)$ becomes $-\infty$ at $x=1$. This feature is reflected in the phonon dispersion relation. Due to the electron-phonon interaction the derivative of the phonon frequency

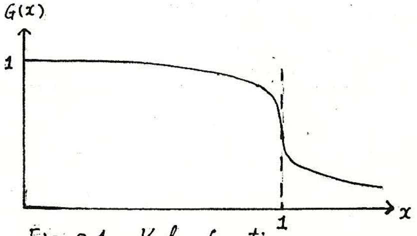

Fig. 2.1 Kohn function

$\omega(q)$ diverges at $q = 2k_F \pm q_c$ ($q_c = 2mv_s/\hbar$, v_s : sound velocity). This Kohn anomaly is directly related to the anomaly of $G(x)$. (2.65) indicates the reason why the Kohn anomaly appears.

Since $\varepsilon(q)$ tends to infinity with $q \to 0$, one might consider that $U_{scr}(q) = U_{eff}(q)/\varepsilon(q)$ goes to zero with $q \to 0$.

However, this is not the case. The cancellation effect due to U_{ps} is operative near the nucleus and in the region far from the nucleus U_{eff} takes the form of the Coulomb potential. Thus, we have

$$\begin{cases} U_{eff}(r) = -e^2/r \quad : \text{ large } r, \\ U_{eff}(q) = -4\pi e^2 n/q^2 \quad : q \sim 0 . \end{cases} \qquad (2.67)$$

In consideration of the potential field outside the Wigner-Seitz cell being zero the Function $F(qr_s)$ introduced in (2.48) and (2.49), appears. On making use of (2.64) for $\varepsilon(q)$ we obtain

$$U_{scr}(q) = \left\{ -\frac{4\pi e^2 n}{q^2} + U_0 \right\} F(qr_s) \Big/ \left\{ 1 + \frac{4\pi e^2}{q^2} N(E_F) \right\} . \qquad (2.68)$$

By applying the free electron approximation (2.66), (2.68) becomes

$$\begin{aligned} U_{scr}(q) &= \left\{ -\tfrac{2}{3} E_F + U_0 (q^2/q_s^2) \right\} F(qr_s) \big/ (1 + q^2/q_s^2), \\ q_s^2 &= 4\pi e^2 N(E_F) = 6\pi e^2 n / E_F \end{aligned} \qquad (2.69)$$

q_s is the screening constant of the Coulomb potential of a point charge immersed in the free electron gas:

$$U_s(r) = -\frac{e^2}{r} e^{-q_s r}. \qquad (2.70)$$

(2.69) is the formula derived by Bardeen.(2)

Since $F(q\hbar r_s) \to 1$ with $q \to 0$, (2.69) becomes

$$U_{scr}(0) = -\frac{2}{3} E_F . \qquad (2.71)$$

The Bardeen formula is useful for the simple metals.

Chapter 3 Deformation Potential

In the preceding Chapter we mentioned that the eigenstates of the simple metals are well approximated by few plane waves. On the other hand in semiconductors their wave functions are more complex and much different from the plane waves. Then, in order to get the electron-phonon interaction a phenomenological approach is more convenient.

In the semiconductors few carriers are located in the vicinity of the bottom of the conduction band or of the top of the valence band, and the wave length of the phonons interacting with the carriers is enough large as compared with the lattice spacing.

Therefore, it is possible to consider the crystal as the continuous medium and the lattice vibrations as the elastic waves. The lattice vibrations induce the slowly varying deformation of the band extremum and the carriers are scattered by the potential field associated with the deformation.

This is the idea on the "Deformation Potential" proposed by Bardeen-Shockley.[13)]

3.1 Bardeen-Shockley Theory

For definiteness, consider the electron band with a single minimum in the conduction band.

If the crystal with the cubic symmetry undergoes a uniform strain e_{ij}, the energy of the band bottom is given by

$$E(e_{ij}) = E_0 + E_1\Delta, \tag{3.1}$$

where Δ is the dilatation given below

$$\Delta = e_{xx} + e_{yy} + e_{zz} = \nabla_r \delta R(\mathbf{r}). \tag{3.2}$$

Though δR is a displacement of the discrete lattice, it can be considered to be a continuous function of the coordinate $\mathbf{r}$, because we are interested in the long wave vibrations.

In general, $E_1\Delta$ should be replaced by $\sum_{i,j} E_{ij}\Delta_{ij}$.

E_1 in (3.1) is a quantity with the dimension of energy, and called the deformation potential.

Bardeen-Shockley verified that if the band energy under the elastic deformation takes the form:

$$E(k, e) = E_0(k) + E_1\Delta + \text{terms in } k^2 \times \text{strains}, \tag{3.3}$$

the matrix element of the electron-phonon interaction V_p becomes

$$\langle k'|V_p|k\rangle = \langle k'|E_1\Delta|k\rangle + \text{terms of order } \left(\text{strain} \times \frac{\hbar^2}{2m}(k^2 \text{ or } k'^2)\right). \tag{3.4}$$

In the following we will verify it.

Consider a unit cell located at $\mathbf{r}_a$, whose strain is given by $e(\mathbf{r}_a)$, and imagine the lattice composed of the deformed unit cell repeated periodically. The corresponding wave function is

$$\psi_k(r, e(r_a)) = e^{ikr} u_k(r, e(r_a)). \quad (3.5)$$

In a unit cell r_a $u_k(r, e(r_a))$ will differ slightly from $u_k(r - \delta R_a)$. In this cell the potential is $V_0 + V_p$ (V_0 is the potential without deformation) and within this cell (3.5) satisfies the equation:

$$(H_0 + V_p)\,\psi_k(r, e(r_a)) = [E_0(k) + E_1\,\Delta(r_a)]\,\psi_k(r, e(r_a)), \quad (3.6)$$

where we have neglected terms like those of (3.3), of the $k^2 \times$ strains which arise from changes in the effective mass with strain.

Now, we define a function

$$\psi_k(r, e(r)) = e^{ikr} u_k(r, e(r)) = \psi_k(r) + \delta\psi_k(r). \quad (3.7)$$

$\delta\psi_k$ is linear in e for small e and therefore, we neglect the terms of order $\delta\psi_k \times$ strain..

Consider the integral

$$I = \int \psi_{k'}(r)^* \, [H_0 + V_p(r)]\, \psi_k(r, e(r))\, dr. \quad (3.8)$$

Operating $H_0 + V_p(r)$ on $\psi_k(r, e(r))$, we get

$$I = \int \psi_{k'}(r)^* \left[E_0(k) + E_1 \Delta(r) \right] (\psi_k + \delta \psi_k) dr$$

$$+ \text{terms involving } \left(\frac{\partial u_k(r, e(r))}{\partial e} \nabla e(r) \right). \tag{3.9}$$

The last terms can be shown to be of the order $(\hbar^2 k^2/2m)e$. Then, they can be neglected.

On the other hand, I becomes

$$I = \int \psi_{k'}(r)^* \left[H_0 + V_p \right] (\psi_k + \delta \psi_k)\, dr \doteqdot E_0(k') \int \psi_{k'}(r)^* \delta \psi_k\, dr$$

$$+ \int \psi_{k'}(r)^* V_p \psi_k(r)\, dr. \tag{3.10}$$

Equating (3.9) to (3.10), we have

$$\int \psi_{k'}^* V_p \psi_k\, dr \doteqdot E_1 \int \psi_{k'}^* \Delta(r) \psi_k\, dr + \{ E_0(k) - E_0(k') \} \int \psi_{k'}^* \delta \psi_k\, dr. \tag{3.11}$$

The second term in the right hand side of (3.11) is a quantity with the order $e \times (k^2 \text{ or } k'^2)$ and therefore, it can be neglected. ~~Accordingly,~~ In consequence (3.4) has been verified.

Dilatation $\Delta(r)$ makes the local electron density change from n to $n(1-\Delta)$ and the Fermi energy change is

$$\delta \zeta(r) = - \frac{n \Delta(r)}{N(E_F)} = - \frac{2}{3} E_F \Delta(r). \tag{3.12}$$

The last relation is valid in the case of free electron system.

(See (2.66)). Electron transfer restores the Fermi level to the original position and as a result a local potential change $-\delta\zeta(r)$ is induced:

$$\delta V(r) = \frac{n\Delta(r)}{N(E_F)}, \quad E_1 = \frac{n}{N(E_F)} = \frac{2}{3}E_F. \tag{3.13}$$

Ultrasonic wave propagating in a metal interacts with the electrons through (3.13).

3.2 Deformation Potentials in Silicon and Germanium

The band minima of the conduction band in Si are located at 80% length from the Γ (0.0.0) point to the Brillouin zone boundary along [100] directions, while in Ge the band minima occur at the zone-boundaries in the [111] directions.

Constant-energy surface near the band minimum in Si is the ellipsoid of revolution along [100] axis and the equivalent pockets are six. In Ge there are four ellipsoidal pockets along the [111] directions (See Fig. 3.1)

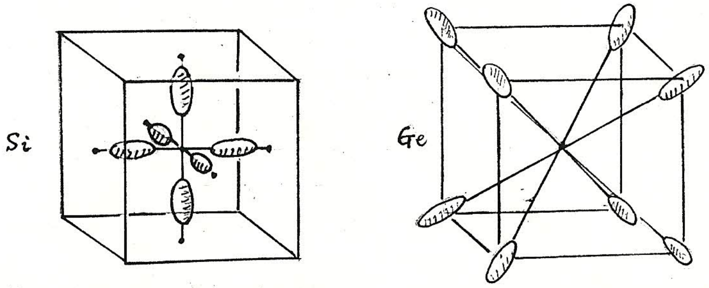

Fig. 3.1 Electron Constant Energy Surfaces in Si and Ge

According to Herring[14)] each pocket is called "valley." Silicon and Germanium are many-valley semiconductors.

Let z-axis be the evolution axis of the λ-th ellipsoid and measure k from the band minimum. Then, we have

$$E^{(\lambda)}(k) = E^{(\lambda)} + \frac{\hbar^2}{2}\left(\frac{k_\perp^2}{m_\perp} + \frac{k_z^2}{m_\parallel}\right), \quad k_\perp^2 = k_x^2 + k_y^2. \qquad (3.14)$$

Values of $m_\perp$ and $m_\parallel$ are

	$m_\perp/m$	$m_\parallel/m$	$(m_\perp^2 m_\parallel)^{1/3}/m$
Si	0.19	0.98$_2$	0.328
Ge	0.082	1.59	0.220

(3.15)

Application of stress on the crystal changes the band edge energy as follows:

$$\delta E^{(\lambda)} = \sum_{ij} \Xi_{ij}^{(\lambda)} e_{ij}, \qquad (3.16)$$

where e_{ij} is the strain tensor. (3.16) is a generalization of (3.1), and $\Xi^{(\lambda)}$ is the deformation potential tensor of the λ-th valley. From the symmetry consideration, $\Xi^{(\lambda)}$ can be expressed by

$$\Xi^{(\lambda)} = \Xi_d \mathbf{1} + \Xi_u K^{(\lambda)} K^{(\lambda)} / K^{(\lambda)2}, \qquad (3.17)$$

where $K^{(\lambda)}$ is the vector corresponding to the λ-th band edge and $\mathbb{1}$ is the unit tensor.

By choosing the ellipsoidal axes as the coordinate axes, (3.17) becomes a diagonal tensor :

$$\Xi^{(\alpha)} = \begin{pmatrix} \Xi_d & 0 & 0 \\ 0 & \Xi_d & 0 \\ 0 & 0 & \Xi_d + \Xi_u \end{pmatrix} . \qquad (3.18)$$

Change of the band edge energy due to the pure dilatation is

$$\frac{1}{3} \mathrm{Tr}\, \Xi^{(\alpha)} = \Xi_d + \frac{1}{3} \Xi_u . \qquad (3.19)$$

Ξ_u corresponds to the deformation potential related to the pure shear. Calculation of the transport coefficients and comparison with the experiments based on (3.16) and (3.17) will be presented in Chapter 7.

Here, we refer to the values of Ξ_u and Ξ_d. From the analyses of the experiments of the piezoresistance and the acoustoelectric effect, the following values were obtained.

n-Ge : $15.8\,\mathrm{eV} < \Xi_u < 19.3\,\mathrm{eV}$. Ξ_u is temperature dependent. It increases with temperature for $T > 60\,\mathrm{K}$ and reaches $\Xi_u = 21\,\mathrm{eV}$ at $T = 100\,\mathrm{K}$.

at $T = 77\,\mathrm{K}$

$$\Xi_d / \Xi_u = \begin{cases} -0.38 & (\text{Herring-Vogt}^{15)}), \\ -0.45 & (\text{J.E. Smith, Jr}^{16)}). \end{cases}$$

n-Si : $8.5\,\text{eV} < \Xi_u < 9.6\,\text{eV}, \quad \Xi_a \ll \Xi_u.$

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Chapter 4 Motion of Wave Packet and the Boltzmann Equation

4.1 Motion of Wave Packet

Now we consider the effect of uniform electric field on an electron. In this case it is not appropriate to apply the ordinary perturbation theory. Perturbation caused by the electric field is larger than the energy difference of the unperturbed Bloch states, because the energy levels specified by wave vector k form the continuum spectrum. Moreover, the Bloch function $\psi_k = e^{ikr} u_k$ are not seitable for studying transport phenomena, since they correspond to a well-defined value of the crystal momentum k, which makes the position coordinate completely undertermined.

These two defects can be remedied by constructing a wave packet from Bloch states. It is desirable to construct a wave packet whose width Δk is as sharp as possible. According to the uncertainty principle, we have

$$\Delta k \, \Delta r \sim 1. \tag{4.1}$$

Since electrons are scattered, they have finite mean free path l. Therefore, the position uncertainty Δr should be smaller than l. Since $\Delta k \ll k$, we obtain the restriction

$$k \gg \Delta k \sim 1/\Delta r \gg 1/l. \tag{4.2}$$

Spatial variations of the temperature, the carrier density fluctuation, and applied fields $\mathcal{E}$ or H should be negligibly small in Δr.

When there is a uniform electric field $\mathcal{E}$, the Schrödinger equation is

$$\frac{\hbar}{i}\frac{\partial \Psi}{\partial t} = -H_0\Psi - e\mathcal{E}\cdot r\,\Psi \quad , (e>0) \tag{4.3}$$

where H_0 denotes the unperturbed Hamiltonian. To solve (4.3), we expand Ψ in terms of the Bloch functions $\psi_{k\cdot m}$ (m: band index)[17)]

$$\Psi(r,t) = \sum_m \int \alpha_m(k\cdot t)\,\psi_{k\cdot m}(r)\,dk. \tag{4.4}$$

We require a number of formulae to get the equations of wave packet subjected to uniform electric and magnetic fields.

(1) Let $\varphi(k\cdot r)$ be a continuous function of k and r such that

$$\varphi(k, r+a_i) = \varphi(k\cdot r), \tag{4.5}$$

where a_i $(i=1.2.3)$ are the vectors forming the unit cell.

Then,

$$\frac{1}{(2\pi)^3}\int d\tau \int e^{i(k'-k)\cdot r}\varphi(k'\cdot r)\,dk' = \frac{1}{\Delta}\int \varphi(k\cdot r)\,d\tau_0, \tag{4.6}$$

where $\Delta = a_1\cdot(a_2\times a_3)$ is the volume of the unit cell and k' is taken over $-\pi \leq k'\cdot a_i \leq \pi$. $d\tau$ means the integral over the whole space while $d\tau_0$ over the unit cell.

Proof of (46) is easy.

(2) Let introduce two wave functions $\psi_k = e^{ikr} u_k$, $\phi_k = e^{ikr} v_k$, which are defined in the reduced wave vector space and normalized in the unit cell. Moreover, consider a function $\alpha(k)$ which is twice differentiable periodic function of the reduced wave vector.

Then, we obtain

$$\frac{\Delta}{(2\pi)^3}\int d\tau \int \alpha(k')\,\phi_k^* x \psi_{k'}\, dk' = -\frac{i\Delta}{(2\pi)^3}\int d\tau \int \alpha(k')\,\phi_k^* \frac{\partial e^{ik'r}}{\partial k_1'} u_{k'}\, dk'$$

$$= i\frac{\partial \alpha(k)}{\partial k_1}\int v_k^* u_k\, d\tau_0 + i\alpha(k)\int v_k^* \frac{\partial u_k}{\partial k_1}\, d\tau_0. \qquad (4.7),$$

(3)

$$\frac{\Delta}{(2\pi)^3}\int d\tau \int \alpha(k')\,\phi_k^* y \frac{\partial \psi_{k'}}{\partial x}\, dk' = \frac{\Delta}{(2\pi)^3}\int d\tau \int \alpha(k')\,\phi_k^* \frac{\partial e^{ik'r}}{\partial k_2'}$$

$$\times \left(k_1' u_{k'} - i\frac{\partial u_{k'}}{\partial x}\right) dk' = i\,\frac{\partial \alpha(k)}{\partial k_2}\int \phi_k^* \frac{\partial \psi_k}{\partial x}\, d\tau_0 - \alpha(k)\int v_k^* k_1 \frac{\partial u_k}{\partial k_2}\, d\tau_0$$

$$- i\alpha(k)\int \frac{\partial v_k^*}{\partial x}\,\frac{\partial u_k}{\partial k_2}\, d\tau_0. \qquad (4.8)$$

(4.7) and (4.8) can be easily proved. Surface integrals, which come from the partial integration over the k-space, become zero, since all functions are periodic in the reduced wave vector space. This relation is employed in the proofs of the above formulae.

Substituting (44) into (43) and integrating over the whole space by multiplying ψ_{km}^*, we get the equation for

$\alpha_m(k)$ from (4.6) and (4.7):

$$\frac{\hbar}{i}\frac{\partial \alpha_m(k)}{\partial t} = -E_{km}\alpha_m(k) - ie\mathcal{E}\cdot\left\{\nabla_k \alpha_m + \sum_{m'} \alpha_{m'} \int u_m^* \nabla_k u_{m'}\, d\tau_0\right\}. \quad (4.9)$$

Combining (4.9) with the complex conjugate equation, we get

$$\left(\hbar\frac{\partial}{\partial t} - e\mathcal{E}\cdot\nabla_k\right)|\alpha_m|^2 = e\mathcal{E}\cdot\left\{\alpha_m^* \sum_{m'} \alpha_{m'} \int u_m^* \nabla_k u_{m'}\, d\tau_0\right.$$

$$\left. + \alpha_m \sum_{m'} \alpha_{m'}^* \int u_m \nabla_k u_{m'}^*\, d\tau_0\right\}. \quad (4.10)$$

Operating $\sum_m \cdots$ on the both sides, we obtain

$$\left(\hbar\frac{\partial}{\partial t} - e\mathcal{E}\cdot\nabla_k\right)\sum_m |\alpha_m|^2 = 0, \quad (4.11)$$

In deriving (4.11), we employed the relation of $\sum_{m.m'} \alpha_m^* \alpha_{m'} \times \nabla_k \int u_m^* u_{m'}\, d\tau_0 = 0$, which is a consequence of the orthogonality relation $\int u_m^* u_{m'}\, d\tau_0 = \delta_{mm'}$.

If an electron belongs to the m-th band at $t=0$, it will remain in the same band after enough short time. Then, (4.11) becomes

$$\hbar\frac{\partial|\alpha_m|^2}{\partial t} = e\mathcal{E}\cdot\nabla_k|\alpha_m|^2. \quad (4.12)$$

Since the solution of (4.12) is given by $|\alpha_m|^2 = f(k + e\mathcal{E}t/\hbar)$, the rate of change of k due to an electric field is

$$\frac{dk}{dt} = -\frac{e\mathcal{E}}{\hbar}, \quad (e>0). \tag{4.13}$$

This is same as the classical equation of motion of the free electron. (4.13) can be easily obtained from the semiclassical approach. In this case the Hamiltonian is given by

$$\mathcal{H}(p.r) = E(p) + U(r). \tag{4.14}$$

where $E(p) = E_k$ $(p = \hbar k)$ and now $E(p)$ is considered to be a classical quantity. Hamilton equation provides

$$\dot{r} = \frac{\partial \mathcal{H}}{\partial p}, \quad \dot{p} = -\frac{\partial \mathcal{H}}{\partial r}. \tag{4.15}$$

Then, we have

$$\dot{r} = v = \frac{\partial E}{\partial p}, \quad \dot{p} = F. \; F = -\frac{\partial U}{\partial r}. \tag{4.16}$$

We must stress that the Newtonian like equation $\dot{p} = -\frac{\partial U}{\partial r}$ includes only forces external to the crystal. Putting $U = e\mathcal{E}\cdot r$, we obtain (4.13). Thus, the equation for the accerlation is given by

$$\frac{dv_i}{dt} = \sum_j \frac{\partial v_i}{\partial k_j}\frac{\partial k_j}{\partial t} = \frac{1}{\hbar}\sum_j \frac{\partial^2 E}{\partial k_i \partial k_j}\frac{dk_j}{dt}$$

$$= -\frac{e}{\hbar^2}\sum_j \frac{\partial^2 E}{\partial k_i \partial k_j}\mathcal{E}_j . \tag{4.17}$$

By introducing the effective mass tensor m_{ij} :

$$m_{ij}^{-1} = \frac{1}{\hbar^2} \frac{\partial^2 E}{\partial k_i \partial k_j} . \qquad (4.18)$$

(4.17) is written as

$$\frac{d v_i}{dt} = -e \sum_j (m_{ij})^{-1} \mathcal{E}_j . \qquad (4.19)$$

Next, we derive the equation of motion in the presence of a magnetic field $\mathbb{H}$. The vector potential $\mathbb{A}$ related to $\mathbb{H}$ by curl $A = H$, is not uniquely defined by $\mathbb{H}$, but there is a degree of arbitrariness. The Schrödinger equation is invariant under the gauge transformation

$$\psi \to \psi e^{ie\Lambda/\hbar c} , \quad A \to A - \nabla \Lambda , \quad V \to V - \frac{e}{c} \frac{\partial \Lambda}{\partial t} , \qquad (4.20)$$

where $\Lambda(r, t)$ is an arbitrary function. Now, we choose $\mathbb{A}$, whose average value is equal to zero.

Namely,

$$A = \frac{1}{2} \mathbb{H} \times (\mathbb{r} - \langle \mathbb{r} \rangle) , \quad \langle \mathbb{r} \rangle = \int r \, \Psi^* \Psi \, d\tau . \qquad (4.21)$$

This corresponds to

$$\Lambda = \frac{1}{2} r . (\mathbb{H} \times \langle \mathbb{r} \rangle) . \qquad (4.22)$$

Therefore,

$$\frac{\partial \langle \mathbf{r} \rangle}{\partial t} = \int \mathbf{r} \frac{\partial}{\partial t}(\Psi^* \Psi)\, d\tau = \langle \mathbf{v} \rangle, \quad \frac{\partial \Lambda}{\partial t} = \frac{1}{2}\mathbf{r}\cdot(\mathbf{H} \times \langle \mathbf{v} \rangle), \tag{4.23}$$

and if $\mathbf{H} = (0, 0, H)$ the Schrödinger equation becomes

$$\Big[\frac{\hbar}{i}\frac{\partial}{\partial t} - \frac{\hbar^2}{2m}\Delta + V + \frac{\hbar e H}{2imc}\Big\{ (x - \langle x \rangle)\frac{\partial}{\partial y} - (y - \langle y \rangle)\frac{\partial}{\partial x} \Big\}$$
$$+ \frac{eH}{2c}\left(x\langle v_y \rangle - y \langle v_x \rangle \right) + \frac{e^2 H^2}{8mc^2}\Big\{ (x - \langle x \rangle)^2 + (y - \langle y \rangle)^2 \Big\} \Big] \Psi = 0. \tag{4.24}$$

Neglecting the terms of $O(H^2)$ and the interband transitions, we can express Ψ by the wave packet belonging to a band:

$$\Psi(\mathbf{r}, t) = \int \alpha(\mathbf{k}, t)\, \psi_{\mathbf{k}}(\mathbf{r})\, d\mathbf{k}, \tag{4.25}$$

Substiting (4.25) into (4.24) and carrying out a similar calculation to (4.9) ~ (4.12), we get

$$\frac{\partial |\alpha|^2}{\partial t} = -\frac{eH}{2\hbar c}\Big\{ (v_x + \langle v_x \rangle)\frac{\partial |\alpha|^2}{\partial k_y} - (v_y + \langle v_y \rangle)\frac{\partial |\alpha|^2}{\partial k_x} \Big\}, \tag{4.26}$$

where (4.8) is employed. If $|\alpha|^2$ is only large near $\mathbf{k}$, $[\mathbf{v}]$ and $\mathbf{v}_{\mathbf{k}}$ will be the same for enough small times, and (4.26) becomes

$$\frac{\partial |\alpha|^2}{\partial t} = -\frac{eH}{\hbar c}\left(v_x \frac{\partial |\alpha|^2}{\partial k_y} - v_y \frac{\partial |\alpha|^2}{\partial k_x} \right) = \frac{e}{\hbar c}(\mathbf{v} \times \mathbf{H})\cdot \nabla_{\mathbf{k}} |\alpha|^2. \tag{4.27}$$

This shows that the equation equivalent to the classical Lorentz equation holds:

$$\frac{d\mathbf{k}}{dt} = -\frac{e}{\hbar c}(\mathbf{v} \times \mathbf{H}). \tag{4.28}$$

In the presence of electric and magnetic fields, we have

$$\frac{dk}{dt} = -\frac{e\mathcal{E}}{\hbar} - \frac{e}{\hbar c}(v \times H). \qquad (4.29)$$

Accordingly, the rate of change of the distribution function $f(k.t)$ is given by

$$\frac{\partial f}{\partial t} = \frac{e}{\hbar}\left(\mathcal{E} + \frac{1}{c} v \times H\right) \cdot \nabla_k f. \qquad (4.30)$$

4.2 Concept of Holes

One of the most important achievement in the band theory is that unoccupied states in the nearly filled band behave like the particles with positive charge. These fictitious particles are called holes. Peierls first proved that in the nearly filled band the Hall coefficient is positive.[18)] Concept of holes is not a conventional one, but it plays an essential role in the semiconductor physics.

Contribution of the electrons in a given band to the current density is given by

$$j = (-e) \sum_{\text{occupied}} v(k). \qquad (4.31)$$

Since a completely filled band carries no current,

$$\sum_{\text{occupied}} v(k) + \sum_{\text{unoccupied}} v(k) = 0, \qquad (4.32)$$

then

$$\boldsymbol{j} = (-e)\sum_{\text{occupied}} \boldsymbol{v}(\boldsymbol{k}) = (+e)\sum_{\text{unocupied}} \boldsymbol{v}(\boldsymbol{k}). \tag{4.33}$$

(4.33) indicates that the current carried by occupied electrons is same as the current carried by unoccupied states - holes with positive charge. The total sum of the crystal momentum $\sum k$ is zero in the completely filled band. Then, the wave vector of a hole is equal to minus of the wave vector of the missing electron:

$$\boldsymbol{k}_h = -\boldsymbol{k}_e. \tag{4.34}$$

From (4.33), it is concluded that

$$\boldsymbol{v}_e = \boldsymbol{v}_h. \tag{4.35}$$

Therefore, we obtain

$$\hbar \frac{d\boldsymbol{k}_h}{dt} = e\boldsymbol{\mathcal{E}} + \frac{e}{c}(\boldsymbol{v}_h \times \boldsymbol{H}). \tag{4.36}$$

This is the semiclassical equation for a positive charge particle. The inverse mass tensor defined by (4.18) is not always positive. For example, near the zone boundary along [111] direction of the noble metals such as Cu, Ag and Au the constant energy surface is described by

$$E_k = \frac{\hbar^2 k_1^2}{2m_1} + \frac{\hbar^2 k_2^2}{2m_2} + \frac{\hbar^2 k_3^2}{2m_3} , \tag{4.37}$$

where $m_1 = m_2 > 0$ and $m_3 < 0$. Then the constant energy surface is the hyperboloid of one sheet. (See Fig. 4.1). More familiar

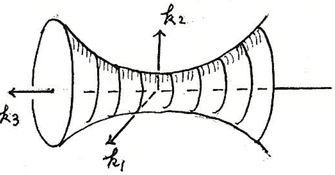


Fig. 4.1 Constant energy surface for (4.37).

examples are seen in semiconductors or semimetals with almost filled bands (see Fig. 4.2). Let k_0 be the point where E_k takes the maximum value.

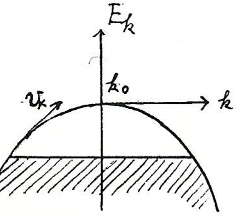


Fig. 4.2 Hole pocket near the almost filled band.

Since $v_k = (1/\hbar)\,\partial E_k/\partial k$ is zero at k_0, the principal values of $\partial^2 E_k/\partial k\partial k$ become zero in the vicinity of k_0. Accordingly, the mass tensor defined by (4.18) is negative. Instead of using the negative effective mass, it is more convenient to introduce the positive mass by

$$E_k = E_{k_0} - \sum_i \frac{\hbar^2}{2m_i}(k - k_0)^2 . \tag{4.38}$$

From (4.36) the rate of change of the hole distribution function $f_h = 1 - f_e$ is given by

$$\frac{\partial f_h}{\partial t} = -\frac{e}{\hbar}\left(\mathcal{E} + \frac{1}{c} v_h \times H\right) \cdot \nabla_k f_h . \tag{4.39}$$

4.3 Boltzmann Equation

(4.30) is the equation for the collision-free case. Let it express by $(\partial f/\partial t)_{drift}$.

According to the Liouville's theorem the density in phase space remains constant in the neighborhood of a point as it moves along its orbit. Therefore, $f(k-\dot{k}\Delta t, r-\dot{r}\Delta t)$ at t is equal to $f(k.r)$ at $t+\Delta t$. This leads to

$$\left(\frac{\partial f}{\partial t}\right)_{drift}\Delta t = f(k-\dot{k}\Delta t, r-v\Delta t) - f(k.r). \qquad (4.40)$$

On making use of (4.29), we obtain

$$\left(\frac{\partial f}{\partial t}\right)_{drift} = \frac{e}{\hbar}\left(\mathcal{E}+\frac{1}{c}v\times H\right)\cdot\nabla_k f - v\nabla_r f. \qquad (4.41)$$

This is the generalization of (4.30). If the temperature gradient and/or the concentration gradient exist, the last term $-v\nabla_r f$ becomes important.

Under the combined action of the applied electromagnetic field and the collisions of the electrons a steady state is set up, and the distribution function in the steady state is determined by the Boltzmann equation

$$\frac{\partial f}{\partial t} - \frac{e}{\hbar}\left(\mathcal{E}+\frac{1}{c}v\times H\right)\cdot\nabla_k f + v\cdot\nabla_r f = \left(\frac{\partial f}{\partial t}\right)_{coll.} \quad (e>0) \qquad (4.42)$$

If the external field does not depend on time, $\partial f/\partial t$ should be zero. The term of $(\partial f/\partial t)_{coll}$ is refered as the collision term.

Generally, it has a complicated structure but very often $(\partial f/\partial t)_{coll}$ can be taken to be of the form

$$\left(\frac{\partial f}{\partial t}\right)_{coll} = -\frac{f-f_0}{\tau}, \tag{4.43}$$

where τ is the relaxation time. Many subtle and ingenious techniques have been developed for solving the Boltzmann equation. Detailed discussions will be given in Chapter 9..

The Boltzmann equation has a wide field of application. However, it is not almighty. For an example the transport phenomena in strong magnetic fields can not be correctly treated by the Boltzmann equation. It needs a different formalism. In this respect we consider in Chapters 11 and 12.

Chapter 5 Motion of Electrons in Slowly Varying Fields

5.1 Wannier Function and Slater's Theory

Let consider a band n with no degeneracy, and expand the Bloch function $\psi_{k,n}$ by the Fourier series:

$$\psi_{kn}(\mathbf{r}) = \frac{1}{\sqrt{N}} \sum_{l} e^{ik \cdot R_l} a_n(\mathbf{r}, R_l), \tag{5.1}$$

N: number of the unit cell; R_l: coordinate of the lattice point.

$a_n(r, R_l)$ is called the Wannier function. It is proved that $a_n(r, R_l)$ is written as $a_n(r - R_l)$. From (5.1) we have

$$\psi_{kn}(r - R_t) = \frac{1}{\sqrt{N}} \sum_{l} e^{ikR_l} a_n(r - R_t, R_l). \tag{5.2}$$

As a consequence of the Bloch's theorem

$$\psi_{kn}(r - R_t) = \frac{1}{\sqrt{N}} \sum_{l} e^{ik(R_l - R_t)} a_n(\mathbf{r}, R_l).$$

By changing $R_l - R_t \to R_l$, we obtain

$$\psi_{kn}(r - R_t) = \frac{1}{\sqrt{N}} \sum_{l} e^{ikR_l} a_n(r, R_l + R_t). \tag{5.3}$$

Comparing (5.2) and (5.3) and putting $R_l = 0$, we have

$$a_n(\mathbf{r} - R_t, 0) = a_n(r, R_l), \tag{5.4}$$

Therefore, we arrive at

$$\psi_{kn}(r) = \frac{1}{\sqrt{N}} \sum_{l} e^{ikR_l} a_n(r-R_l). \qquad (5.5)$$

The Wannier function $a_n(r-R_l)$ in (5.1) is given by the inversion formula

$$a_n(r-R_l) = \frac{1}{\sqrt{N}} \sum_{k} e^{-ikR_l} \psi_{kn}(r). \qquad (5.6)$$

It can be easily verified that the Wannier functions satisfy the relation :

$$\int a_n^*(r-R_l)\, a_m(r-R_t)\, dr = \delta_{nm}\delta_{lt}. \qquad (5.7)$$

This indicates that the Bloch functions and the Wannier functions are interrelated through the unitary transformation.

If the Bloch function is assumed in the form $e^{ikr}u(r)/\sqrt{N}$, $a(r)$ is given by

$$a(r-R_n) = u(r) \prod_i \frac{\sin\{\pi(x_i-X_i)/d\}}{\{\pi(x_i-X_i)/d\}}, \quad r=(x_1,x_2,x_3),\ R_n=(X_1,X_2,X_3), \qquad (5.8)$$

where the crystal structure is considered to be the simple cubic type with a lattice constant d. (5.8) shows that for $x_i - X_i \cong 0$ $a(r-R_n) \cong u(r)$ and for $x_i - X_i \gg d$ $a(r-R_n) \to 0$. Thus the Wannier function assumes its largest value within the lattice point R_n and it decreases as we go out from the central cell.

Now we verify the Slater's theorem.[19] Let $U(r)$ be a slowly varying perturbational potential and $E_n(k)$ the eigenvalue of the unperturbed Hamiltonian H_0. The solution of the Schrödinger equation

$$\{ H_0 + U(\mathbf{r}) \} \psi(\mathbf{r}) = E \psi(r), \qquad (5.9)$$

can be obtained by solving

$$\{ E_n(-i\nabla) + U(r) \} f(r) = E f(r). \qquad (5.10)$$

The proof of (5.10) is given in the following.
Expanding $\psi(r)$ in terms of the Wannier functions

$$\psi(r) = \sum_{n,l} f_n(\mathbf{R}_l)\, a_n(\mathbf{r} - R_l), \qquad (5.11)$$

inserting (5.11) into (5.9) and operating $\int d\mathbf{r}\, a^*_{n'}(r - R_{l'}) \cdots$ on both sides, we obtain

$$\sum_{n,l} \int a^*_{n'}(\mathbf{r} - R_{l'}) (H_0 + U) a_n(r - \mathbf{R}_l) f_n(\mathbf{R}_l) = E f_{n'}(\mathbf{R}_{l'}). \qquad (5.12)$$

Since $H_0 \psi_{kn} = E_n(k) \psi_{kn}$, we have

$$H_0 a_n(\mathbf{r} - R_l) = \frac{1}{\sqrt{N}} \sum_k e^{-ikR_l} H_0 \psi_{kn} = \frac{1}{\sqrt{N}} \sum_k e^{-ikR_l} E_n(k) \psi_{kn}$$

$$= \frac{1}{N} \sum_k e^{-ikR_l} E_n(k) \sum_{l'} e^{ikR_{l'}} a_n(r - R_{l'})$$

$$= \sum_{l'} E_{n, R_l - R_{l'}}\, a_n(\mathbf{r} - R_{l'}), \qquad (5.13)$$

where
$$E_{n,R_l} = \frac{1}{N}\sum_k e^{ikR_l} E_n(k).$$

Then, (5.12) becomes

$$\sum_{n,l}\left\{\delta_{nn'} E_{n,R_l-R_{l'}} + U_{nn'}(R_l,R_{l'})\right\} f_n(R_l) = E f_{n'}(R_{l'}), \tag{5.14}$$

where $U_{nn'}(R_l,R_{l'}) = \int a_n^*(r-R_l)\, U(r)\, a_{n'}(r-R_{l'})\, dr.$

By replacing k by $-i\nabla$ in $E_n(k) = \sum_l E_{n,R_l} e^{ikR_l}$,

$$E_n(-i\nabla) f(r) = \sum_l E_{n,R_l} e^{iR_l(-i\nabla)} f(r) = \sum_l E_{n,R_l}\left\{\sum_p \frac{1}{p!}(R_l\cdot\nabla)^p\right\} f(r)$$

$$= \sum_l E_{n,R_l}\left\{ f(r) + R_l\cdot\nabla f(r) + \frac{1}{2}\left[X_l^2 \frac{\partial^2 f}{\partial x^2} + \cdots\right] + \cdots\right\}$$

$$= \sum_l E_{n,R_l} f(r+R_l). \tag{5.15}$$

Therefore,

$$\left[E_{n'}(-i\nabla) f_{n'}(r)\right]_{r=R_{l'}} + \sum_{n,l} U_{nn'}(R_l,R_{l'}) f_n(R_l) = E f_{n'}(R_{l'}). \tag{5.16}$$

Up to now we have not introduced any approximation.

Since $U(r)$ is a slowly varying function, we can use the approximation

$$U_{nn'}(R_l,R_{l'}) \cong U(R_{l'})\,\delta_{nn'}\delta_{ll'}. \tag{5.17}$$

Though $f_n(R_l)$ is defined at the discrete lattice point, we consider f_n as the continuous function $f_n(r)$.

Then, one obtains

$$\left[E_n(-i\nabla) + U(r) \right] f_n(r) = E f_n(r) . \qquad (5.18)$$

(5.18) is a very useful equation. In the presence of a magnetic field it is not straightfoward to get the corresponding equation to (5.18). However, in this case we can obtain a similar equation. Namely, the effective Schrödinger equation is given by[20]

$$\left\{ E_n\left(-i\nabla + \frac{e}{\hbar c} A(r)\right) + U(r) \right\} f_n(r) = E f_n(r), \qquad (5.19)$$

where $A(r)$ is the vector potential.

5.2 Effect of the Magnetic Field on an Electron moving in the Periodic Lattice Potential

Without lack of generality, it is possible to put $U(r) = 0$.

Thus, the Hamiltonian becomes

$$\mathcal{H} = \frac{1}{2m}\left(\mathbb{P} + \frac{e}{c}\mathbb{A}(r)\right)^2 + V(r), \qquad (5.20)$$

where $V(r)$ is the periodic crystal potential. Here, we set $\mathcal{H} \equiv \mathcal{H}\left(p + \frac{e}{c}\mathbb{A}(r)\right)$.

At first, we prove the following relation.

i) $$e^{(ie/\hbar c)G}\,\mathbf{H}\left(\mathbf{p}+\frac{e}{c}\mathbf{A}(r)\right)e^{-(ie/\hbar c)G} = \mathbf{H}\left(\mathbf{p}+\frac{e}{c}\mathbf{A}(r-R)\right), \qquad (5.21)$$

where $G = \mathbf{A}(R)\cdot \mathbf{r}.$

Proof: (5.21) can be proved if the following relation :

$$e^{(ie/\hbar c)G}\left(p+\frac{e}{c}A(r)\right)e^{-(ie/\hbar c)G} = p+\frac{e}{c}[\mathbf{A}(r)-\mathbf{A}(R)]$$

$$= \mathbf{p}+\frac{e}{c}\mathbf{A}(r-R). \qquad (5.22)$$

is verified.

Because,

$$e^{(ie/\hbar c)G}\left(\mathbf{p}+\frac{e}{c}\mathbf{A}(r)\right)^2 e^{-(ie/\hbar c)G} = e^{(ie/\hbar c)G}\left(\mathbf{p}+\frac{e}{c}\mathbf{A}\right)e^{-(ie/\hbar c)G}e^{(ie/\hbar c)G}\left(\mathbf{p}+\frac{e}{c}\mathbf{A}\right)e^{-(ie/\hbar c)G}$$

$$= \left(\mathbf{p}+\frac{e}{c}\mathbf{A}(r-R)\right)^2. \qquad (5.23)$$

For arbitrary operators a and b, we have

$$e^{a}\,b\,e^{-a} = b + [a,b] + \frac{1}{2!}[a,[a,b]] + \frac{1}{3!}[a,[a,[a,b]]] + \cdots . \qquad (5.24)$$

Putting $a = (ie/\hbar c)G$, $b = \mathbf{p}+\frac{e}{c}\mathbf{A}(r)$ and using the relations

$$\begin{cases} [a,b] = \left(\dfrac{ie}{\hbar c}\right)\left(\dfrac{\hbar}{i}\right)[G,\nabla] = -\dfrac{e}{c}\mathbf{A}(R), \\[2ex] [a,[a,b]] = [a,[a,[a,b]]] = \cdots = 0, \end{cases} \qquad (5.25)$$

we can verify (5.22) and, then (5.21).

ii) If $E_n(k)$ is the eigenvalue of the Hamiltonian $H_0 = \frac{1}{2m} p^2 + V(r)$, the solution of the Schrödinger equation,

$$i\hbar \frac{\partial \psi}{\partial t} = H\psi$$

is approximately given by the solution of

$$i\hbar \frac{\partial f}{\partial t} = E_n\left(-i\nabla + \frac{e}{\hbar c}\mathbb{A}(r)\right) f. \tag{5.26}$$

Proof : We assume that magnetic field is weak enough so that we may neglect contributions from different bands and then, omit the band index n. By suitably modifying the expansion (5.11), we shall be able to use most of the procedures of Slater's proof. Let us replace (5.11) by

$$\psi(r,t) = \sum_l f(R_l,t)\, e^{-(ie/\hbar c)\mathcal{G}_l} a(r-R_l) = \sum_l f_l\, e^{-(ie/\hbar c)} a_l, \tag{5.27}$$

where $\mathcal{G}_l = \mathbb{A}(R_l) . r$.

We must now calculate $H\psi$. Using (5.21), we have

$$i\hbar\dot{\psi} = H\psi = \sum_l f_l \left\{ \frac{1}{2m}\left(\mathbb{P} + \frac{e}{c}\mathbb{A}(r)\right)^2 + V(r) \right\} e^{-(ie/\hbar c)\mathcal{G}_l} a_l$$

$$= \sum_l f_l\, e^{-(ie/\hbar c)\mathcal{G}_l} \left\{ \frac{1}{2m}\left(\mathbb{P} + \frac{e}{c}\mathbb{A}(r-R_l)\right)^2 + V(r) \right\} a_l. \tag{5.28}$$

Since the Wannier function a_l is localized around R_l, we can neglect $A(r-R_l)$ as a small quantity.

Then,

$$\mathcal{H}\psi \doteqdot \sum_{l} f_l\, e^{-(ie/\hbar c)G_l}\left(\frac{\mathbb{P}^2}{2m}+V(r)\right)a_l=\sum_{l} f_l\, e^{-(ie/\hbar c)G_l} H_0 a_l . \qquad (5.29)$$

As is well known, $E(k)$ is a periodic function of k, having the periodicity of the reciprocal lattice. Thus we may expand

$$E(k)=\sum_{s} B_s\, e^{-ikR_s} . \qquad (5.30)$$

Using (5.1), (5.6) and (5.30) we obtain

$$H_0 a_l=\left(\frac{\mathbb{P}^2}{2m}+V(r)\right)a_l=\sum_{s} B_s\, a_{l+s} . \qquad (5.31)$$

Substitution of (5.31) into (5.29) then yields

$$\mathcal{H}\psi \doteqdot \sum_{l} f_l\, e^{-(ie/\hbar c)G_l}\sum_{s} B_s\, a_{l+s}=\sum_{l} a_l \sum_{s} B_s\, e^{-(ie/\hbar c)G_{l-s}} f_{l-s} . \qquad (5.32)$$

On making use of

$$f_{l-s}=e^{-R_s\cdot\nabla_l} f_l , \qquad (5.33)$$

and the localization property of a_l, we have

$$\begin{aligned} G_{l-s}&=\mathbb{A}(R_l-R_s)\cdot r=\mathbb{A}(R_l-R_s)(r-(R_l-R_s))=\mathbb{A}(R_l-R_s)(r-R_l)\\ &+\mathbb{A}(R_l-R_s)\cdot R_s \doteqdot \mathbb{A}(R_l-R_s)\cdot R_s=\mathbb{A}(R_l)\cdot R_s . \end{aligned} \qquad (5.34)$$

From (5.33) and (5.34), (5.32) becomes

$$\mathcal{H}\psi \doteqdot \sum_{l} a_l \sum_{s} B_s\, e^{-(ie/\hbar c)\mathbb{A}(R_l)\cdot R_s}\, e^{-R_s\cdot\nabla_l} f_l=\sum_{l} a_l\left(\sum_{s} B_s\, e^{-i[-i\nabla_l+\frac{e}{\hbar c}\mathbb{A}(R_l)]\cdot R_s}\right) f_l$$

$$= \sum_{l} a_l E\left(-i\nabla_l + \frac{e}{\hbar c} A(R_l)\right) f_l. \qquad (5.35)$$

Using

$$\frac{\partial \psi}{\partial t} = \sum_{l} \dot{f}_l e^{-(ie/\hbar c) G_l} a_l \doteqdot \sum_{l} \dot{f}_l a_l, \qquad (5.36)$$

and the orthogonal relation of a_l, we get the required result

$$i\hbar \frac{\partial f_l}{\partial t} \doteqdot E\left(-i\nabla_l + \frac{e}{\hbar c} A(R_l)\right) f_l. \qquad (5.37)$$

Chapter 6 Transport Phenomena

6.1 Bloch Equation

We assume that the wave functions of the system can be described by one-electron Bloch functions $\psi_k(r) = e^{ik.r} u_k(r)$. The number of electrons per unit volume whose wave vectors lie in the interval $(k, k+dk)$ is

$$\frac{2}{(2\pi)^3} f(k.r)\,dk, \qquad (6.1)$$

where factor 2 is the spin weight. In equilibrium $f(k.r)$ becomes the Fermi function $f_0(E)$.

The change with time of the distribution function $f(k r)$ due to a constant electric and magnetic fields is determined by the Boltzmann equation, which was derived in Section 4.3:

$$-\frac{e}{\hbar}\left(\mathcal{E} + \frac{1}{c} v \times H\right) \cdot \nabla_k f + v \cdot \nabla_r f = \left(\frac{\partial f}{\partial t}\right)_{coll.} \qquad (e > 0) \qquad (6.2)$$

In consideration of the exclusion principle, the collision term $(\partial f / \partial t)_{coll}$ is expressed by

$$\left(\frac{\partial f}{\partial t}\right)_{coll} = \sum_{k'} \left[W(k', k) f(k') (1 - f(k)) - W(k, k') f(k) (1 - f(k')) \right], \qquad (6.3)$$

where $W(k.k')$ is the transition probability per unit time from the state k to the state k'. In general, W is a complex function. If electrons interact with other dynamical system, for instance, the phonon system or the magnon system, W includes their distribution functions. This situation makes (6.2) difficult to solve. Now we assume that the system interacting with electron is in thermal equilibrium.

If the electron system is in equilibrium, the right hand side in (6.3) should be zero.

Substituting

$$f_0(E_{\mathbf{k}}) = \left[e^{(E_{\mathbf{k}}-\zeta)/k_0T} + 1 \right]^{-1}, \quad (\zeta : \text{Fermi energy}) \tag{6.4}$$

into (6.3), we have

$$W(\mathbf{k}',\mathbf{k})\, e^{E_{\mathbf{k}}/k_0T} = W(\mathbf{k},\mathbf{k}')\, e^{E_{\mathbf{k}'}/k_0T}, \tag{6.5}$$

where we assume that W does not change due to the external field and the temperature gradient.

If the applied electric field and temperature gradient are sufficiently small, the deviation from equilibrium is also small, and we can write

$$\left\{ \begin{aligned} & f(\mathbf{k},\mathbf{r}) = f_0(E_{\mathbf{k}}) + f_1(\mathbf{k},\mathbf{r}), \quad |f_1| \ll f_0 \\ & f_1 = -\Phi(\mathbf{k},\mathbf{r}) \frac{\partial f_0}{\partial E} = \Phi f_0 (1-f_0)(k_0T)^{-1}. \end{aligned} \right. \tag{6.6}$$

Inserting (6.6) into (6.3) and retaining the first order terms in f_1, we get

$$\left(\frac{\partial f}{\partial t}\right)_{coll} = \frac{1}{k_0 T}\sum_{k'} W(k,k') f_0(E_k)[1-f_0(E_{k'})][\Phi(k')-\Phi(k)]. \qquad (6.7)$$

(6.7) corresponds to the equation in the region where the linear laws - the Ohm's law $j = \sigma \mathcal{E}$ and the Fourier's law $w = -\varkappa \nabla T$ are valid. In semiconductors so called "hot electron" state is easily realized in strong electric fields. In this case the linearlized approximation is not valid. The right hand side in (6.7) is called the collision integral.

From (6.2), (6.7) and $v = (1/\hbar)\nabla_k E_k$, (6.2) becomes

$$-\frac{e}{\hbar}\left[\mathcal{E}+\frac{1}{c\hbar}\nabla_k E_k \times H\right]\cdot\nabla_k f(k,r) + \frac{1}{\hbar}\nabla_k E_k\cdot\nabla_r f(k,r)$$
$$= \frac{1}{k_0 T}\sum_{k'} W(k,k') f_0(E_k)[1-f_0(E_{k'})][\Phi(k')-\Phi(k)]. \qquad (6.8)$$

(6.8) is called the Bloch equation and the basic equation for the transport phenomena.

Let introduce the quantity

$$V(k,k') = W(k,k') f_0(E_k)(1-f_0(E_{k'})). \qquad (6.9)$$

From (6.4) and (6.5), it is shown that V satisfies the symmetry relation:

$$V(k,k') = V(k',k). \tag{6.10}$$

(6.10) plays an important role in solving the Boltzmann equation by using the variation principle.

Substituting (6.6) into the left hand side of (6.8) and considering ζ and T being smooth functions of $\mathbf{r}$, (6.8) becomes

$$-e\left(\mathcal{E}+\frac{\nabla\zeta}{e}\right)\cdot v\frac{\partial f_0}{\partial E_k} + \frac{e}{\hbar c}(v\times H)\cdot\nabla_k\Phi\frac{\partial f_0}{\partial E_k} - \frac{(E_k-\zeta)}{T}(v\cdot\nabla T)\frac{\partial f_0}{\partial E_k}$$
$$= \frac{1}{k_0T}\sum_{k'}V(k,k')\left[\Phi(k')-\Phi(k)\right]. \tag{6.11}$$

Since the observed electric field is $\mathcal{E}+\frac{\nabla\zeta}{e}$, hereafter it is rewritten by $\mathcal{E}$.

Due to the complex structure of the collision term, it is not easy to solve (6.11). Here, we assume that $(\partial f/\partial t)_{\text{coll}}$ can be taken to be of the form,

$$\left(\frac{\partial f}{\partial t}\right)_{\text{coll}} = -\frac{f-f_0}{\tau} = -\frac{f_1}{\tau}, \quad = \frac{1}{k_BT}\sum_{k'}V(k,k')\left[\Phi(k') - \Phi(k\right. \tag{6.12}$$

which has already been introduced in Section 4.3.

6.2 Relaxation Time Approximation

The solution of (6.11) under the relaxation time approximation

(6.12) is obtained by the differential equation:

$$\begin{cases} \Phi = \frac{\tau}{\hbar}(\mathbb{P}\cdot\nabla_k E) - \frac{e\tau}{\hbar^2 c}\mathbb{H}\cdot\Omega\Phi, \\ \mathbb{P} = -e\mathcal{E} - \frac{(E-\zeta)}{T}\nabla T, \quad \Omega = \nabla_k E \times \nabla_k . \end{cases} \tag{6.13}$$

To obtain a formal solution of (6.13) is easy, but the solution is incovenient to carry out a concrete calculation. Jones and Zener [21)] solved (6.13) in ascending powers of H by iteration as follows:

$$\Phi = \sum_{n=0}^{\infty}(-1)^n\left(\frac{e}{\hbar^2 c}\right)^n(\tau\mathbb{H}\cdot\Omega)^n\left(\frac{\tau}{\hbar}\mathbb{P}\cdot\nabla_k E\right). \tag{6.14}$$

In order to be able to define the relaxation time τ, it is necessary that τ is a quantity independent of $\mathcal{E}$ and ∇T. Let us examine briefly in what conditions it is realized.

For simplicity, we consider the case for no magnetic field.

From (6.11) and (6.12), we have

$$\frac{1}{\tau(k)} = -\frac{(\partial f/\partial t)_{\text{coll.}}}{f_1} = -\frac{1}{k_0 T(\partial f_0/\partial E)}\sum_{k'} V(k,k')\left\{1-\frac{\Phi(k')}{\Phi(k)}\right\}. \tag{6.15}$$

Inserting $\Phi = \frac{\tau}{\hbar}(\mathbb{P}\cdot\nabla_k E)$ into (6.15), we obtain

$$\frac{1}{\tau(k)} = -\frac{1}{k_0 T\,(\partial f_0/\partial E)} \sum_{k'} V(k,k') \left\{ 1 - \frac{\tau(k')}{\tau(k)} \frac{\left(e\mathcal{E} + \frac{E'-\zeta}{T}\nabla T\right)\cdot\nabla_{k'} E(k')}{\left(e\mathcal{E} + \frac{E-\zeta}{T}\nabla T\right)\cdot\nabla_{k} E(k)} \right\}. \quad (6.16)$$

On inspection of (6.16), it is shown that if the scattering is elastic $(E=E')$ τ does not depend on $\mathcal{E}$ and ∇T.

Even if the scattering process is not elastic in the strict sence, we can define τ approximately in the case of $|E'-E| \ll k_0 T$.

Scattering due to impurity centers, acoustic phonon scattering in semiconductors, phonon scattering in metals at the temperatures higher than the Debye temperature and magnon scattering in magnetic semiconductors, are the examples where the relaxation time approximation is valid.

In the next Section the transport coefficients are calculated in terms of the relaxation time approximation.

6.3 Electrical and Thermal Conductivities

In the absence of a magnetic field, f_1 becomes

$$f_1 = \left(e\mathcal{E} + \frac{E-\zeta}{T}\nabla T\right)\cdot v\tau \frac{\partial f_0}{\partial E}. \quad (6.17)$$

The electric and heat current densities are given by

$$\begin{cases} \mathbf{j} = -\dfrac{e}{4\pi^3}\displaystyle\int \left(e\mathcal{E} + \frac{E-\zeta}{T}\nabla T\right)\cdot(v\tau)\,v\,\frac{\partial f_0}{\partial E}\,dk, \\ \mathbf{w} = \dfrac{1}{4\pi^3}\displaystyle\int \left(e\mathcal{E} + \frac{E-\zeta}{T}\nabla T\right)\cdot(v\tau)\,(E-\zeta)\,v\,\frac{\partial f_0}{\partial E}\,dk. \end{cases} \quad (6.18)$$

Let assume that τ and E_k only depend on $|k|$.

If a small temperature gradient, as well as an electric field are set up in a crystal, both an electric and a heat current will flow:

$$\boldsymbol{j} = \sigma \mathcal{E} - \beta \nabla T, \qquad \boldsymbol{w} = \chi \mathcal{E} - \lambda \nabla T. \tag{6.19}$$

The coefficients β and χ are related through the Onsager relation, Namely,

$$T\beta_{ij}(H) = \chi_{ji}(-H), \quad (i, j = x, y, z). \tag{6.20}$$

Now we consider a simple case if $H = 0$ and $\mathcal{E} \parallel \nabla T \parallel x$.
From (6.18), we get

$$\sigma_{xx} = -\frac{e^2}{12\pi^3}\int dE \frac{\partial f_0}{\partial E}\int \tau v^2 \frac{dS}{|\nabla_k E|} \doteqdot \frac{e^2}{12\pi^3}\int_{E=\zeta} \tau v^2 \frac{dS}{|\nabla_k E|}, \tag{6.21}$$

$$\begin{aligned}\beta_{xx} &= \frac{e}{12\pi^3}\,\frac{1}{T}\int dE\,(E-\zeta)\frac{\partial f_0}{\partial E}\int \tau v^2 \frac{dS}{|\nabla_k E|}. \\ &\doteqdot -\frac{e}{36\pi}\,\frac{(k_0 T)^2}{T}\left[\frac{\partial}{\partial E}\int_E \tau v^2 \frac{dS}{|\nabla_k E|}\right]_{E=\zeta},\end{aligned} \tag{6.22}$$

$$\left\{\begin{aligned}\chi_{xx} &\doteqdot -\frac{e}{36\pi}(k_0 T)^2\left[\frac{\partial}{\partial E}\int_E \tau v^2 \frac{dS}{|\nabla_k E|}\right]_{E=\zeta}, \\ \lambda_{xx} &\doteqdot \frac{1}{36\pi}\,\frac{(k_0 T)^2}{T}\int_{E=\zeta} \tau v^2 \frac{dS}{|\nabla_k E|}.\end{aligned}\right. \tag{6.23}$$

In deriving (6.21) ~ (6.23), the following relations are employed:

$v_x{}^2 \to \frac{1}{3} v^2$, $\quad dk = dE\, dS/|\nabla_k E_k|$ (S: constant energy surface),

$$\left\{ \begin{aligned} & -\int \phi(E) \frac{\partial f_0}{\partial E}\, dE = \phi(\zeta) + 2 \sum_{n=1}^{\infty} C_{2n} (k_0 T)^{2n} \frac{d^{2n} \phi(\zeta)}{d\zeta^{2n}}, \\ & C_{2n} = \sum_{s=1}^{\infty} \frac{(-1)^{s+1}}{s^{2n}}, \quad \left(C_2 = \frac{\pi^2}{12}, \quad C_4 = \frac{7\pi^4}{720} \right). \end{aligned} \right. \tag{6.24}$$

The Onsager relation $T\beta_{xx}(H=0) = \chi_{xx}(H=0)$ is satisfied in (6.22). It should be noted that the phonon contribution to $\mathbf{j}$ and $\mathbf{w}$ are completely neglected in the present case.

The thermal conductivity is determined by the heat flow produced by a temperature gradient in condition such that there is no electric current.

From (6.19), we obtain

$$\kappa = (\sigma_{xx} \lambda_{xx} - \beta_{xx} \chi_{xx})/\sigma_{xx} = \lambda_{xx} - T\beta_{xx}{}^2/\sigma_{xx}, \tag{6.25}$$

where we employed (6.20). The second term in (6.25) is usually much smaller than the first one in metals. On the other hand, the adiabatic conductivity which is measured under the condition of $w_x = 0$ is given by

$$\sigma = \sigma_{xx} + T\beta_{xx}{}^2/\lambda_{xx}, \tag{6.26}$$

and the second term is also much smaller than the first one in usual metals. σ is called the adiabatic conductivity and σ_{xx} the isothermal conductivity. Exceptionally, we encounter with the case where the difference between σ and σ_{xx} is appreciable.

From (6.21) and (6.23), we obtain

$$\frac{\varkappa}{\sigma T} = \frac{\lambda_{xx}}{\sigma_{xx} T} = \frac{\pi^2}{3}\left(\frac{k_0}{e}\right)^2 = L_0 = 2.718 \times 10^{-13} \text{ esu.} \qquad (6.27)$$

This is the Wiedemann-Frantz law and L_0 is called the Lorentz number. If the scattering process is elastic and the electric and thermal conductions are described by the same relaxation time, (6.27) holds. In the typical monovalent metals such as sodium the magnitude of $\varkappa/\sigma T L_0$ is nearly unity at low temperatures and after passing a minimum at intermediate temperatures it approaches to unity with increasing temperatures (see Fig. 6.1).

This indicates that at intermediate temperatures the relaxation mechanisms controlling the electric conduction and the heat conduction are different, and the inelastic scattering process plays an important role in the heat conduction. We will discuss this problem in Chapter 9.

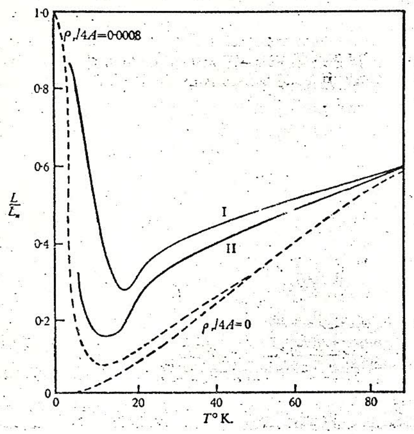


Fig. 6.1 Experimental and theoretical curves for the Lorentz number of two specimens of Na.[22)] Experimental curves —, theoretical curves ···.

In Fig. 6.1 ρ_r is the residual resistivity which is essentially controlled by the elastic scattering. A is a quantity related to the resistivity limited by the phonon scattering process. Detailed treatment will be given in Chapter 9. The phonon scattering resistivity ρ_i includes A in the following form:

$$\rho_i = 4A\left(\frac{T}{\Theta_D}\right)^5 J_5\left(\frac{\Theta_D}{T}\right), \quad J_n(x) = \int_0^x \frac{z^n\,dz}{(e^z-1)(1-e^{-z})}. \tag{6.28}$$

Sample I has $\rho_r/4A = 0.0008$ and II has $\rho_r/4A = 0.0001$.

If we put $v/|\nabla_k E| = 1/\hbar$ and $\tau v = \Lambda$ (mean free path) in (6.21), we have

$$\sigma = \frac{e^2}{12\pi^3\hbar} A_F \Lambda_F \tag{6.29}$$

where A_F denotes the area of the Fermi surface and Λ_F is the average value of $\Lambda = \tau v$ on the Fermi surface. In the most simple case we have $A_F = 4\pi k_F^2$ and $\Lambda_F = \tau(\zeta)\hbar k_F/m^*$.

Then, (6.29) becomes

$$\sigma = \frac{ne^2\tau(\zeta)}{m^*}, \quad n = \frac{k_F^3}{3\pi^2} : \text{electron density} \qquad (6.30)$$

At a glance of (6.30), one might consider that all electrons contribute the conduction process. However, it is not the case. (6.21) and (6.29) indicate that only the electrons near the Fermi surface participate in the conduction process.

For multivalent metals and semimetals carriers are distributed over several bands. In this case we have

$$\sigma = \frac{e^2}{12\pi^3\hbar}\sum_i A_F^{(i)}\Lambda_F^{(i)} = e^2\sum_i \frac{n_i\tau_i(\zeta)}{m_i^*} \qquad (6.31)$$

6.4 Thermoelectric Effects, Kelvin Relation and Onsager Relations

We consider now a wire made of two metals 1 and 2. The two junctions B and C are at temperatures T' and T'', and in the wire made of metal 1 there is a condenser, whose temperature is kept at T_0. There are three important thermoelectric effects, which are closely related to each other.. Namely, they are a) the Seebeck effect, b) the Peltier effect and c) the Thomson effect.

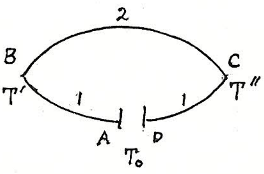


Fig. 6.2 The thermoelectric circuit

a) Seebeck Effect:

In an open circuit as shown in Fig. 6.2 there exists a potential difference $V_A - V_B \equiv \Theta_{12}$. Θ_{12} is independent of T_0 and is a function of T' and T'' only. This is called the thermoelectric force. If T' is fixed and $T'' = T$ is varied, the quantity $d\Theta_{12}/dT$ is called the thermoelectric power (thermopower, TEP) or the Seebeck coefficient.

b) Peltier Effect:

Let consider a closed circuit by joining A and D and keep B and C at a constant temperature. If a current J passes through the junction, heat is generated or absorbed at the junction in addition to the Joule heat. This heat is directly proportional to J and is known as the Peltier heat. The Peltier coefficient Π_{12} is defined as follows:

Π_{12} = the heat generaled per unit time when unit current flows from 1 to 2.

The Peltier heat is the reversible heat and $\Pi_{12} = -\Pi_{21}$.

Π_{12} and Θ_{12} are related to each other by the Kelvin relation as

$$\Pi_{12} = T\frac{d\Theta_{12}}{dT}. \tag{6.32}$$

c) Thomson Effect :

If a current J flows through a homogeneous wire whose temperature difference is ΔT. A heat $\mu J \Delta T$ is generated or absorbed in addition to the Joule heat. It is called the Thomson effect. μ is defined as positive, if the heat is emitted while the current J flows from the higher temperature region to the lower region. Between μ and Θ there exists the Kelvin relation :

$$\mu_1 - \mu_2 = T \frac{d^2\Theta_{12}}{dT^2}. \tag{6.33}$$

Among the three thermoelectric effects μ is only the quantity related to a single metal and we define the absolute thermoelectric power S by

$$S = \frac{d\Theta}{dT} = \int_0^T \frac{\mu}{T} dT. \tag{6.34}$$

In order to determine $S = d\Theta/dT$ it is necessary to measure μ of a metal down to the absolute zero temperature and this can be used as the standard data. Practically, it is difficult to measure μ to the zero temperature. Instead of this, the absolute thermoelectric power S is determined by exploiting the fact that no thermoelectric voltage develops across a superconducting metal. This is due to the reason that superconducting electrons carry no entropy..

Putting $j_x = 0$ in (6.19) and utilizing (6.21), (6.22) we get

$$S = \frac{\mathcal{E}_x}{\nabla_x T} = \frac{\beta_{xx}}{\sigma_{xx}} = -\frac{\pi^2}{3}\frac{k_0^2 T}{e}\left[\frac{\partial}{\partial E}\ln\sigma(E)\right]_{E=\zeta}, \quad (e>0) \qquad (6.35)$$

Consider the following simple case :

$$\sigma(E) \propto n(E)\tau(E), \quad n(E) \propto E^{3/2}, \quad \tau(E) \propto E^p. \qquad (6.36)$$

In this case, we have

$$S = -\frac{\pi^2}{3}\frac{k_0^2 T}{e}\left[\frac{n'(\zeta)}{n(\zeta)} + \frac{\tau'(\zeta)}{\tau(\zeta)}\right] = -\frac{\pi^2}{3}\left(\frac{3}{2}+p\right)\frac{k_0^2 T}{e\zeta}. \qquad (6.37)$$

As will be shown in Chapter 7, the energy dependence of $\tau(E)$ in simple metals is given by

$$\tau(E) \propto \begin{cases} E^{3/2} : & \text{acoustic phonon scattering,} \\ E^{-1/2} : & \text{impurity scattering,} \end{cases} \qquad (6.38)$$

and then,

$$S = \begin{cases} -\dfrac{\pi^2 k_0^2 T}{e\zeta} : & \text{acoustic phonon scattering,} \\ -\dfrac{\pi^2 k_0^2 T}{3e\zeta} : & \text{impurity scattering.} \end{cases} \qquad (6.39)$$

At the temperature where the phonon scattering is predominant, we estimate the thermoelectric power of Na - a typical monovalent metal.

Inserting $T = 300\,\mathrm{K}$ and $\zeta = 3.23\,\mathrm{eV}$ into (6.39), we obtain

$$S = -6.82\ \mu V/\text{deg}. \tag{6.40}$$

It is well established theoretically that a simple free electron system should have a negative thermopower – just what we observe at room temperature in all the alkali metals except Li.

The fact that S is positive for the pure noble metals such as Au, Ag and Cu is due to the sort of a multiply-connected Fermi surfaces[23] (See Fig. 4.1). By checking (6.35) we can see that there is a possibility of observing the positive thermopower in the nearly filled bands.

From (6.29), we have

$$\sigma(E) \propto A(E)\Lambda(E). \text{ Then,}$$

$$\frac{\partial \ln \sigma(E)}{\partial E} = \frac{\Lambda'(E)}{\Lambda(E)} + \frac{A'(E)}{A(E)}. \tag{6.41}$$

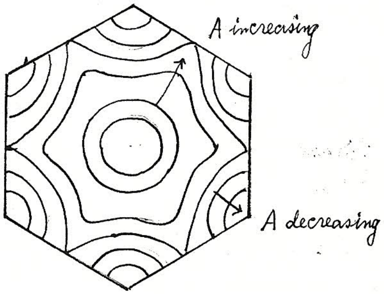


Fig 6.3 Change in area of Fermi surfaces with energy.

As shown in Fig. 6.3 $A(E)$ increases with E in a case of the small Fermi surface, while it decreases with E near the Brillouin zone boundary.

Therefore, in the latter case there is a possibility that S becomes positive due to the predominant contribution from $A'(E)/A(E)$ term. In other words it corresponds to the hole contribution to the thermopower.

There is another problem related to the thermoelectric power besides its sign. MacDonald et al found that the magnitudes of the thermopower of the alkali metals at helium temperatures were many times that predicted by (6.39), for an example in sodium about 10 times larger.[24] In order to explain the observed results, it needs a careful calculation which takes into consideration of the phonon drag effect and the Umklapp process.[25] We do not touch this problem further.

Next, we consider the mixed conduction in multivalent metals and/or semimetals. In this case electrons and holes simultaneously participate in the conduction process.

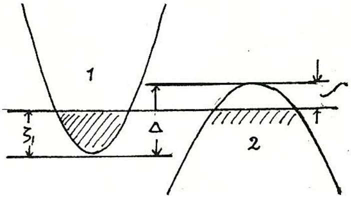


Fig. 6.4 Electron and hole bands. ζ_1 and ζ_2 denote the Fermi levels and Δ the overlapping energy.

Consider the simple parabolic bands as shown in Fig. 6.4. Energy is measured from the bottom of the electron band 1.

Then putting

$$\begin{cases} n_2(E) \propto (\Delta - E)^{3/2}, \\ \tau_2(E) \propto (\Delta - E)^{p}. \end{cases} \qquad (6.42)$$

we obtain

$$S = \frac{3/2 + p}{3} \frac{\pi^2 k_0^2 T}{e} \frac{\sigma_2/\zeta_2 - \sigma_1/\zeta_1}{\sigma_1 + \sigma_2} = \frac{S_1\sigma_1 + S_2\sigma_2}{\sigma_1 + \sigma_2}, \qquad (6.43)$$

where $S_1 < 0$ and $S_2 > 0$. The last expression has a general validity irrespective carriers.

From (6.19), the Peltier coefficient is given by

$$\Pi = \frac{\chi_{xx}}{\sigma_{xx}}, \tag{6.44}$$

and then the Kelvin relation (6.32) is equivalent to

$$T\beta_{xx} = \chi_{xx}. \tag{6.45}$$

As already mentioned in the previous section, (6.45) is a relation in the Onsager relations.

In the following we trace the procedures of the derivation 'due to Kelvin, who arrived at (6.32) and (6.33) based on the unjustified assumption. And show how the Kelvin relation is justified by the Onsager's treatment.

We return again to Fig. 6.2.

Joining AD by a high resistance, we make a closed circuit.

Let consider a unit charge passing through ABCDA.

The work done on the unit charge is Θ_{12}, and the Peltier heat generated at B and C is given by $(\Pi_{12})_{T'} - (\Pi_{12})_{T''}$.

The Thomson heat generated in the metal 2 is given by $-\int_B^C \mu_2 \frac{\partial T}{\partial x} dx = -\int_{T'}^{T''} \mu_2 dT$, and a similar expression is obtained for the metal 1.

Energy conservation law is expressed by

$$\Theta_{12} + (\Pi_{12})_{T'} - (\Pi_{12})_{T''} + \int_{T'}^{T''} (\mu_1 - \mu_2)\, d\,T = 0. \tag{6.46}$$

Kelvin assumed that in the entropy production the irreversible contribution associated with the Joule heat and the thermal conduction can be separated from the reversible part related to the Peltier effect and the Thomson effect, and put the entropy change in the reversible process to be zero.

Namely,

$$\frac{(\Pi_{12})_{T'}}{T'} - \frac{(\Pi_{12})_{T''}}{T''} + \int_{T'}^{T''} \frac{\mu_1 - \mu_2}{T}\, d\,T = 0. \tag{6.47}$$

However, we can not justify the assumption even if the final conclusion is correct.[26)]

Keeping T' as a constant and differentiating (6.46) and (6.47) on T'', we get

$$\begin{cases} \dfrac{d\Theta_{12}}{dT} - \dfrac{d\Pi_{12}}{dT} + \mu_1 - \mu_2 = 0, \\[2ex] \dfrac{d}{dT}\left(\dfrac{\Pi_{12}}{T}\right) = \dfrac{\mu_1 - \mu_2}{T}. \end{cases} \tag{6.48}$$

Then, we get the Kelvin relation:

$$\Pi_{12} = T\,\frac{d\Theta_{12}}{dT}, \quad T\,\frac{d^2\Theta_{12}}{dT^2} = \mu_1 - \mu_2. \tag{6.49}$$

The Peltier coefficient changes its sign by reversing the current direction. Similarly, in the Thomson effect μ becomes $-\mu$ by reversing the temperature gradient. In this meaning, we call these effect the "reversible process", but it does not correspond to the reversible process in the thermodynamics.

Kelvin mentioned in his book that the relation (6.46) is only an assumption which should be checked by experiment.[26]

Now, we consider the relation between the Kelvin's theory and the Onsager principle.

Consider a system subjected to a set $X_1, \cdots, X_n$ of generalized forces which induce generalized fluxes $J_1, \cdots, J_n$. They are linearly related by the phenomenological law,

$$J_i = \sum_j L_{ij} X_j \, . \tag{6.50}$$

Onsager's fundamental theorem states that provided a proper choice is made for the "fluxes" J_i and "forces" X_i, the matrix of phenomenological coefficient L_{ij} is symmetric, i.e.,

$$L_{ij} = L_{ji} \quad (i, j = 1, 2, \cdots, n) . \tag{6.51}$$

These identies are called the Onsager reciprocal relations. We must still explain what is meant by "a proper choice"[7] of the fluxes and forces. According to Onsager in this choice J_i and X_i are defined so as to satisfy the relation :

$$\dot{s} = \sum_i J_i X_i , \qquad (6.52)$$

where $\dot{s}$ denotes the entropy production per unit time during an irreversible process. When a magnetic field is applied to the system, the Onsager relations (6.51) have to be modified to read

$$L_{ij}(H) = L_{ji}(-H). \qquad (6.53)$$

In the following we consider the case for $H = 0$.[27] Consider a unit volume in the interior of an open system. The change in entropy can be expressed by

$$ds = (du - \tilde{\mu}\, dn)/T, \quad \tilde{\mu} = \mu - e\varphi \ (e>0), \qquad (6.54)$$

where

u : internal energy/vol, s : entropy/vol, $\tilde{\mu}$: electrochemical potential/particle, n : electron density, μ : chemical potential, φ : electrical potential.

From (6.54) the entropy production is given by

$$\frac{ds}{dt} = \frac{1}{T}\frac{du}{dt} - \left(\frac{\tilde{\mu}}{T}\right)\frac{dn}{dt} . \qquad (6.55)$$

The energy conservation and the particle number conservation are

$$\frac{du}{dt} + \nabla Q = 0, \quad \frac{dn}{dt} + \nabla J_e = 0, \qquad (6.56)$$

where $\mathbf{Q}$ is the energy flux density and J_e the particle flux density.

Inserting (6.56) into (6.55) and after appropriate manipulation, we get

$$\frac{ds}{dt} + \nabla\cdot[(\mathbf{Q} - \tilde{\mu} J_e)/T] = \mathbf{Q}\cdot\nabla(1/T) - J_e\cdot\nabla(\tilde{\mu}/T). \tag{6.57}$$

$\mathbf{Q} - \tilde{\mu} J_e$ corresponds to the thermal current density $\mathbf{w}$ in (6.19), and $(\mathbf{Q} - \tilde{\mu} J_e)/T$ denotes the entropy flux density. The right hand side of (6.57) is the local entropy production.

By rewriting this in terms of $\mathbf{w} = \mathbf{Q} - \tilde{\mu} J_e$ and $\mathbf{j} = -e J_e$, we have

$$\mathbf{Q}\cdot\nabla(1/T) - J_e\cdot\nabla(\tilde{\mu}/T) = \mathbf{w}\cdot\nabla(1/T) + \mathbf{j}\cdot\mathcal{E}/T, \tag{6.58}$$

where $\mathcal{E} = \nabla(\tilde{\mu}/e)$. Clearly, (6.58) corresponds to the entropy production due to the thermal and electrical conductions.

Let introduce the notation Θ for (6.58). Integrating (6.57) over the total volume, we obtain

$$\int \frac{ds}{dt}\, d\tau + \int \frac{W_n}{T}\, df = \int \Theta\, d\tau, \tag{6.59}$$

where in the second term of the left hand side the Green's theorem is employed. By extending the integration region infinity the surface integral term tends to zero.

At this point it is worthwhile to consider the reason why the Kelvin treatment arrived at the correct conclusion.

We express the entropy production in the form

$$\left\{\begin{aligned} &\Theta = \sum_i J_i X_i = J_s X_s + J_e X_e , \\ &J_s = \frac{1}{T}(Q - \tilde{\mu} J_e) = \frac{W}{T}, \quad X_s = T \nabla (1/T), \\ &J_e = J_e, \quad X_e = -\frac{1}{T}\nabla \tilde{\mu} . \end{aligned}\right. \qquad (6.60)$$

Θ is equal to $\dot{S}$ in (6.52). The phenomenological linear relations are

$$J_e = L_{ee} X_e + L_{es} X_s, \quad J_s = L_{se} X_e + L_{ss} X_s. \qquad (6.61)$$

Eliminating J_s and X_e by use of (6.61) and inserting into Θ, one obtains

$$\Theta = J_e^2/L_{ee} + [(L_{se} - L_{es})/L_{ee}] J_e \cdot X_s + [L_{ss} - (L_{es} L_{se}/L_{ee})] X_s^2 . \qquad (6.62)$$

Consider (6.61) applied to an isothermal sample. Then, we have $J_e = (e L_{ee}/T) \nabla \varphi$. The current density is given by $j = -e J_e = (e^2 L_{ee}/T) \mathcal{E}$.

Therefore,

$$\Theta = j^2/\sigma T . \qquad (6.63)$$

where σ is the electrical conductivity given by $e^2 L_{ee}/T$.

This is just the entropy production related to the Joule heat.

If one assumes $J_e = 0$, (6.61) gives

$$J_s = [L_{ss} - (L_{es}L_{se})/L_{ee}]\, T\nabla(1/T). \qquad (6.64)$$

Since TJ_s is equal to Q for $J_e = 0$,

$$T J_s = Q = -[L_{ss} - (L_{es}L_{se}/L_{ee})]\cdot\nabla T = -\varkappa\nabla T. \qquad (6.65)$$

In this case, the entropy production becomes

$$\theta = J_s X_s = T^2\varkappa[\nabla(1/T)]^2 = [L_{ss} - (L_{es}L_{se})/L_{ee}]X_s^2. \qquad (6.66)$$

This is the entropy production due to the heat transfer by thermal conduction. Generally, (6.62) shows that θ is composed of the three terms:

$$\theta = (\text{Contribution due to the Joule heat}) + (\text{term proportional to } J_e\cdot\nabla T) + (\text{Contribution due to the thermal conduction}). \qquad (6.67)$$

Kelvin assumed that the middle term is equal to zero.

This is justified by the Onsager relation $L_{es} = L_{se}$.

This does not mean that Kelvin's reasoning is justified.

6.5 Phonon Drag Effect

In deriving the expression of the thermopower in the preceding Section, the system interacting with electrons is assumed to be in thermal equilibrium. In the electron-phonon system, the phonon distribution function is described by the Planck function, and all properties of the phonons interacting with electrons are included in the electron relaxation time due to the electron-phonon interaction. However, the deviation of the equilibrium distribution in the phonon system plays an important role in the thermoelectric effects, and this induces an extra contribution to the thermopower. This effect is called the phonon drag effect. In some magnetic semiconductors the magnon drag effect can be observed.

Detailed treatment will be given in Chapter 14. Here, we present a qualitative consideration.

Let consider a phonon gas system with energy density $E(T)$. The pressure exerted on the electron system by the phonon gas is given by

$$P = \frac{1}{3} E(T). \tag{6.68}$$

In the presence of a temperature gradient dT/dx the phonon gas affects the electrons through the force density given by

$$K_x = -\frac{dP}{dx} = -\frac{1}{3}\frac{dE}{dT}\frac{dT}{dx}. \tag{6.69}$$

In an open circuit, this force should be balanced by the phonon drag electric field $\mathcal{E}_x$. Thus, we have

$$-ne\mathcal{E}_x + K_x = 0, \tag{6.70}$$

where n is the electron density, and the thermopower due to the phonon drag effect is

$$S_p = \frac{\mathcal{E}_x}{dT/dx} = -\frac{1}{3e}\left(\frac{1}{n}\frac{dE}{dT}\right) = -\frac{C_p}{3e}, \qquad (6.71)$$

where C_p is the phonon specific heat per electron. Since the electron-phonon interaction is not included in (6.71), it does not represent the correct phonon drag contribution to the thermoelectric power. To obtain the correct result, (6.71) should be multiplied by a factor $\langle R \rangle$ which is smaller than unity:

$$S_p = -\frac{C_p}{3e}\langle R \rangle, \ \langle R \rangle = \langle t/t^{(e)} \rangle, \ 1/t = 1/t^{(e)} + 1/t^{(r)}; \qquad (6.72)$$

where $t^{(e)}$ is the phonon relaxation time associated with the electron-phonon scattering and $t^{(r)}$ includes the remaining relaxation processes except the electron-phonon interaction. Definition of $\langle \dots \rangle$ is given in Chapter 14. Electron-magnon interaction in antiferromagnets is formally similar to the electron-longitudinal phonon interaction, and in some antiferromagnets the magnon drag effect plays an important role in the thermoelectric effect.

Let consider the electrons in monovalent metals interacting only with the longitudinal acoustic phonons. C_p at low temperatures is given by

$$C_p = \frac{4\pi^4}{5} k_0 \left(\frac{T}{\Theta_D}\right)^3, \quad \Theta_D = \text{Debye temperature.} \tag{6.73}$$

Then, the ratio of S_p to (6.37) is given by

$$\frac{S_p}{S} = \frac{4\pi^2}{5(3/2+p)} \left(\frac{T}{\Theta_D}\right)^3 \left(\frac{\zeta}{k_0 T}\right) \langle R \rangle . \tag{6.74}$$

If $\langle R \rangle$ is not so much smaller than unity, (6.74) indicates that S_p can be comparable to S.

A relation equivalent to (6.72) can be derived by a different approach.

As shown in (2.30) and (2.48), the crystal momentum is conserved in the electron-phonon scattering process, i. e.,

$$\mathbf{k} = \mathbf{k}' \pm \mathbf{q} + \mathbf{G}, \quad \mathbf{G} : \text{reciprocal lattice vector.} \tag{6.75}$$

In semiconductors and semimetals it is permissible to put $\mathbf{G} = 0$, and

$$\mathbf{k} = \mathbf{k}' \pm \mathbf{q} . \tag{6.76}$$

This indicates that the total momentum $\mathbb{K} + \mathbb{P}_{ph}$ remains constant, where $\mathbb{K}$ is the total electron momentum and $\mathbb{P}_{ph}$ the total phonon momentum.

~~Accordingly~~, we have

Consequently

$$\left[d(\mathbb{K} + \mathbb{P}_{ph}) / dt \right]_{scatt.} = 0. \tag{6.77}$$

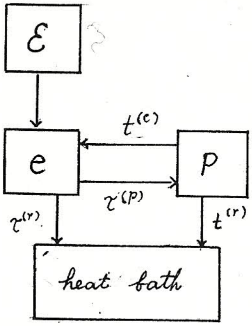


Fig. 6.5 Momentum exchange between electrons and phonons and other systems.

In Fig. 6.5 transfer of the crystal momentum between electrons and phonons and other systems, are schematically shown. Since the heat bath has a very large degree of freedom, reaction effect may be neglected. τ, τ, t and t are the momentum relaxation times. Change of K with time due to an electric field $\mathcal{E}$ is already given in (4.13) as

$$\frac{dK}{dt} = -\frac{ne\mathcal{E}}{\hbar}. \qquad (6.78)$$

Then, dK/dt and dP_{ph}/dt take the following forms:

$$\left\{ \begin{aligned} \frac{dK}{dt} &= -\frac{K}{\tau^{(p)}} - \frac{K}{\tau^{(r)}} + \frac{P_{ph}}{t^{(e)}} - \frac{ne\mathcal{E}}{\hbar}, \\ \frac{dP_{ph}}{dt} &= \frac{K}{\tau^{(p)}} - \frac{P_{ph}}{t^{(e)}} - \frac{P_{ph}}{t^{(r)}}. \end{aligned} \right. \qquad (6.79)$$

In the stationary state we have $dK/dt = dP_{ph}/dt = 0$, and

$$K = -\frac{ne\mathcal{E}\tau}{\hbar}(1-\Gamma)^{-1}, \quad \Gamma = \frac{\tau}{\tau^{(p)}}\frac{t}{t^{(e)}} < 1, \qquad (6.80)$$

where $1/\tau = 1/\tau^{(p)} + 1/\tau^{(r)}$, $\quad 1/t = 1/t^{(e)} + 1/t^{(r)}$.

From (6.80) the electrical conductivity σ is given by

$$\sigma = -\frac{e\hbar K}{m^* \mathcal{E}} = \frac{ne^2\tau}{m^*}(1-P)^{-1}, \qquad (6.81)$$

and the phonon heat flux becomes

$$W_p = \hbar v_s^2 P_{ph} = -ne\, v_s^2\, \mathcal{E}\, t\left(\frac{\tau}{\tau^{(p)}}\right)(1-P)^{-1}. \qquad (6.82)$$

By using the Onsager relation (6.20) the thermoelectric power S_p is given by

$$S_p = \frac{\chi}{T\sigma} = -\frac{m^* v_s^2}{eT}\,\frac{t}{\tau^{(p)}}, \qquad (6.83)$$

where χ is related to W_p by $W_p = \chi\,\mathcal{E}$ (see (6.19)).

If the electrons are degenerated and the phonon distribution can be approximated by the classical distribution, there is the relation between $t^{(e)}$ and $\tau^{(p)}$ (See Chapter 14):

$$\frac{t^{(e)}}{\tau^{(p)}} = \frac{k_0 T}{\frac{1}{2} m^* v_s^2}. \qquad (6.84)$$

Combining (6.84) ~~and~~ with (6.83) we obtain

$$S_p = -\frac{2k_0}{e}\,\frac{t}{t^{(e)}} = -\frac{2k_0}{e}\langle R\rangle. \qquad (6.85)$$

(6.85) is equivalent to (6.72), since at enough high temperatures $C_p \sim k_0$.

The quantity P, which is smaller than unity, is called the mutual drag coefficient. In some cases Γ plays an important role in the transport phenomena. On this point we discuss in Chapter 14. The reason why $\sigma \to \infty$ with $\Gamma \to 1$ is easily understood from Fig. 6.5.

6.6 Transport Coefficients of Semiconductors

In Section 6.3 we paid our attentions mainly to the degenerate system and calculated the transport coefficients. In this Section the electrical conductivity and the thermoelectric power are calculated for the non-degenerate semiconductors.

Consider an isotropic electron band with effective mass m^*..

Since $e^{-\beta\zeta} \gg 1$, the distribution becomes

$$f(E) = [e^{\beta(E-\zeta)} + 1]^{-1} \doteqdot e^{\beta(\zeta - E)} = A e^{-\beta E}, \qquad (6.86)$$

where $\beta = 1/k_0 T$. The electron density n is calculated by

$$n = \frac{2}{(2\pi)^3} \int dk\, f(E_k). \qquad (6.87)$$

Inserting (6.86) into (6.87), one obtains

$$A = e^{\zeta / k_0 T} = 4n \left(\frac{\pi \hbar^2}{2m^* k_0 T} \right)^{3/2}, \qquad (6.88)^{\#)}$$

where $E_k = \hbar^2 k^2 / 2m^*$ is employed. In the non-degenerate system (6.88) should be much smaller than unity. Therefore,

$$n \ll \frac{1}{4}\left(\frac{2m^* k_0 T}{\pi \hbar^2}\right)^{3/2} = 2.51\times 10^{19}\left(\frac{m^*}{m}\right)^{3/2}\left(\frac{T}{300}\right)^{3/2}. \qquad (6.89)$$

For an example $m^*/m = 0.014$ in n-InSb, and then we have

$$n \ll 4.16\times 10^{16}\left(\frac{T}{300}\right)^{3/2}. \qquad (6.90)$$

From (6.18), (6.86) and (6.88) the electrical conductivity is expressed by

$$\sigma = \frac{ne^2}{m^*}\langle \tau \rangle_{3/2}, \qquad (6.91)$$

where

$$\langle F(x)\rangle_{3/2} = \frac{4}{3\sqrt{\pi}}\int_0^\infty dx\, e^{-x} x^{3/2} F(x), \quad x = \frac{E}{k_0 T}. \qquad (6.92)$$

As will be shown in Chapter 7, in semiconductors the relaxation rate due to the longitudinal acoustic phonon scattering has a dependence on T and E as

$$1/\tau \propto T E^{1/2}. \qquad (6.93)$$

Then, we get

$$\tau = \tau_0 x^p, \quad \tau_0 \propto T^{-3/2}, \quad p = -1/2. \qquad (6.94)$$

In ionized impurity scattering (see Chapter 7),

$$\tau \propto E^{3/2}, \quad \tau = \tau_0 x^p, \quad \tau_0 \propto T^{3/2}, \quad p = 3/2. \qquad (6.95)$$

(6.90) leads to

$$\sigma = \frac{ne^2\tau_0}{m^*}\,\frac{\Gamma(5/2+p)}{\Gamma(5/2)}. \qquad (6.96)$$

Similarly, one readily finds from (6.18), (6.19), (6.86) and (6.88) that

$$\chi = -\frac{5}{2}\frac{n e k_0 T}{m^*}\langle\tau\rangle_{5/2} + \frac{\zeta}{e}\sigma, \tag{6.97}$$

$$\langle F(x)\rangle_{5/2} = \frac{8}{15\sqrt{\pi}}\int_0^\infty dx\, e^{-x} x^{5/2} F(x), \tag{6.98}$$

$$S = -\frac{5}{2}\frac{k_0}{e}\frac{\langle\tau\rangle_{5/2}}{\langle\tau\rangle_{3/2}} + \frac{\zeta}{eT}. \tag{6.99}$$

Assuming again that the energy dependence of the relaxation time is given by $\tau = \tau_0 x^p$, we obtain

$$S = -\frac{k_0}{e}\left(\frac{5}{2} + p - \frac{\zeta}{k_0 T}\right), \quad (k_0/e = 86.26\,\mu V/\mathrm{deg}). \tag{6.100}$$

From (6.88), ζ/k_0T is given by

$$e^{\zeta/k_0T} = 3.98\times10^{-20}\, n\left(\frac{m}{m^*}\right)^{3/2}\left(\frac{300}{T}\right)^{3/2}. \tag{6.101}$$

It is easily shown that (6.100) is much lager than (6.39).

6.7 General Theory of the Transport Phenomena in Magnetic Field

In Section 6.2 a solution of the Bloch equation in the presence of a magnetic field was presented on the assumption that a relaxation time can be defined. The solution (6.14) is clearly the power series in the expansion of $\omega_c\tau$, $\omega_c = eH/m^*c$.

If the expression for E_k is of the form $E_k = (\hbar^2/2) \sum_i k_i^2/m_i$, the series (6.14) can be given in closed form.

For a moment we consider the simple case of $E_k = (\hbar^2/2m^*) k^2$. If the magnetic field is parallel to z-axis, (6.13) becomes

$$\Phi \doteq \frac{\tau}{\hbar}(\mathbb{P} \cdot \nabla_k E) - \frac{e^2 \tau}{\hbar^2 c} H \left(\frac{\partial E}{\partial k_x} \frac{\partial \Phi}{\partial k_y} - \frac{\partial E}{\partial k_y} \frac{\partial \Phi}{\partial k_x} \right). \qquad (6.102)$$

Assuming Φ in the form

$$\Phi = \Psi(k) \cdot v = \sum_{i=x,y,z} \Psi_i(k) v_i, \qquad (6.103)$$

substituting into (6.102) and equating the terms with same v_i in both sides, we obtain

$$\Psi_x = \frac{\tau(P_x - \theta P_y)}{1+\theta^2}, \quad \Psi_y = \frac{\tau(P_y + \theta P_x)}{1+\theta^2}, \quad \Psi_z = \tau P_z, \qquad (6.104)$$

where $\theta = \omega_0 \tau$. Therefore, Φ is written in the form

$$\Phi = \tau \{ v \cdot P - \theta (v \times P)_z + \theta^2 v_z P_z \} / (1+\theta^2). \qquad (6.105)$$

(6.105) is generalized to the case with an arbitrary direction of $\mathbb{H}$, namely

$$\Phi = \tau \left\{ v \cdot P - \frac{e\tau}{m^* c} \mathbb{H} \cdot (v \times \mathbb{P}) + \left(\frac{e\tau}{m^* c} \right)^2 (\mathbb{H} \cdot v)(\mathbb{H} \cdot P) \right\} / (1+\theta^2). \qquad (6.106)$$

As is shown clearly from (6.104), the electric current and thermal current do not depend on $\mathbf{H}$, if $\mathbf{H}$ is parallel to z-axis. Accordingly, the longitudinal magnetoresistance vanishes in this case. However, it remains finite if E_k has an anisotropic dependence on k.

In a configuration of $\mathbf{H} \parallel z$ and $\mathbf{P} \perp \mathbf{H}$, we estimate the magnetoresistance, Hall coefficient and thermomagnetic coefficients by use of (6.106).

Expressions of j_x and w_x are

$$j_x = e\sum_k v_x \Phi \frac{\partial f_0}{\partial E} = -e\sum_k v_x^2 \tau \frac{\partial f_0}{\partial E_k}\Big\{ e\mathcal{E}_x + \frac{(E_k-\zeta)}{T}\nabla_x T - \theta\Big[e\mathcal{E}_y + \frac{(E_k-\zeta)}{T}\nabla_y T\Big]\Big\}(1+\theta^2)^{-1},$$

$$w_x = -\sum_k v_x (E_k-\zeta)\Phi\frac{\partial f_0}{\partial E_k} = \sum_k v_x^2\tau(E_k-\zeta)\frac{\partial f_0}{\partial E_k}\Big\{ e\mathcal{E}_x + \frac{(E_k-\zeta)}{T}\nabla_x T - \theta\Big[e\mathcal{E}_y + \frac{(E_k-\zeta)}{T}\nabla_y T\Big]\Big\}(1+\theta^2)^{-1}. \qquad (6.107)$$

The coefficients σ, β, χ and λ introduced in (6.19) are given by

$$\begin{cases} \sigma_{xx} = -e^2\sum_k v_x^2\tau \dfrac{\partial f_0}{\partial E_k}\dfrac{1}{1+\theta^2}, \\[2ex] \sigma_{xy} = e^2\sum_k v_x^2\tau\dfrac{\partial f_0}{\partial E_k}\dfrac{\theta}{1+\theta^2}, \end{cases} \qquad (6.108)$$

$$\left\{\begin{aligned} \beta_{xx} &= \frac{e}{T}\sum_k v_x^2 \tau \frac{\partial f_0}{\partial E_k}\frac{(E_k-\zeta)}{1+\theta^2}, \\ \beta_{xy} &= -\frac{e}{T}\sum_k v_x^2 \tau \frac{\partial f_0}{\partial E_k}(E_k-\zeta)\frac{\theta}{1+\theta^2}, \end{aligned}\right. \qquad (6.109)$$

$$\left\{\begin{aligned} \chi_{xx} &= e\sum_k v_x^2 \tau \frac{\partial f_0}{\partial E_k}\frac{(E_k-\zeta)}{1+\theta^2}, \\ \chi_{xy} &= -e\sum v_x^2 \tau \frac{\partial f_0}{\partial E_k}(E_k-\zeta)\frac{\theta}{1+\theta^2}, \end{aligned}\right. \qquad (6.110)$$

$$\left\{\begin{aligned} \lambda_{xx} &= -\frac{1}{T}\sum_k v_x^2 \tau \frac{\partial f_0}{\partial E_k}\frac{(E_k-\zeta)^2}{1+\theta^2}, \\ \lambda_{xy} &= \frac{1}{T}\sum_k v_x^2 \tau \frac{\partial f_0}{\partial E_k}(E_k-\zeta)^2\frac{\theta}{1+\theta^2}. \end{aligned}\right. \qquad (6.111)$$

In the case of hole conduction, we should replace θ by $-\theta$ in (6.108) ~ (6.112).

On making use of the replacements $1-f_0 = f_0'$, $\Delta - E_k = E_k'$, $E_k-\zeta = \zeta' - E_k'$ (In Fig. 6.4 $\zeta = \zeta_1$, $\zeta' = \zeta_2$) it is readily shown that σ_{xy}, β_{xx}, χ_{xx} and λ_{xy} change their sign in the hole conduction. Magnetoresistivity $\rho(H)$ and Hall coefficient R are obtained by putting $j_y = 0$:

$$\left\{\begin{aligned} \rho(H) &= \frac{\mathcal{E}_x}{j_x} = \frac{\sigma_{yy}}{\sigma_{xx}\sigma_{yy} - \sigma_{xy}\sigma_{yx}} = \frac{\sigma_{yy}}{\sigma_{xx}\sigma_{yy} + \sigma_{xy}^2}, \\ R &= \frac{\mathcal{E}_y}{H j_x} = \frac{-\sigma_{yx}}{H(\sigma_{xx}\sigma_{yy} - \sigma_{xy}\sigma_{yx})} = \frac{\sigma_{xy}}{H(\sigma_{xx}\sigma_{yy} + \sigma_{xy}^2)}. \end{aligned}\right. \qquad (6.112)$$

To obtain the last expressions in $\rho(H)$ and R, the relation of $\sigma_{yx}(H) = -\sigma_{xy}(H)$ is employed. However, generally this is not always valid, because the Onsager relation guarantees

$$\sigma_{ij}(H) = \sigma_{ji}(-H), \tag{6.113}$$

but does not justify $\sigma_{ij}(H) = -\sigma_{ij}(-H)$ and $\sigma_{ij}(H) = -\sigma_{ji}(H)$.

Generally speaking $\sigma_{xy}(H)$ includes the symmetric part and antisymmetric one for $H \to -H$. Now, let consider the simple case that the relations of $\sigma_{yx}(H) = -\sigma_{xy}(H)$ and $\sigma_{xx} = \sigma_{yy}$ are satisfied.

By retaining the lowest order term in the power of k_0T/ζ, (6.109) ~ (6.111) become as follows:

$$\sigma_{xx} = \frac{e^2}{12\pi^3}\,\frac{\tau(\zeta)}{1+\theta(\zeta)^2}\int_{E=\zeta} v^2 \frac{dS}{|\nabla_k E|}, \quad \sigma_{xy} = -\theta(\zeta)\sigma_{xx}, \tag{6.114}$$

$$\begin{cases} \beta_{xx} = -\dfrac{e}{36\pi}\,\dfrac{(k_0T)^2}{T}\left[\dfrac{\partial}{\partial E}\displaystyle\int_E \frac{\tau v^2}{1+\theta^2}\,\frac{dS}{|\nabla_k E|}\right]_{E=\zeta}, \\ \beta_{xy} = \dfrac{e}{36\pi}\,\dfrac{(k_0T)^2}{T}\left[\dfrac{\partial}{\partial E}\displaystyle\int_E \tau v^2 \frac{\theta}{1+\theta^2}\,\frac{dS}{|\nabla_k E|}\right]_{E=\zeta}, \end{cases} \tag{6.115}$$

$$\chi_{xx} = T\beta_{xx}, \quad \chi_{xy} = T\beta_{xy}, \tag{6.116}$$

$$\lambda_{xx} = \frac{1}{36\pi}\,\frac{(k_0T)^2}{T}\,\frac{\tau(\zeta)}{1+\theta(\zeta)^2}\int_{E=\zeta} v^2 \frac{dS}{|\nabla_k E|}, \quad \lambda_{xy} = -\theta(\zeta)\lambda_{xx}. \tag{6.117}$$

In this approximation $\rho(H)$ is independent of H. This is due to the situation that the Hall field exactly cancel the deflection of electron orbit due to magnetic field.

In a cubic crystal the current is of the form

$$\mathbf{j} = \sigma_0 \boldsymbol{\mathcal{E}} + \lambda \boldsymbol{\mathcal{E}} \times \mathbf{H} + \mu \boldsymbol{\mathcal{E}} H^2 + \nu \mathbf{H}(\boldsymbol{\mathcal{E}} \cdot \mathbf{H}) + \xi \sum_i \mathbf{e}_i \mathcal{E}_i H_i^2, \qquad (6.118)$$

if we neglect terms of order H^3 and higher.[28)] $\mathbf{e}_i$ is the unit vector along the i-axis. Let take the crystal axes as the coordinate axes, and we consider the configuration of

$\mathbf{j} = (j_x, 0, 0)$. $\mathbf{H} = (H_x, 0, H_z)$ and $\boldsymbol{\mathcal{E}} = (\mathcal{E}_x, \mathcal{E}_y, 0)$.

From (6.118) we have

$$j_x = \left\{ \sigma_0 + \mu H^2 + (\nu + \xi) H_x^2 \right\} \mathcal{E}_x + \lambda \mathcal{E}_y H_z,$$

$$0 = -\lambda \mathcal{E}_x H_z + (\sigma_0 + \mu H^2) \mathcal{E}_y.$$

Therefore, in the weak field approximation

$$\left\{ \begin{aligned} R &= \frac{\mathcal{E}_y}{j_x H} = \frac{\lambda}{\sigma_0^2} \sin\theta \\ \sigma &= \frac{j_x}{\mathcal{E}_x} = \sigma_0 \left[1 + \left\{ \left(\frac{\mu}{\sigma_0} + \frac{\lambda^2}{\sigma_0^2} \right) \sin^2\theta + \frac{\mu + \nu + \xi}{\sigma_0} \cos^2\theta \right\} H^2 \right], \end{aligned} \right. \qquad (6.119)$$

where $\mathbf{H} = (\cos\theta, 0, \sin\theta) H$.

Substituting (6.14) into the general expression of electric current

$$j = \frac{e}{4\pi^3\hbar}\int \nabla_k E\, \Phi \frac{\partial f_0}{\partial E}\, dk, \tag{6.120}$$

and comparing with (6.118), we get 28)

$$\left\{\begin{aligned}
\sigma_0 &= -\frac{e^2}{4\pi^3\hbar^2}\int \tau\left(\frac{\partial E}{\partial k_x}\right)^2\frac{\partial f_0}{\partial E}\, dk, \\
\lambda &= \frac{e^3}{4\pi^3\hbar^4 c}\int \tau\frac{\partial E}{\partial k_x}\,\Omega_z\left(\tau\frac{\partial E}{\partial k_y}\right)\frac{\partial f_0}{\partial E}\, dk, \\
\mu &= -\frac{e^4}{4\pi^3\hbar^6 c^2}\int \tau\frac{\partial E}{\partial k_x}\,\Omega_z\left\{\tau\Omega_z\left(\tau\frac{\partial E}{\partial k_x}\right)\right\}\frac{\partial f_0}{\partial E}\, dk, \\
\nu &= -\frac{e^4}{4\pi^3\hbar^6 c^2}\int \tau\frac{\partial E}{\partial k_x}\left[\Omega_x\left\{\tau\Omega_y\left(\tau\frac{\partial E}{\partial k_y}\right)\right\} + \Omega_y\left\{\tau\Omega_x\left(\tau\frac{\partial E}{\partial k_x}\right)\right\}\right]\frac{\partial f_0}{\partial E}\, dk, \\
\mu+\nu+\xi &= -\frac{e^4}{4\pi^3\hbar^6 c^2}\int \tau\frac{\partial E}{\partial k_x}\,\Omega_x\left\{\tau\Omega_x\left(\tau\frac{\partial E}{\partial k_x}\right)\right\}\frac{\partial f_0}{\partial E}\, dk.
\end{aligned}\right. \tag{6.121}$$

By integrating by parts, the expressions for μ and $\mu+\nu+\xi$ are transformed into

$$\left\{\begin{aligned}
\mu &= \frac{e^4}{4\pi^3\hbar^6 c^2}\int \tau\left\{\Omega_z\left(\tau\frac{\partial E}{\partial k_x}\right)\right\}^2\frac{\partial f_0}{\partial E}\, dk, \\
\mu+\nu+\xi &= \frac{e^4}{4\pi^3\hbar^6 c^2}\int \tau\left\{\Omega_x\left(\tau\frac{\partial E}{\partial k_x}\right)\right\}^2\frac{\partial f_0}{\partial E}\, dk.
\end{aligned}\right. \tag{6.122}$$

Since $\partial f_0/\partial E$ is negative, μ and $\mu+\nu+\xi$ are both negative. $\lambda^2 \leq -\mu\sigma_0$ is concluded from Schwarz's inequality, so that σ is less than σ_0, and the resistance always increases in the presence of a magnetic field.

If the electrons are completely degenerate and the energy is given by $E_k = \hbar^2 k^2/2m^*$, we obtain $\lambda^2 = -\mu\sigma_0$, $\mu + \nu + \xi = 0$, so that the conductivity is independent of magnetic field.

In the case of a metal having cubic symmetry whose conduction band has an extremum at $k=0$, Davis expanded k and τ in spherical harmonics and calculated the Hall coefficient and transverse and longitudinal magnetoresistance coefficients in the limit of vanishing magnetic fields.29)

When the several kinds of carriers participate in the conduction phenomena, the Hall field can not cancel out the deflecting effect of the magnetic field since the Hall angle of each carrier is not the same.

Let consider two types of carriers 1 and 2. The resistivity and the Hall coefficient are given by

$$\rho = \frac{\dfrac{\sigma_1}{1+\theta_1^2} + \dfrac{\sigma_2}{1+\theta_2^2}}{\left(\dfrac{\sigma_1}{1+\theta_1^2} + \dfrac{\sigma_2}{1+\theta_2^2}\right)^2 + \left(\dfrac{\lambda_1\sigma_1\theta_1}{1+\theta_1^2} + \dfrac{\lambda_2\sigma_2\theta_2}{1+\theta_2^2}\right)^2}, \qquad (6.123)$$

$$R = \frac{\dfrac{1}{H}\left(\dfrac{\lambda_1 \sigma_1 \theta_1}{1+\theta_1{}^2} + \dfrac{\lambda_2 \sigma_2 \theta_2}{1+\theta_2{}^2}\right)}{\left(\dfrac{\sigma_1}{1+\theta_1{}^2} + \dfrac{\sigma_2}{1+\theta_2{}^2}\right)^2 + \left(\dfrac{\lambda_1 \sigma_1 \theta_1}{1+\theta_1{}^2} + \dfrac{\lambda_2 \sigma_2 \theta_2}{1+\theta_2{}^2}\right)^2} , \tag{6.124}$$

where

$$\lambda = \begin{cases} -1 : \text{electron}, \\ +1 : \text{hole} , \end{cases} \quad \sigma_i = \frac{n_i e^2 \tau_i}{m_i}, \quad \theta_i = \frac{eH}{m_i c} \tau_i .$$

The relative change in resistivity due to the magnetic field is

$$\frac{\rho(H) - \rho(0)}{\rho(0)} = \frac{\Delta \rho}{\rho_0} = \frac{\sigma_1 \sigma_2 (\lambda_1 \theta_1 - \lambda_2 \theta_2)^2}{(\sigma_1 + \sigma_2)^2 + (\lambda_1 \theta_1 \sigma_2 + \lambda_2 \theta_2 \sigma_1)^2} . \tag{6.125}$$

Rewriting (6.124),

$$R = \frac{1}{ec} \frac{\left\{ \dfrac{\lambda_1 \sigma_1{}^2}{n_1} + \dfrac{\lambda_2 \sigma_2{}^2}{n_2} + \sigma_1{}^2 \sigma_2{}^2 \left(\dfrac{H}{ec}\right)^2 \left(\dfrac{\lambda_1 n_1 + \lambda_2 n_2}{n_1{}^2 n_2{}^2}\right) \right\}}{(\sigma_1 \pm \sigma_2)^2 + \left(\dfrac{H}{ec}\right)^2 \sigma_1{}^2 \sigma_2{}^2 \left(\dfrac{\lambda_1}{n_1} + \dfrac{\lambda_2}{n_2}\right)^2} . \tag{6.126}$$

In the case of $\lambda_1 = \lambda_2$ and $\theta_1 = \theta_2$, $\Delta \rho / \rho_0$ becomes zero and R vanishes if $\lambda_1 = -\lambda_2$, $n_1 = n_2$ and $\theta_1 = \theta_2$ are realized.

σ_{xx} and σ_{xy} are expressed by

$$\sigma_{xx} = \frac{c}{H} \sum_i \frac{e n_i \theta_i}{1+\theta_i{}^2} , \quad \sigma_{xy} = \frac{c}{H} \sum_i \frac{e_i n_i \theta_i{}^2}{1+\theta_i{}^2} , \tag{6.127}$$

where $e_i = \begin{cases} -e : \text{electron} \\ +e : \text{hole} , \end{cases}$ and $H \parallel z$-axis.

If the field intensity is strong enough and the conditions of $\theta_1, \theta_2 \gg 1$ is satisfied, $\Delta\rho/\rho_0$ approaches to a constant value and R converges to a scattering independent value:

$$R(H\to\infty) = \frac{1}{ec(\lambda_1 n_1 + \lambda_2 n_2)} . \qquad (6.128)$$

(6.128) is a general formula which does not depend on the special model employed in the calculation.

In weak magnetic field $\theta_i \ll 1$, R takes the form

$$R(H\to 0) = \frac{1}{e^3 c} \frac{\left\{\lambda_1 n_1 \left(\frac{\tau_1}{m_1}\right)^2 + \lambda_2 n_2 \left(\frac{\tau_2}{m_2}\right)^2\right\}}{\left(\frac{n_1\tau_1}{m_1} + \frac{n_2\tau_2}{m_2}\right)^2} . \qquad (6.129)$$

Since $n_i \propto m_i^{3/2}$ in semiconductors (See (6.88)), (6.129) becomes

$$R(H\to 0) \propto \frac{\lambda_1 \frac{\tau_1^2}{m_1^{1/2}} + \lambda_2 \frac{\tau_2^2}{m_2^{1/2}}}{(m_1^{1/2}\tau_1 + m_2^{1/2}\tau_2)^2} . \qquad (6.130)$$

(6.130) indicates that if the mass ratio m_1/m_2 is very much larger than unity, the light carriers play a dominant role. In semimetals we have $n_1 = n_2 \,(\equiv n)$ and $\lambda_1 = -\lambda_2$, then,

$$R(H\to 0) = \frac{\lambda_1}{ecn} \frac{\left(\frac{\tau_1}{m_1}\right)^2 - \left(\frac{\tau_2}{m_2}\right)^2}{\left(\frac{\tau_1}{m_1} + \frac{\tau_2}{m_2}\right)^2} . \qquad (6.131)$$

Therefore, weight of the light carriers in the Hall coefficient particularly increases.

On making use of (6.108) ~ (6.111), expressions of the magneto-resistance, the Hall coefficient and the thermomagnetic coefficients in semiconductors, can be easily obtained.

Namely,

$$j_x = \frac{ne^2}{m^*}\left\{\mathcal{E}_x\langle\tau\rangle - \mathcal{E}_x\,\omega_c^2\left\langle\frac{\tau^3}{1+(\omega_c\tau)^2}\right\rangle + \mathcal{E}_y\left\langle\frac{\omega_c\tau^2}{1+(\omega_c\tau)^2}\right\rangle\right\}. \tag{6.132}$$

$$\left\{\begin{aligned} A_\perp &= \frac{\Delta\rho}{H^2\rho_0} = \left(\frac{e}{m^*c}\right)^2\frac{1}{\langle\tau\rangle}\left[\left\langle\frac{\tau^3}{1+(\omega_c\tau)^2}\right\rangle - \frac{\left\langle\frac{\tau^2}{1+(\omega_c\tau)^2}\right\rangle^2}{\left\langle\frac{\tau}{1+(\omega_c\tau)^2}\right\rangle}\right], \\ R &= -\frac{1}{nec}\,\frac{\left\langle\frac{\tau^2}{1+(\omega_c\tau)^2}\right\rangle}{\left\langle\frac{\tau}{1+(\omega_c\tau)^2}\right\rangle}\left\{\langle\tau\rangle + \omega_c^2\left[\frac{\left\langle\frac{\tau^2}{1+(\omega_c\tau)^2}\right\rangle^2}{\left\langle\frac{\tau}{1+(\omega_c\tau)^2}\right\rangle}\right.\right. \\ &\qquad \left.\left. - \left\langle\frac{\tau^3}{1+(\omega_c\tau)^2}\right\rangle\right]\right\}^{-1}, \end{aligned}\right. \tag{6.133}$$

where $\langle\cdots\rangle$ is defined by (6.92).

Here, we consider the two limiting cases: i) weak field limit $\omega_c\tau \ll 1$ and ii) strong field limit $\omega_c\tau \gg 1$. Of course the present discussions are limited to the classical case in which the

Boltzmann equation is appliable. A physically interesting case except i) and ii) is the quantum region, in which $\omega_c \tau \gg 1$ and $\hbar\omega_c / k_0 T \gg 1$ (quantization of orbit) are satisfied, and the Boltzmann equation is no longer applicable. Concering the transport phenomena in the quantum region a detailed consideration will be done in Chapter 11.

i) Weak field region:

$$\begin{cases} A_\perp = \left(\dfrac{e}{m^* c}\right)^2 \dfrac{\langle\tau^3\rangle\langle\tau\rangle - \langle\tau^2\rangle^2}{\langle\tau\rangle^2}, \\[2ex] R = -\dfrac{1}{nec}\,\dfrac{\langle\tau^2\rangle}{\langle\tau\rangle^2}. \end{cases} \tag{6.134}$$

Assuming $\tau = \tau_0 (E/k_0 T)^p = \tau_0 x^p$, one obtains

$$\begin{cases} A_\perp = \left(\dfrac{e}{m^* c}\right)^2 \tau_0^2 \,\dfrac{\Gamma(5/2+3p)\,\Gamma(5/2+p) - \Gamma(5/2+2p)^2}{\Gamma(5/2+p)^2}, \\[2ex] R = -\dfrac{1}{nec}\,\dfrac{\Gamma(5/2)\,\Gamma(5/2+2p)}{\Gamma(5/2+p)^2}. \end{cases} \tag{6.135}$$

ii) Strong field region:

$$\begin{cases} A_\perp = \dfrac{1}{H^2}\left[1 - \dfrac{1}{\langle\tau\rangle\langle\tau^{-1}\rangle}\right] = \dfrac{1}{H^2}\left[1 - \dfrac{\Gamma(5/2)^2}{\Gamma(5/2+p)\,\Gamma(5/2-p)}\right], \\[2ex] R = -\dfrac{1}{nec}. \end{cases} \tag{6.136}$$

The quantity defined by $c|R|\sigma$ is called the Hall mobility μ_H. From (6.91) and (6.134)

$$\mu_H = \frac{e}{m^*}\frac{\langle \tau^2 \rangle}{\langle \tau \rangle}. \tag{6.137}$$

The drift mobility is related to σ by $\sigma = ne\mu_d$. There exists the following relation between μ_H and μ_d:

$$\mu_H = \frac{\Gamma(5/2+2p)\,\Gamma(5/2)}{\Gamma(5/2+p)^2}\,\mu_d. \tag{6.138}$$

- Among the thermomagnetic effects in semiconductors usually measured quantities are the thermoelectric power (Magneto-Seebeck coefficient) and the Nernst coefficient or the Nernst-Ettingshausen coefficient.

Under the configuration of $H \parallel z$-axis, $j = 0$, $\nabla_x T \neq 0$ and $\nabla_y T = 0$ (isothermal condition), these coefficients are written as follows:

$$\left\{\begin{aligned} S &= \frac{\mathcal{E}_x}{\nabla_x T} = \frac{\sigma_{yy}\beta_{xx} - \sigma_{xy}\beta_{yx}}{\sigma_{xx}\sigma_{yy} - \sigma_{xy}\sigma_{yx}} = \frac{\sigma_{yy}X_{xx}(-H) - \sigma_{xy}X_{xy}(-H)}{T(\sigma_{xx}\sigma_{yy} - \sigma_{xy}\sigma_{yx})}, \\ A_{NE} &= \frac{\mathcal{E}_y}{H\nabla_x T} = \frac{\sigma_{xx}\beta_{yx} - \sigma_{yx}\beta_{xx}}{H(\sigma_{xx}\sigma_{yy} - \sigma_{xy}\sigma_{yx})} = \frac{\sigma_{xx}X_{xy}(-H) - \sigma_{yx}X_{xx}(-H)}{HT(\sigma_{xx}\sigma_{yy} - \sigma_{xy}\sigma_{yx})}. \end{aligned}\right. \tag{6.139}$$

β and X are the quantities defined in (6.19).

The usual configuration experimentally employed is not the isothermal condition but the adiabatic condition $w_y = 0$.

However, the difference between the isothermal coefficient and the adiabatic one is usually very small, and then we employ the expression (6.139), which is convenient to the theoretical treatment.

More unfamiliar coefficients are the Ettingshausen and Righi-Leduc coefficients, and they are defined as follows.

If we pass an electric current in the x-direction and apply a magnetic field in the z-direction, a temperature gradient is set up if the sample faces are thermally insulated. The Ettingshausen coefficient is usually defined by

$$A_E = \frac{\nabla_y T}{H j_x}, \tag{6.140}$$

under the condition of $j_x = \nabla_x T = w_y = 0$.

The Righi-Leduc effect is the thermal analogue of the Hall effect and defined by

$$B_{RL} = \frac{\nabla_y T}{H \nabla_x T},$$

or $\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad$ (6.141)

$$A_{RL} = -\frac{\nabla_y T}{H w_x},$$

where the conditions of $H \parallel z$, $j = w_y = 0$ are imposed. Usually the Righi-Leduc effect is too small to observe. However, if it is measured, it provides a useful information on the mutual drag coefficient Γ introduced in Section 6.5.

The thermal conductivity $\varkappa$ is composed of the two parts, $\varkappa$(electronic) and $\varkappa$(lattice). If we apply a magnetic field, we can change $\varkappa$(electronic), leaving $\varkappa$(lattice) unchanged. The change in $\varkappa$(electronic) is related to the scattering mechanism, mobility and degree of degeneracy of the electrons, and in a favorable condition we can separate $\varkappa$ into the electronic and lattice components. Field dependence of the thermal conduction is called the Maggi-Righi-Leduc effect.

In the thermomagnetic effects the phonon drag and mutual drag effects play dominant role. Especially in semimetals where electrons and holes coexist, variegated phenomena are observed. They are treated in Chapter 14.

Expressions of X_{xx} and X_{xy} in semiconductors are from (6.110)

$$\left\{ \begin{aligned} X_{xx} &= -\frac{5}{2}\frac{nek_0T}{m^*}\left\langle \frac{\tau}{1+\theta^2} \right\rangle_{5/2} + \frac{\zeta ne}{m^*}\left\langle \frac{\tau}{1+\theta^2} \right\rangle_{3/2}, \\ X_{xy} &= \frac{5}{2}\frac{nek_0T}{m^*}\left\langle \frac{\tau\theta}{1+\theta^2} \right\rangle_{5/2} - \frac{\zeta ne}{m^*}\left\langle \frac{\tau\theta}{1+\theta^2} \right\rangle_{3/2}. \end{aligned} \right. \qquad (6.142)$$

$\Psi = \tau P + \frac{e\tau}{c} B \times (\alpha \tau P) + \left(\frac{e\tau}{c}\right) B \times \{\alpha [B \times (\alpha \tau P)]\}.$

$\downarrow$

$O(\mathcal{E}, \nabla T),\ O(B \times \mathcal{E}),\ O(B \times \nabla T),\ O(B^2) \times O(\mathcal{E}, \nabla T)$

Until now we have restricted our considerations to the simple case in which the electron energy is given by $E_k = \hbar^2 k^2/2m^*$.

It is desirable to extend the our considerations to the many valley semiconductors such as Ge and Si and to the semimetals with several Fermi pockets such as Bi and Sb. Discussions on the semiconductors with an isotropic relaxation time were done by Abeles-Meiboom and Shibuya.[30] Here, we extend their results to the case with an anisotropic relaxation time.[31]

In the Boltzmann equation:

$$-\frac{e}{\hbar}\left(\mathcal{E} + \frac{1}{c} v \times H\right) \cdot \nabla_k f + v \cdot \nabla_r f = -\frac{f - f_0}{\tau}, \qquad (6.143)$$

we assume

$$f = f_0 - \Phi \frac{\partial f_0}{\partial E}, \quad \Phi = v \cdot \Psi(E), \qquad (6.144)$$

and $\tau^{-1} = \nu$ is replaced by a tensor $\tilde{\nu}$, then

$$-\frac{f - f_0}{\tau} \longrightarrow v \cdot \tilde{\nu} \cdot \Psi \frac{\partial f_0}{\partial E}. \qquad (6.145)$$

The reciprocal mass tensor is introduced by

$$\tilde{\alpha}_{ij} = \frac{1}{\hbar^2} \frac{\partial^2 E}{\partial k_i \partial k_j}. \qquad (6.146)$$

Thus, we obtain from (6.143)

$$P \cdot v + \frac{e}{c}(v \times H)\underbrace{(\Psi \cdot \tilde{\alpha})}_{\|} = v \cdot \tilde{\nu} \cdot \Psi, \qquad (6.147)$$

$\Sigma (v \times H)_i \Sigma \alpha_{ij} \Psi_j$

where P is the quantity defined by (6.13). From (6.147), we have

$$\mathbb{P} + \frac{e}{c} \mathbb{H} \times (\Psi \tilde{\alpha}) - \tilde{\nu} \Psi = 0 . \tag{6.148}$$

Define $\tilde{\tau}$ by $\tilde{\nu} \tilde{\tau} = 1$ and Ψ^* by $\Psi = \tilde{\tau} \Psi^*$.

(6.148) becomes

$$\mathbb{P} = \Psi^* + \frac{e}{c} [(\tilde{\tau} \Psi^*) \tilde{\alpha}] \times \mathbb{H} . \tag{6.149}$$

To solve (6.149) we operate $[(\tilde{\tau} \cdot [\dots]) \cdot \tilde{\alpha}] \times \mathbb{H}$ on both sides, then

$$[(\tilde{\tau} \cdot P) \tilde{\alpha}] \times \mathbb{H} = [(\tilde{\tau} \cdot \Psi^*) . \tilde{\alpha}] \times \mathbb{H} + \frac{e}{c} \{ [\tilde{\tau} \{ [(\tilde{\tau} \cdot \Psi^*) \tilde{\alpha}] \times \mathbb{H} \}] . \tilde{\alpha} \} \times \mathbb{H} , \tag{6.150}$$

Let denote the principal axes of the constant energy surface, which we assume ellipsoidal, by (x', y', z') and along the axes $\tilde{\tau}$ and $\tilde{\alpha}$ are diagonal as follows :

$$\tilde{\tau} = \begin{bmatrix} \tau_{x'} & 0 & 0 \\ 0 & \tau_{y'} & 0 \\ 0 & 0 & \tau_{z'} \end{bmatrix} , \quad \tilde{\alpha} = \begin{bmatrix} 1/m_{x'} & 0 & 0 \\ 0 & 1/m_{y'} & 0 \\ 0 & 0 & 1/m_{z'} \end{bmatrix} . \tag{6.151}$$

In consideration of (6.151), we get the following identity,

$$\left[\tilde{\tau}\left\{\left[(\tilde{\tau}\,\Psi^{*})\cdot\tilde{\alpha}\right]\times H\right\}\right]\cdot\tilde{\alpha} = \Psi^{*}\times(\tilde{\mathbb{C}}\cdot H), \tag{6.152}$$

where

$$\tilde{\mathbb{C}} = \tilde{M}\,\tilde{\nu}/|\tilde{M}||\tilde{\nu}|, \quad \tilde{M} = \tilde{\alpha}^{-1}, \quad \tilde{\nu} = \tilde{\tau}^{-1},$$

$$|\tilde{M}| = \det\tilde{M}, \quad |\tilde{\nu}| = \det\hat{\nu}.$$

Substituting (6.152) into (6.150), one obtains

$$[(\tilde{\tau}\cdot P)\cdot\alpha]\times H = [(\tilde{\tau}\cdot\Psi^{*})\tilde{\alpha}]\times H + \frac{e}{c}[\Psi^{*}\times(\tilde{\mathbb{C}}\times H)]\times H. \tag{6.153}$$

On operating $\cdot H(\tilde{\mathbb{C}}\cdot H)$ on both sides of (6.149), the second term in the right hand side vanishes and

$$(P\cdot H)(\tilde{\mathbb{C}}\cdot H) = (\Psi^{*}\cdot H)(\tilde{\mathbb{C}}\cdot H). \tag{6.154}$$

By using the identity

$$[\Psi^{*}\times(\tilde{\mathbb{C}}\times H)]\times H = (\Psi^{*} H)(\tilde{\mathbb{C}}\, H) - [H\cdot(\tilde{\mathbb{C}}\cdot H)]\Psi^{*}, \tag{6.155}$$

and (6.154), (6.153) is transformed into

$$[(\tilde{\tau}\, P)\tilde{\alpha}]\times H = [(\tilde{\tau}\,\Psi^{*})\tilde{\alpha}]\times H + \frac{e}{c}\left\{(P\cdot H)(\tilde{\mathbb{C}}\, H) - [H\cdot(\tilde{\mathbb{C}}\cdot H)]\Psi^{*}\right\}. \tag{6.156}$$

Employing (6.149) and rewriting the first term in the right hand side of the above equation, we get the solution

$P = -e\mathcal{E} - \frac{(E-\zeta)}{T}\cdot\nabla T$

$$\Psi = \tilde{\tau}\,\Psi^{*} = \frac{\tilde{\tau}\left\{P + \left(\frac{e}{c}\right)^2 (P\cdot H)(\hat{C}\cdot H) - \frac{e}{c}\left[(\tilde{\tau}\cdot P)\cdot\tilde{\alpha}\right]\times H\right\}}{1 + \left(\frac{e}{c}\right)^2\left[H\cdot(\hat{C}\cdot H)\right]}. \qquad (6.157)$$

From (6.157) we can calculate the transport coefficients due to one valley, and by summing up the contributions from all valleys the transport coefficients of the system are obtained.

Now, we pay our attention to the results obtained by Abeles - Meiboom and Shibuya,$^{30)}$ where they calculated the Hall coefficient and magnetoresistance for the ellipsoidal energy surface whose principal axes are parallel to [100] or [111]. They assumed that the relaxation time is a scalar. We do not follow the calculation processes but present a brief review of the results obtained by them.

Inverting the Seitz's relation (6.118), we get

$$\mathcal{E} = \rho_0 j + R(j\times H) + \rho_0\left[bH^2 j + cH(j\cdot H) + d\,\mathbb{T} j\right], \qquad (6.158)$$

where $\mathbb{T}$ is a diagonal tensor defined by $T_{ij} = \delta_{ij} H_i^2$.

Shibuya remarked that the coefficients b, c and d, which are related to the magnetoresistance in weak magnetic fields, are connected with the symmetry of the constant energy surface as follows :

Symmetry of the constant energy surface	Condition of the symmetry
1) spherical	$b+c=0,\ d=0$
2) [111] ellipsoid	$b+c=0,\ d>0$
3) [100] ellipsoid	$b+c+d=0,\ d<0$
4) [110] ellipsoid	$b+c=d,\ d>0$

Table 6.1. The magnetoresistance and the symmetry condition

Experimentally, the condition 2) is approximately satisfied for n-Ge. Similarly, 3) explains qualitatively the observed magnetoresistance of n-Si. These predictions were undoubtedly ascertained by the cyclotron experiment.

Another important conclusion obtained by Abeles-Meiboom and Shibuya's theories is the one on the longitudinal magnetoresistance $\Delta\rho_{11}/\rho_0$. The theories expect that $\Delta\rho_{11}/\rho_0$ takes a very large value for the [111]-ellipsoid and becomes zero for the [100]-ellipsoid, and these expectations are in good agreement with the experiments in Ge and Si.

Next, we mention about McClure's theory,33) which provides a useful tool in considering the magnetoresistance of the crystal with a warped energy surface. This theory is also useful in discussing the harmonics of the cyclotron resonance.

The Boltzmann equation with a scalar relaxation time is

$$\frac{e}{\hbar}\left(\mathcal{E}+\frac{1}{c}v\times H\right)\cdot\nabla_k f+\frac{f_0-f}{\tau}=0. \qquad (6.159)$$

From (6.144),

$$-\frac{e}{\hbar c}(v\times H)\cdot\nabla_k\Phi+\frac{\Phi}{\tau}+e\mathcal{E}\cdot v=0. \qquad (6.160)$$

The first term represents the differentiation along the trajectory on the constant energy surface, which is perpendicular to the magnetic field. This trajectory is called the hodograph (see (4.28)). Let introduce the variable s defined by

$$\frac{\partial k}{\partial s}=-\frac{e}{\hbar c}(v\times H). \qquad (6.161)$$

$s(k)$ denotes the time at a point k, when an electron moves along the hodograph under the influence of the magnetic field. On making use of s (6.160) is rewritten as

$$\frac{\partial \Phi}{\partial s} + \frac{\Phi}{\tau} + e\mathcal{E}\cdot v = 0. \qquad (6.162)$$

Integrating (6.162), we get

$$\Phi = -\int_r^s ds' e\mathcal{E}\cdot v(s') \exp\left[-\int_{s'}^{s} ds''/\tau(s'')\right], \qquad (6.163)$$

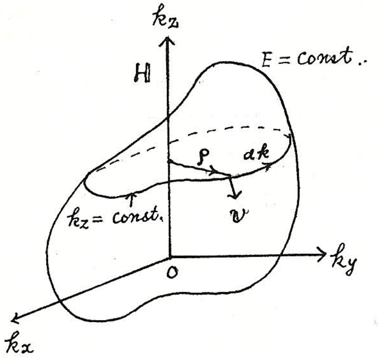


Fig. 6.6 Hodograph perpendicular to the magnetic field.

where r is the integration constant.

Since Φ is a single valued function, s should be a periodic function. v and τ are the periodic functions with the same period as Φ. Therefore, we get $r = -\infty$.

The period T is given by

$$T = 2\pi/\omega_c = \frac{\hbar c}{eH}\oint \frac{dk}{v_\perp}, \qquad (6.164)$$

where ω_c is the cyclotron frequency and $v_\perp$ denotes the velocity component perpendicular to H. $\oint$ is the contour integral along the hodograph. The motion of an electron in a magnetic field has an interesting feature in the case when the constant energy contour perpendicular to the magnetic field is open. In this case the electron escapes to infinity in the plane perpendicular to the magnetic field and

T becomes infinite. Another interesting case is illustrated in Fig. 6.7. This is the case when the electron trajectory is closed but passes through a saddle point of the constant energy surface.

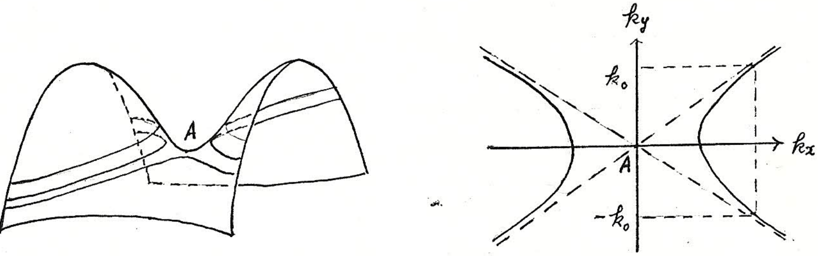


Fig. 6.7 Trajectory of an electron near a saddle point A, where its velocity is zero.$^{34)}$

An electron located at the saddle point can not move at all and the electrons which move along the trajectories passing near the saddle point, spend a very long time. This means that the period T increases when the electron trajectory approaches the A point (See Fig. 6.7). Near A the electron energy can be expressed in the following way:

$$E = E_0(k_z) + \frac{1}{2}\left(\frac{\hbar^2 k_x^2}{m_1} - \frac{\hbar^2 k_y^2}{m_2}\right), \qquad (6.165)$$

where $E_0(k_z)$ is the energy at the saddle point and the k_z axis is parallel to the magnetic field. In the vicinity of the point A the velocity in k_x-k_y plane is infinitesimally small, then we get

$$T \cong \frac{\hbar c}{eH} \int_{-k_0}^{k_0} \sqrt{\frac{1+\left(\frac{dk_x}{dk_y}\right)^2}{v_x^2+v_y^2}}\, dk_y \cong \frac{2c}{eH}\sqrt{\frac{m_1+m_2}{m_2}} \int_0^{k_0} \frac{dk_y}{\sqrt{\frac{k_x^2}{m_1}+\frac{k_y^2}{m_2}}}, \tag{6.166}$$

where k_0 is the value of k_y at the point far from the saddle point A (See Fig. 6.7). Expressing k_x in terms of $\Delta E = E - E_0(k_z)$, we obtain

$$T \cong \frac{2c}{eH} (m_1 m_2)^{1/2} \left| \ln \frac{\Delta E}{E_0} \right| . \tag{6.167}$$

Thus, the period T increases logarithmically infinity when the electron trajectory approaches the saddle point.

In this Section we do not consider the energy band with saddle point.

Since the velocity v is a periodic function of s, it can be expressed as

$$v = \sum_{m=-\infty}^{\infty} v(m) \exp(im\omega_c s), \tag{6.168}$$

and the requirement of the real number for v leads to $v(-m) = v(m)^*$. Substituting (6.168) into (6.163) and assuming τ being independent of s, we obtain

$$\Phi = -\tau \sum_m e\, \mathcal{E} \cdot v(m) \exp(im\omega_c s) / (1 + im\omega_c s). \tag{6.169}$$

Current density j is given by

$$j = -\frac{2e}{(2\pi)^3}\int dk\, v\Phi\left(-\frac{\partial f_0}{\partial E}\right). \tag{6.170}$$

By averaging $v\Phi$ over each hodograph, (6.170) is rewritten as

$$j = \frac{2e^2}{(2\pi)^3}\int dk\left(-\frac{\partial f_0}{\partial E}\right)\tau M,$$

$$M = -\frac{1}{eT\tau}\oint ds\, \Phi v, \tag{6.171}$$

where T is the period defined by (6.164) and M denotes the average of Φv over a hodograph. From (6.168) and (6.169) M becomes

$$M = \sum_m [\mathcal{E}\cdot v(m)]\, v(-m)/(1+im\omega_c\tau). \tag{6.172}$$

Introducing the tensor S by $M = S\cdot\mathcal{E}$, we get

$$\begin{cases} S_{xx} = \displaystyle\sum_{m=-\infty}^{\infty} \frac{|v_x(m)|^2}{1+im\omega_c\tau} = 2\sum_{m=1}^{\infty}\frac{|v_x(m)|^2}{1+(m\omega_c\tau)^2}, \\ S_{xy} = \displaystyle\sum_{m=1}^{\infty}\left\{\frac{v_x(m)v_y(-m)+v_x(-m)v_y(m)}{1+(m\omega_c\tau)^2} + i\,\frac{[v_x(-m)v_y(m)-v_x(m)v_y(-m)]\,m\omega_c\tau}{1+(m\omega_c\tau)^2}\right\}, \\ S_{zz} = v_z^2(0) + \displaystyle\sum_{m=1}^{\infty}\frac{2|v_z(m)|^2}{1+(m\omega_c\tau)^2}. \end{cases} \tag{6.173}$$

Similary, S_{yy}, S_{xz} and S_{yz} can be easily obtained. The Onsager relation $S_{ij}(H) = S_{ji}(-H)$ is satisfied in (6.173). In deriving

(6.174) we employ the relation of $v_x(0)=0$, and it is verified in the following. From (6.168) $v_x(0)$ is given by

$$v_x(0) = \frac{\omega_c}{2\pi}\oint ds\, v_x . \tag{6.174}$$

Changing the integral on s to the one on the hodograph, we obtain

$$v_x(0) = \frac{\omega_c \hbar c}{2\pi e H}\oint dk\,(v_\perp \cdot e)/v_\perp , \tag{6.175}$$

where e is a unit vector parallel to the x-axis. Since dk along the hodograph is perpendicular to $v_\perp$, we have

$$dk\, v_\perp / v_\perp = dk \times H/H . \tag{6.176}$$

then

$$v_x(0) = \frac{\omega_c \hbar c}{2\pi e H}\left(H \times \oint dk\right)\cdot e . \tag{6.177}$$

(6.177) leads to $v_x(0)=0$ since $\oint dk = 0$. Similarly, we obtain the relation $v_y(0)=0$. This means that the electron trajectory can not drift along the direction perpendicular to the magnetic field without electric field.

In general the first term in S_{xy} remains finite in the absence of the magnetic field. In this case, the electric conductivity is anisotropic. However, this term disappears if the hodograph is highly symmetric.

The electric conductivity is expressed in terms of S as

$$\sigma = \frac{2e^2}{(2\pi)^3}\int dk\left(-\frac{\partial f_0}{\partial E}\right)\tau\,\mathbb{S}. \qquad (6.178)$$

By introducing the cylindrical coordinate (ρ, θ, k_z), where $\rho = \sqrt{k_x^2 + k_y^2}$, $\tan\theta = k_y/k_x$, energy E is written by

$$E = \sum_n E_n(\rho, k_z)\, e^{in\theta} \quad (E_{-n} = E_n^*). \qquad (6.179)$$

If the k_z axis is the p-th fold symmetry axis, E_n is non-zero only for n being a multiple of p. From (6.179) v_x and v_y are given by

$$\begin{aligned} v_x &= \frac{1}{\hbar}\sum_n \left(E_n'\cos\theta - \frac{n}{\rho}E_n\sin\theta\right)e^{in\theta}, \quad \left(E_n' = \frac{\partial E_n}{\partial \rho}\right) \\ v_y &= \frac{1}{\hbar}\sum_n \left(E_n'\sin\theta + \frac{n}{\rho}E_n\cos\theta\right)e^{in\theta}. \end{aligned} \qquad (6.180)$$

Rewriting the above expressions, we get

$$\begin{cases} v_x = \dfrac{1}{\sqrt{2}}(g + g^*), \quad v_y = \dfrac{i}{\sqrt{2}}(g - g^*), \\ g = \dfrac{1}{\hbar\sqrt{2}}\displaystyle\sum_n \left(E_n' - \frac{n}{\rho}E_n\right)e^{i(n+1)\theta}. \end{cases} \qquad (6.181)$$

Next, let v_x and v_y express as the function of s. Since, θ is given by $\theta = \omega_c s +$ (periodic function of s) and ρ is a periodic function of θ, g takes the form :

$$g = \sum_{n} A(n) \exp\left[i (n+1) \omega_c s \right] . \qquad (6.182)$$

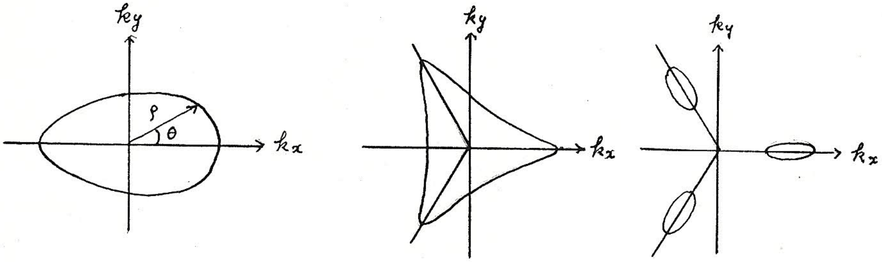
Accordingly, the Fourier components of v_x and v_y becomes

$$v_x(m) = \frac{1}{\sqrt{2}} \left[A(m-1) + A(-m-1)^* \right], \qquad (6.183)$$

$$v_y(m) = \frac{i}{\sqrt{2}} \left[-A(m-1) + A(-m-1)^* \right]. \qquad (6.184)$$

As is readily understood from (6.181) and (6.182), if E_n is zero, the corresponding factor $A(n)$ also vanishes.

Consider the following three cases represented by Fig. 6.8.



(a). (b) (c)

Fig. 6.8 Examples of the hodograph.

Combinations of v_x and v_y which appear in S_{xy} are as follows:

$$\begin{cases} v_x(m)\, v_y(-m) + v_x(-m)\, v_y(m) = -i \left[A(m-1) A(-m-1) - A(m-1)^* A(-m-1)^* \right], \\ v_x(m)\, v_y(-m) - v_x(-m)\, v_y(m) = -\left[|A(m-1)|^2 - |A(-m-1)|^2 \right]. \end{cases} \qquad (6.185)$$

In the case of Fig. 6.8 (a) k_xk_z-plane is a mirror plane. In this case $A(n)$ is real. Then, we have

$$S_{xy} = \sum_{m=1}^{\infty} \frac{m\omega_c\tau\left[A(-m-1)^2 - A(m-1)^2\right]}{1+(m\omega_c\tau)^2} . \tag{6.186}$$

In Fig. 6.8(b), where the hodograph is a singly connected trigonal symmetrical curve, non-vanishing elements are $A(3p)$ $(p = 0, \pm 1, \pm 2, \cdots)$. Therefore, (6.186) becomes

$$S_{xy} = -\sum_{n=0}^{\infty} \frac{(3n+1)\,\omega_c\tau\, A(3n)^2}{1+[(3n+1)\,\omega_c\tau]^2} + \sum_{n=1}^{\infty} \frac{(3n-1)\,\omega_c\tau\, A(-3n)^2}{1+[(3n-1)\,\omega_c\tau]^2} , \tag{6.187}$$

and S_{xx} is given by

$$S_{xx} = \sum_{n=0}^{\infty} \frac{A(3n)^2}{1+[(3n+1)\omega_c\tau]^2} + \sum_{n=1}^{\infty} \frac{A(-3n)^2}{1+[(3n-1)\omega_c\tau]^2} . \tag{6.188}$$

It should be noted that ω_c is positive for electrons and negative for holes (See (6.164)). It is interesting that negative and positive terms appear alternately in (6.187).

Finally, we shall consider Fig. 6.8 (c). In this case the hodograph is separated into three pieces. Each piece has a mirror plane and as a whole the hodograph is trigonally symmetric.

S_{xy} and S_{xx} are given by

$$\left\{\begin{aligned} S_{xy} &= \frac{\omega_c\tau\left[A(-2)^2-A(0)^2\right]}{1+(\omega_c\tau)^2}+\frac{2\omega_c\tau\left[A(-3)^2-A(1)^2\right]}{1+(2\omega_c\tau)^2}+\frac{3\omega_c\tau\left[A(-4)^2-A(2)^2\right]}{1+(3\omega_c\tau)^2}+\cdots, \\ S_{xx} &= \frac{A(-2)^2+A(0)^2}{1+(\omega_c\tau)^2}+\frac{A(-3)^2+A(1)^2}{1+(2\omega_c\tau)^2}+\frac{A(-4)^2+A(2)^2}{1+(3\omega_c\tau)^2}+\cdots. \end{aligned}\right. \tag{6.189}$$

In the crystals with large band warping it is expected that the higher harmonics $A(n)$ $(|n| \geqq 1)$ play an important role in S_{xx} and S_{xy} in weak magnetic field $(n\omega_c\tau < 1)$ and there is a large difference between $\sigma_{ij}(H)$ with the band warping and the one without the warping. One of such examples is graphite. Behaviors of the Hall effect of the well-crystalline graphite at low temperatures is ascribed to the trigonal warping of the bands (See Chapter 8).

Chapter 7 Mechanisms of Scattering Process

7.1 Acoustic Phonon Scattering

The electron - phonon interaction of the monovalent metals such as the alkali metals was treated in detail in Chapter 2.
A simple and useful formula is (2.69) due to Bardeen.

From (2.30), (2.48) and (2.69) the matrix elements of the electron phonon interaction is given by

$$\langle k', n_{q\lambda}\pm 1 \mid H_{ep} \mid k, n_{q\lambda}\rangle = -i\sqrt{\frac{\hbar}{2MN\omega_{q\lambda}}}\, e_{q\lambda}\cdot(k-k')\,U(|k-k'|)$$

$$\times\, \delta_{k',k\pm q+G} \begin{cases}\sqrt{n_{q\lambda}} \\ \sqrt{n_{q\lambda}+1}\end{cases}, \tag{7.1}$$

where $e_{q\lambda}$ is the polarization vector of the phonon $(q\lambda)$, G a reciprocal vector and $U(|k-k'|)$ is a function of the scattering angle and represents the strength of the electron-phonon interaction.

- In the normal process (N-process) with $G=0$ only the longitudinal phonons interact with electrons, while in the Umklapp process (U-process) with $G\neq 0$ the transverse phonons also participate in the scattering events.

If the scattering angle is sufficiently small, the coupling constant $U(|k-k'|)$ becomes $-\frac{2}{3}E_F$.

In semiconductors and semimetals their energy surfaces are small and then U-process can be disregarded. In these materials the deformation potential approximation is valid (see Chapter 3). For simplicity, we consider the interaction with the longitudinal phonons and put $U(|k-k'|) = D =$ constant.

(7.1) takes the form

$$\langle k', n_q \mp 1 | H_{e\text{-}p} | k, n_q \rangle = \mp i D \sqrt{\frac{\hbar}{2NM\omega_q}}\, q\, \delta_{k', k\pm q} \begin{cases} \sqrt{n_q} \\ \sqrt{n_q+1} \end{cases} . \qquad (7.2)$$

From (1.59) and (1.66) the lattice displacement vector $\xi(R)$ becomes

$$\xi(R) = \sum_{q,\lambda} \sqrt{\frac{\hbar}{2NM\omega_{q\lambda}}}\, e_{q\lambda} (b_{q\lambda} + b_{-q\lambda}^{+}) e^{iq\cdot R} , \qquad (7.3)$$

Since we are interested in the long wave length phonons, the discrete lattice point R can be considered to be a continuous variable. The electron phonon interaction $H_{e\text{-}p}$ is represented in the operator form:

$$H_{ep} = -D \operatorname{div} \xi(r) = -iD \sum_q \sqrt{\frac{\hbar}{2d\Omega\omega_q}}\, q\, (b_q e^{iqr} - b_q^{+} e^{-iqr}), \qquad (7.4)$$

where d is the density of the crystal and Ω the volume.

(7.4) is formally identical with (3.1).

The transition probability from (k, n_q) to $(k', n_q \mp 1)$ is

$$W(k', n_q \mp 1 ; k, n_q) = \frac{2\pi}{\hbar} \left| \langle k', n_q \mp 1 | H_{e\text{-}p} | k, n_q \rangle \right|^2 \delta(E_k - E_{k'} \pm \hbar\omega_q), \qquad (7.5)$$

Assuming $\omega_q = v_s q$ and $E_k = \hbar^2 k^2/2m^*$, we get

$$W(k', n_q \mp 1; k, n_q) = \frac{\pi D^2 q}{d\Omega\, v_s} \begin{pmatrix} n_q \\ n_q+1 \end{pmatrix} \delta\left[\frac{\hbar^2}{2m^*}(\mp 2k\cdot q - q^2) \pm \hbar v_s q\right], \qquad (7.6)$$

From the δ-function, which guarantees the energy conservation, we have

$$2k\cos\Theta \pm q - \frac{2m^* v_s}{\hbar} = 0, \qquad (7.7)$$

where Θ is the angle between k and q. The third term in (7.7) is usually small and can be neglected. For instance, if we put $m^*/m_0 = 0.1$ and $v_s = 4\times10^5$ cm/sec, we obtain $2m^* v_s/\hbar = 0.69\times10^5\,\mathrm{cm}^{-1}$. Then, the energy conservation law becomes

$$2k\cos\Theta \pm q = 0. \qquad (7.8)$$

This corresponds to the relation for the elastic scattering process. To obtain the relation

$$f_0(E_k)(1-f_0(E_{k'})) \doteqdot f_0(E_k)(1-f_0(E_k)), \qquad (7.9)$$

where the left hand side appears in the Bloch equation (6.8), the condition of $|E_{k'} - E_k| = \hbar\omega_q \ll k_0 T$ should be satisfied.

If we choose $k \cong 10^6\,\mathrm{cm}^{-1}$ ($\gg 2m^* v_s/\hbar$), we have $(\hbar\omega_q)_{max} \cong 2v_s k \cong 8.4\times10^{-16}$ erg $= 6.1$K. Therefore, except at low temperatures the acoustic phonon scattering is considered to be elastic.

In metals with large Fermi momentum the scattering process is also nearly elastic at $T \gg \Theta_D$.

In the following we calculate the relaxation time due to the acoustic phonon scattering in semimetals and semiconductors.

Assuming the elastic scattering and putting $\nabla T = 0$, we get from (6.9) and (6.16)

$$\frac{1}{\tau(k)} = \sum_{k'} W(k,k') \left\{ 1 - \frac{\mathcal{E}\cdot v(k')}{\mathcal{E}\cdot v(k)} \right\}, \qquad (7.10)$$

where $v(k) = (\hbar/m^*)\,k$, $v(k') = (\hbar/m^*)\,k'$ and $|k'| = |k|$.

By decomposing k' into the two components — one is the parallel to k and the other perpendicular to k, the curly bracket term becomes

$$1 - \frac{\mathcal{E}\{k_\perp' + k(k'\cdot k)/k^2\}}{\mathcal{E}\cdot k} \qquad (7.11)$$

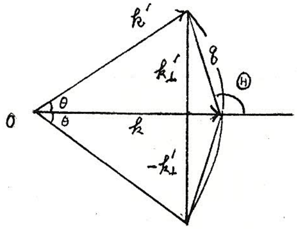


Fig. 7.1 Momentum change in the elastic scattering process. (Phonon absorption process).

Since W is a function of θ or Θ (See Fig. 7.1), it does not change by $k_\perp' \to -k_\perp'$, then the term related to $k_\perp'$ in (7.11) vanishes after the summation over k'.

Consequently, the relaxation time is given by

$$\frac{1}{\tau(k)} = \sum_{k'} W(\theta)\,(1-\cos\theta)\,. \tag{7.12}$$

At high temperatures the phonon distribution is well described by the classical one : $n_q \cong n_q + 1 \triangleq k_0 T/\hbar v_s q$, and (7.6) becomes

$$\left\{\begin{aligned} W &= \frac{\pi D^2 m^* k_0 T}{\Omega \hbar^3 d\, v_s^2\, k\, q}\,\delta(\cos\Theta - \cos\Theta_0), \\ \cos\Theta_0 &= \begin{cases} -q/2k : & \text{phonon absorption} \\ q/2k : & \text{phonon emission} \end{cases} \end{aligned}\right. \tag{7.13}$$

and θ is related to Θ by

$$\cos\theta = -\cos 2\Theta. \tag{7.14}$$

By substituting (7.13) into (7.12), we obtain

$$\frac{1}{\tau} = \frac{D^2}{2\pi\hbar}\left(\frac{k_0 T}{d\, v_s^2}\right)\left(\frac{2m^*}{\hbar^2}\right)^{3/2} \underline{E^{1/2}} \propto E^{1/2}\, T. \tag{7.15}$$

Let estimate (7.15) for n-type InSb. Choosing a set of parameters

$$\left\{\begin{aligned} & D = 7.2\,\mathrm{eV},\quad m^* = 0.014\, m_0,\quad d = 5.775, \\ & v_s = 3.7\times 10^5\ \mathrm{cm/sec}, \end{aligned}\right. \tag{7.16}$$

and $T = 77\mathrm{K}$, $E = 10^{-14}\,\mathrm{erg}$ ($k = 0.48\times 10^6\ \mathrm{cm}^{-1}$)

, we get

$$\tau = 3.36\times 10^{-10}\ \mathrm{sec}. \tag{7.17}$$

Similarly, we can estimate τ of the monovalent metals. In this case the integration limit on q is different from those of semiconductors and semimetals. In the latter case (7.8) shows $q \leq 2k$. On the other hand in the monovalent metals the Debye cut off vector q_D is given by

$$\frac{1}{(2\pi)^3}\frac{4\pi}{3} q_D{}^3 = N \quad (N: \text{number density of atom}), \tag{7.18}$$

and the Fermi momentum is $k_F = (3\pi^2 N)^{1/3}$, then we have

$$q_D = (6\pi^2 N)^{1/3} = 2^{1/3} k_F < 2k_F . \tag{7.19}$$

This indicates that the upper limit is not $2k_F$ but q_D. In consideration of this point, the relaxation rate on the Fermi surface is

$$\frac{1}{\tau} = \frac{m^* q_D{}^4}{16\pi d\, v_s{}^2}\,\frac{k_0 T D^2}{\hbar^3 k_F{}^3} \propto T, \tag{7.20}$$

and by using $D = -(2/3)E_F$ (see (2.71)) (7.20) becomes

$$\frac{1}{\tau} = \frac{m^* q_D E_F{}^2 k_0 T}{18\pi \hbar^3 d\, v_s{}^2} . \tag{7.21}$$

(7.21) is evaluated for sodium, which is a typical monovalent metal. On making use of the paramters

$$\begin{cases} E_F = 3.1\,\mathrm{eV}, \; q_D = 1.14 \times 10^8\,\mathrm{cm}^{-1}, \; v_s = 3.2 \times 10^5\,\mathrm{cm/sec}, \\ d = 0.97, \; m^* = m_0 \end{cases} \tag{7.22}$$

we obtain

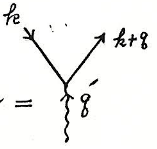
$$\tau = 6.20 \times 10^{-14} \text{sec} \quad \text{at } T = 300\,K, \qquad (7.23)$$

which is much smaller than (7.17).

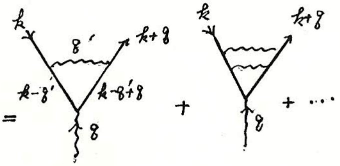
Before finishing this Section, we present an important theorem on the higer order terms in the electron-phonon interaction (Migdal theorem). This theorem states that the higher order corrections to $H_{e\text{-}p}$ give only the small quantities of order of $\sqrt{m/M}$, where m and M are the masses of the electron and nucleus, respectively. This may be easily verified by utilizing the Green's function method.35) Now we prove it by an elementary procedure.

We calculate the first-order correction to $H_{e\text{-}p}$ in the phonon absorption process. Diagramatically, the zeroth-order term and the higher order ones are represented by

zeroth order term =



, higher order terms =



+ ···. (7.24)

From (7.4) the matrix element corresponding to the first term in the higher order term is given by

$$-iDC_q \sum_{q'} D^2 C_{q'}^2 \frac{(n_{q'}+1)(1-f_{k-q'})(1-f_{k-q'+q})}{(E_k - E_{k-q'} - \hbar\omega_{q'})(E_k - E_{k-q'+q} + \hbar\omega_{q'})}, \qquad (7.25)$$

where $C_q = \sqrt{\hbar/2NM\omega_q}\, q$ and $D = -\frac{2}{3}E_F$. It is easily shown that

$$\sum_{q'} \cdots \simeq \frac{\hbar k_F}{M v_s} = \frac{m v_F}{M v_s} \simeq \sqrt{\frac{m}{M}}, \qquad (7.26)$$

where Bohm-Staver relation (1.82) is employed. The estimate just made is not changed by taking account of higher-order diagrams.

7.2 Phonon Cloud

The existence of the electron-phonon interaction (7.4) indicates that an electron in a state k accompanying no phonons can not be an exact eigenstate of the system but the electron is always surrounded by a cloud of virtual phonons. Such an electron is called a polaron. Typical example of the polaron is the slow electron which interacts strongly with the optical phonons in ionic crystals.

In the following we calculate the number of virtual phonons around a slowly moving electron by perturbation theory. The first order perturbed state is given by

$$\Phi_k = \phi_k + \sum_q \phi_{k-q}\chi_q \frac{\langle k-q ; n_q = 1 | \mathcal{H}_{ep} | k ; n_q = 0 \rangle}{E_k - E_{k-q} - \hbar\omega_q}, \qquad (7.27)$$

where χ_q is the phonon wave function for $n_q = 1$ (See (1.26)).

The average number of virtual phonons in the state Φ_k is

$$\langle n \rangle = \langle \sum_q b_q^+ b_q \rangle = \sum_q \frac{|\langle k-q ; n_q = 1 | \mathcal{H}_{ep} | k ; n_q = 0 \rangle|^2}{(E_k - E_{k-q} - \hbar\omega_q)^2}$$

$$= \frac{\hbar D^2}{2(2\pi)^3 d v_s} \int_0^{q_D} d\mathbf{q} \frac{q}{\left\{ \frac{\hbar^2}{2m^*}(2\mathbf{k}\cdot\mathbf{q} - q^2) - \hbar v_s q \right\}^2}$$

$$= \frac{D^2 m^{*2}}{(2\pi)^2 d v_s \hbar^3 k} \left\{ (q_c - 2k) \ln \left| \frac{q_c - 2k}{q_D + q_c - 2k} \right| + (q_c + 2k) \ln \left| \frac{q_D + q_c + 2k}{q_c + 2k} \right| \right\}, \qquad (7.28)$$

where $\hbar q_c = 2m^* v_s$.

Taking

$$\begin{cases} D = 10\ \mathrm{eV}, \quad m^* = 0.1\, m_0, \quad v_s = 4 \times 10^5\ \mathrm{cm/sec}, \\ d = 5, \quad q_D = 10^8\ \mathrm{cm}^{-1}, \quad k = 10^6\ \mathrm{cm}^{-1}, \end{cases} \qquad (7.29)$$

we have

$$\langle n \rangle \cong 3.5 \times 10^{-4} \ll 1. \qquad (7.30)$$

Then, we can describe the crystal wave functions as a product of separate electronic and phonon functions.

In a similar way, the average number of virtual LO-phonons around each electron is obtained by use of He-Lo defined by (1.134). Namely, we have

$$\langle n \rangle = \frac{e^2}{4\hbar\omega_l}\left(\frac{2m^*\omega_l}{\hbar}\right)^{1/2}\left(\frac{1}{\varepsilon_\infty}-\frac{1}{\varepsilon_0}\right) = \frac{\alpha}{2}. \qquad (7.31)$$

In deriving (7.31) $2k.q$ term in the energy denominator of (7.28) is neglected as compared with q^2 term. In ionic crystals such as KCl and AgBr the number of virtual phonons $\langle n \rangle$ is of the order of unity (See Table 1.1), then the first order perturbation calculation is no longer valid.

7.3 Scattering Process in Many Valley Semiconductors

In semiconductors the carrier density n is a function of the temperature and impurity concentration. Then, the mobility μ defined by $\sigma = ne\mu$ is a more fundamental quantity than the conductivity σ.

From (6.95) and (7.15) the mobility related to the deformation potential scattering is

$$\mu_L = \frac{(8\pi)^{1/2}}{3}\frac{e\hbar^4 d v_s^2}{(k_0T)^{3/2} m^{*5/2} D^2} \propto T^{-3/2}. \qquad (7.32)$$

As stated in Section 3.2, Si and Ge are the many valley semiconductor and the energy near the band edge is written in the form

$$E^{(\lambda)}(k) = E_0^{(\lambda)} + \frac{\hbar^2}{2}\left(\frac{k_\perp^2}{m_\perp} + \frac{k_\parallel^2}{m_\parallel}\right). \tag{7.33}$$

Interaction with the acoustic phonons is given by

$$\mathcal{H}_{e\text{-}p}^{(\lambda)} = \delta E^{(\lambda)} = \sum_{\alpha,\beta} e_{\alpha\beta}\left(\Xi_d \delta_{\alpha\beta} + \Xi_u a_\alpha^{(\lambda)} a_\beta^{(\lambda)}\right), \tag{7.34}$$

where $a_\alpha^{(\lambda)}$ is the direction cosine of the vector $k^{(\lambda)}$ corresponding to the band edge λ and $e_{\alpha\beta}$ is the strain tensor defined by

$$\xi(r) = (\xi_1, \xi_2, \xi_3), \quad \xi_\alpha = \sum_\beta e_{\alpha\beta} x_\beta, \quad r = (x_1, x_2, x_3). \tag{7.35}$$

Choosing the coordinate axes as the principal axes of the ellipsoid λ, we obtain

$$\delta E^{(\lambda)} = \Xi_d\left(e_{xx} + e_{yy} + e_{zz}\right) + \Xi_u e_{zz}. \tag{7.36}$$

Herring - Vogt calculated the transport coefficients of Si and Ge by use of (7.36).(15) Their theory is briefly explained in the next Section.

7.4 Herring - Vogt Theory

Along the principal axes of an ellipsoidal energy surface the relaxation time tensor τ becomes diagonal:

$$\tau = \left[\begin{array}{ccc} \tau_\perp & 0 & 0 \\ 0 & \tau_\perp & 0 \\ 0 & 0 & \tau_\parallel \end{array}\right]\begin{array}{c} x \\ y \\ z \end{array}. \tag{7.37}$$

Squares of the matrix elements due to the longitudinal and transverse phonon scatterings, are given by

$$|\langle k \pm q | H_l' | k \rangle|^2 = \frac{(\Xi_d + \Xi_u \cos^2\theta)^2 \hbar\omega_l(q)}{2\Omega d v_l^2} \begin{cases} n_{ql}, \\ n_{ql}+1, \end{cases} \qquad (7.38)$$

$$|\langle k \pm q | H_t' | k \rangle|^2 = \frac{\Xi_u^2 \sin^2\theta \cos^2\theta\, \hbar\omega_t(q)}{2\Omega d v_t^2} \begin{cases} n_{qt}, \\ n_{qt}+1 , \end{cases} \qquad (7.39)$$

where θ is the angle between q and z-axis.

If $\Xi_d + \Xi_u \cos^2\theta$ is replaced by E_1, (7.38) gives the same matrix element as given earlier for spherical constant energy surface (See Section 3.1).

It is convenient to write the above expressions in the coordinate system in which the constant energy surface is sphere. To transform to this system, we use the substitution

$$k_i = k_i^* (m_i/m_0)^{1/2}, \quad (m_i = m_\perp \text{ or } m_\parallel). \qquad (7.40)$$

In the new system

$$E^{(\lambda)} = E_0^{(\lambda)} + (\hbar^2/2m_0) k^{*2}. \qquad (7.41)$$

Let denote the transition probability for $k^* \to k^{*\prime}$ by Λ.

After a lengthy calculation, we get the expressions for $\tau_\parallel$ and $\tau_\perp$ as follows:

$$
\left\{
\begin{aligned}
\frac{1}{\tau_{\parallel}} &= 3\pi \int_{-1}^{1}\int_{-1}^{1} \cos\beta\,(\cos\beta - \cos\beta')\,\langle\langle \Lambda \rangle\rangle\, d(\cos\beta')\, d(\cos\beta), \\
\frac{1}{\tau_{\perp}} &= \frac{3\pi}{2} \int_{-1}^{1}\int_{-1}^{1} [\sin^2\beta\,\langle\langle \Lambda \rangle\rangle - \sin\beta\sin\beta' \langle \cos(\alpha'-\alpha)\langle\Lambda\rangle\rangle\, d(\cos\beta')\, d(\cos\beta),
\end{aligned}
\right.
\tag{7.42}
$$

where α is the azimuthal angle of k^* and β the corresponding polar angle. α' and β' are related to $k^{*\prime}$.

The outer angular bracket $\langle\cdots\rangle$ in $\langle\langle\cdots\rangle\rangle$ indicates an average over $(\alpha'-\alpha)$ and the inner one an average over α' for fixed $(\alpha'-\alpha)$.

Λ takes the form

$$
\Lambda = \frac{m_\perp m_\parallel^{1/2}\,\Omega}{2^{3/2}\,\pi^2\hbar^4}\, E^{1/2} \sum_\alpha |H_\alpha'|^2, \tag{7.43}
$$

where H_α' indicates the combined matrix elements for emission and absorption of acoustic phonons with polarization α (See (7.38) and (7.39)). Expressing $\cos^2\theta$ in terms of β, β', $(\alpha'-\alpha)$ and carrying out the integration, we get the relaxation times

$$
\left\{
\begin{aligned}
\frac{1}{\tau_\parallel} &= (3\pi C k_0 T E^{1/2}/C_l)\,[\xi_\parallel \Xi_d^2 + \eta_\parallel \Xi_d \Xi_u + \zeta_\parallel \Xi_u^2], \\
\frac{1}{\tau_\perp} &= (3\pi C k_0 T E^{1/2}/C_l)\,[\xi_\perp \Xi_d^2 + \eta_\perp \Xi_d \Xi_u + \zeta_\perp \Xi_u^2],
\end{aligned}
\right.
\tag{7.44}
$$

where C_l is an averaged elastic constant associated with the longitudinal wave given by

$$C_l = C_{12} + 2C_{44} + \frac{3}{5}C^*, \quad C^* = C_{11} - C_{12} - 2C_{14}, \tag{7.45}$$

and C is given by

$$C = (m_\perp^2 m_\parallel)^{1/2} / 2^{3/2} \pi^2 \hbar^4. \tag{7.46}$$

ξ, η, and ζ are dimensionless coefficients that depend on the elastic constants, $m_\perp/m_\parallel$ and the orientation of the ellipsoids.

Concrete expressions of $[\cdots]$ of (7.44) for n-Ge and n-Si are

$$n\text{-Ge}\quad \begin{cases} [\parallel] = \Xi_u^2 \left[1.24\,(\Xi_d/\Xi_u)^2 + 2.32\,(\Xi_d/\Xi_u) + 1.22\right], \\ [\perp] = \Xi_u^2 \left[1.31\,(\Xi_d/\Xi_u)^2 + 1.61\,(\Xi_d/\Xi_u) + 1.01\right]. \end{cases} \tag{7.47}$$

$$n\text{-Si}\quad \begin{cases} [\parallel] = \Xi_u^2 \left[1.40\,(\Xi_d/\Xi_u)^2 + 2.40\,(\Xi_d/\Xi_u) + 1.62\right], \\ [\perp] = \Xi_u^2 \left[1.33\,(\Xi_d/\Xi_u)^2 + 1.15\,(\Xi_d/\Xi_u) + 1.07\right]. \end{cases} \tag{7.48}$$

7.5 Piezoresistance and Deformation Potential

Many valley structures of n-Ge and n-Si were decisively determined by the cyclotron resonance experiment.36)

Piezoresistance experiment performed by Smith 37) provided a key for elucidation of the many valley structure prior to the cyclotron resonance experiment. Moreover, it is a useful tool for the determination of Ξ_u.

If a stress X is applied under the condition of constant current density, the electric field and resistivity change as

$$\delta \mathcal{E} = \delta\rho\, \mathbf{j} \ , \tag{7.49}$$

where in general $\delta\rho$ is a tensor. For a cubic crystal, it is convenient to divide through by the scalar resistivity ρ giving

$$\delta \mathcal{E}/\rho = \Delta \mathbf{j} \ , \quad (\Delta = \delta\rho/\rho) \, . \tag{7.50}$$

If $\mathbf{X}$ is small enough, there is a linear relation between Δ and $\mathbf{X}$,

$$\Delta = \boldsymbol{\Pi} \mathbf{X} \, , \tag{7.51}$$

where $\boldsymbol{\Pi}$ is a six by six matrix of piezoresistance constants. Instead of $\mathbf{X}$, Δ can be related to the strain $\mathbf{e}$ by the elastoresistance coefficients $\mathbf{m}$,

$$\Delta = \mathbf{m}\, \mathbf{e} \, . \tag{7.52}$$

Since we have for the relation between stress and strain $\mathbf{X} = \mathbf{C}\, \mathbf{e}$, where $\mathbf{C}$ is the elastic constant matrix, it follows using (7.51) that

$$\mathbf{m} = \boldsymbol{\Pi}\, \mathbf{C} \, . \tag{7.53}$$

In the crystal with the symmetry of any one of the classes Td, O or Oh, $\mathbf{m}$ reduces to

$$\mathbf{m} = \begin{bmatrix} m_{11} & m_{12} & m_{12} & 0 & 0 & 0 \\ m_{12} & m_{11} & m_{12} & 0 & 0 & 0 \\ m_{12} & m_{12} & m_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & m_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & m_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \, . \tag{7.54}$$

Π and C have same structure as (7.54). m_{44} and
can be measured by using the arrangements shown in F

(Actually, uniaxial s
applied to crystal ro
different crystallographi
and from these meas
m is determined)

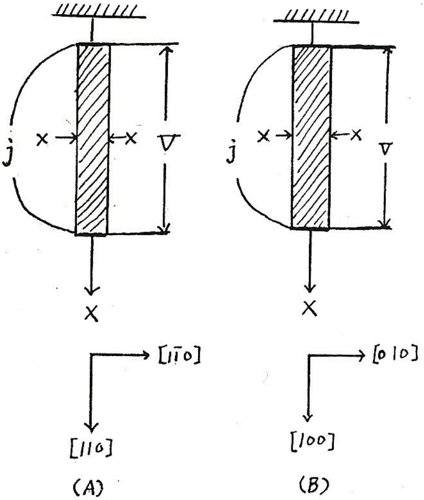


Fig. 7.2 Experimental arrangements for the measurement of the elastoresistance tensor.

(A) Configuration for measuring m_{44},

(B) Configuration for measuring $(m_{11}-m_{12})$.

In the arrangement (A) of Fig. 7.2, $X_1 = X_2 = X_3 = X_4 = X_5$
and $X_6 = X$, then we have

$$\Delta_{12} = \pi_{44} X, \quad m_{44} = \pi_{44} C_{44}, \quad \frac{1}{X}\frac{\delta\rho}{\rho} = \pi_{44},$$

7-55

In the arrangement (B), $X_1 = -X_2 = X$, and $X_3 = X_4 =$
$= X_6 = 0$, then we have

$$\frac{1}{X}\frac{\delta\rho}{\rho} = \pi_{11} - \pi_{12}, \quad m_{11} - m_{12} = (\pi_{11} - \pi_{12})(C_{11} - C_{12}).$$

7-56

m_{44} and $(m_{11}-m_{12})/2$ of n-Ge and n-Si obtained by Smith are listed in Table 7.1. It should be noted that in n-Ge $|m_{44}| \gg (m_{11}-m_{12})/2$, while in Si $|m_{44}| \ll |m_{11}-m_{12}|/2$. These feature are well explained by introducing the many valley model.

	Resistivity	m_{44}	$(m_{11}-m_{12})/2$
n-Ge	1.5 Ω cm	−93.0	+0.4
n-Ge	16.6 Ω cm	−93.4	+0.1
n-Si	11.7 Ω cm	−10.8	−79.5

Table 7.1 Elastoresistance coefficients of n-Ge and n-Si.

According to (7.34) the change of the band edge i is represented by

$$\delta E^{(i)} = \Xi^{(i)} \cdot \mathbf{e}, \quad \Xi^{(i)} = \Xi_d \mathbf{1} + \Xi_u \mathbf{a}^{(i)}\mathbf{a}^{(i)}, \tag{7.57}$$

Conductivity $\sigma^{(i)}$ is

$$\sigma^{(i)} = n^{(i)} e \mu^{(i)}, \tag{7.58}$$

By applying an elastic strain to the sample, the band edge and Fermi level change and then $n^{(i)}$ varies. From the microscopic point of view this variation is caused by the two different mechanisms: 1) electron transfer effect and 2) variation of the intervalley scattering. Contribution from 2) to the piezoresistance in Si is about 1/3 of 1) and 15% in Ge at room temperature.[38] Now we neglect the effect 2), and $\delta\sigma^{(i)}$ is given by

Accordingly, $\delta\sigma$ becomes

$$\delta\sigma = \sum_i \delta\sigma^{(i)} = -ne\,(1/k_0T)\sum_i \mu^{(i)}\left[\Xi^{(i)} - \nu^{-1}\sum_j \Xi^{(j)}\right]\cdot \mathbf{e}, \tag{7.63}$$

Let introduce a fourth-rank tensor M:

$$M = -ne\,(1/k_0T)\sum_i \mu^{(i)}\left[\Xi^{(i)} - \nu^{-1}\sum_j \Xi^{(j)}\right]. \tag{7.64}$$

From these relations several conclusions are derived as follows.

(i). $\mathrm{Tr}\,\delta\sigma = 0$. $\because$ $\mathrm{Tr}\,\delta\sigma = \sum_i \delta n^{(i)} e\,\mathrm{Tr}\,\mu^{(i)} = e\,\mathrm{Tr}\,\mu \sum_i \delta n^{(i)}$ $= 0$, because of $\mathrm{Tr}\,\mu^{(i)}$ being independent on i.

$$\mu^{(i)} = \frac{3\mu_0}{2K+1}\left[K\mathbb{1} + (1-K)\mathbf{a}^{(i)}\mathbf{a}^{(i)}\right], \tag{7.66}$$

where

$$K = \frac{\mu_\perp}{\mu_\parallel} = \frac{\tau_\perp m_\perp}{\tau_\parallel m_\parallel}, \quad \mu_0 = \frac{1}{3}(2\mu_\perp + \mu_\parallel). \tag{7.67}$$

$\mu_\parallel$ and $\mu_\perp$ denote the mobility component parallel and perpendicular to the ellipsoid axis, respectively.

From (7.57), (7.64), (7.65) and (7.67) we can derive **m** for n-Ge with [111]-valley and n-Si with [100]-valley as follows:

$$\text{Ge}: \begin{cases} m_{11} = m_{12} = 0, \\ m_{44} = \dfrac{1}{3}\dfrac{\Xi_u}{k_0T}\dfrac{1-K}{2K+1} = \dfrac{1}{9}\dfrac{\mu_\parallel - \mu_\perp}{\mu_0}, \end{cases} \tag{7.68}$$

$$\mathrm{Si}: \begin{cases} m_{11} = -2m_{12} = \dfrac{2}{3}\dfrac{\Xi_u}{k_0T}\dfrac{1-K}{2K+1} = \dfrac{2}{9}\dfrac{\mu_{\parallel}-\mu_{\perp}}{\mu_0}, \\ \\ m_{44} = 0. \end{cases} \qquad (7.69)$$

Above relations were derived by Herring-Vogt,15) and they are in qualitative agreement with Table 7.1.

From the piezoresistance experiment and the acoustoelectric effect Ξ_u of n-Ge was estimated as

$$15.8\,\mathrm{eV} < \Xi_u < 19.3\,\mathrm{eV}, \qquad (7.70)$$

and Herring-Vogt obtained

$$\Xi_d/\Xi_u \cong -0.38, \qquad (7.71)$$

while in n-Si

$$8.5\,\mathrm{eV} < \Xi_u < 9.6\,\mathrm{eV}, \quad \Xi_d \ll \Xi_u. \qquad (7.72)$$

7.6 Scattering due to Non-Polar Optical phonon

As discussed in Section 1.6, the electron-polar optical interaction is represented by

$$H'_{op} = \mathbf{D}\cdot\delta\mathbf{r}, \qquad (7.73)$$

where $\delta\mathbf{r}$ is the relative displacement of + and − ions. The interaction with the non-polar optical phonon is also given by (7.73), where D is called the optical deformation potential constant, and its order of magnitude is $\sim 10^8\,\mathrm{eV/cm}$.39)

There are two non-equivalent atoms in the unit cell of Ge and Si, and their relative displacement is represented in the form of (7.3), in which the dispersion of ω_q can be disregarded ($\omega_q \simeq \omega_0$).

Square of the matrix element of H'_{op} is

$$|\langle k \pm q | H'_{op} | k \rangle|^2 = \frac{D^2 \hbar}{2 d \Omega \omega_0} \begin{cases} n_q : \text{phonon absorption,} \\ n_q + 1 : \text{phonon emission,} \end{cases} \qquad (7.74)$$

and the corresponding transition probability is given by

$$\frac{1}{\tau_{op}} = \frac{2\pi}{\hbar} \frac{D^2 \hbar}{2 d \Omega \omega_0} \sum_q \left\{ n_q \, \delta(E_k - E_{k \mp q} + \hbar\omega_q) + (n_q + 1)\, \delta(E_k - E_{k \pm q} - \hbar\omega_q) \right\}. \qquad (7.75)$$

From the δ-function the integration range on q becomes

$$\begin{cases} k\left[\sqrt{1 + \frac{\hbar\omega_0}{E}} - 1\right] < q < k\left[\sqrt{1 + \frac{\hbar\omega_0}{E}} + 1\right] : \text{phonon absorption,} \\ k\left[1 - \sqrt{1 - \frac{\hbar\omega_0}{E}}\right] < q < k\left[1 + \sqrt{1 - \frac{\hbar\omega_0}{E}}\right] : \text{phonon emission} \end{cases} \qquad (7.76)$$

After carrying out the integration over q, (7.75) gives

$$\frac{1}{\tau_{op}} = \frac{D^2 m^{*3/2}}{\sqrt{2}\pi \hbar^3 d \omega_0} \left[n (E + \hbar\omega_0)^{1/2} + (n+1)(E - \hbar\omega_0)^{1/2} \right], \qquad (7.77)$$

where

$$n = [\exp(\hbar\omega_0 / k_0 T) - 1]^{-1}.$$

The phonon emission term appears only in the case for $E > \hbar\omega_0$. In the many valley model, $m^{*3/2}$ should be replaced by $m_\perp m_{\parallel}^{1/2}$.

Optical phonon scattering is essentially inelastic except at high temperatures ($k_0T \gg \hbar\omega_0$), then τ_{op} represented by (7.75) and (7.77) does not correspond to the relaxation time. Therefore, it is not easy to calculate the conductivity.

7.7 Intervalley Scattering and Mobilities of n-Ge and n-Si

In Fig. 7.3 an example of the intervalley scattering is shown. The relaxation rate from μ-valley to ν-valley takes the same form as (7.77):

$$\frac{1}{\tau_\mu^{(l)}} = \sum_\nu{}' \frac{1}{\tau_{\mu\nu}^{(l)}} = \sum_\nu{}' \frac{D_{\mu\nu}^2 (m_\perp^2 m_\parallel)^{1/2}}{\sqrt{2}\pi\hbar^3 d\,\omega_{\mu\nu}}$$

$$\times \left[n_{\mu\nu}(E_\mu - E_\nu + \hbar\omega_{\mu\nu})^{1/2} + (n_{\mu\nu}+1)(E_\mu - E_\nu - \hbar\omega_{\mu\nu})^{1/2} \right]. \quad (7.78)$$

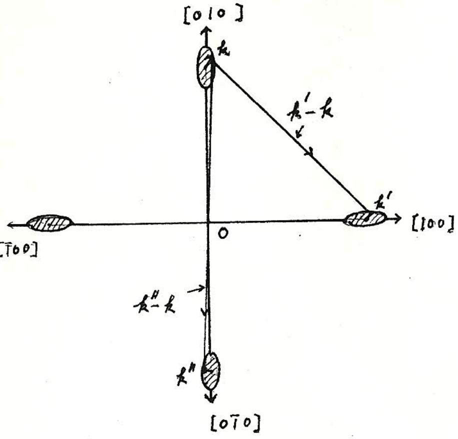


Fig. 7.3 Intervalley Scattering (n-Si)

Let introduce the notations ; $\omega_{\mu\nu} = \omega_i$, $\hbar\omega_i = k_0\Theta_i$ and $\hbar\omega_0 = k_0\Theta_0$. In n-Ge values of Θ_i and Θ_0 are obtained as follows:40)

$$\Theta_i = 315\,K, \quad \Theta_0 = 430\,K. \qquad (7.79)$$

In n-Ge it is shown that the intervalley transition is forbidden due to the selection rule.15) Since the band edges are located at the L-points, which correspond to the centers of the hexagonal faces in the Brillouin zone, and the intervalley phonons must have wave vectors $k_\mu - k_\nu$ which end at the centers of the square faces (X-points).

If $D_X^{(p)}$ is the representation of the full space group to which the phonon belongs, and $D_L^{(e)}$ that to which the electronic band-edge state belongs, the intervalley matrix element connecting two band-edge states does not vanish only if $D_L^{(e)} \times D_X^{(p)}$ includes $D_L^{(e)}$. In the present case $D_L^{(e)} \times D_X^{(p)}$ does not contain $D_L^{(e)}$, then only the weak transitions corresponding to $(k_\mu + \Delta k_\mu) \to (k_\nu + \Delta k_\nu)$ remain finite.

In Table 7.2 the observed mobilities of n, p-Ge and n, p-Si in the phonon scattering region are shown. Except n-Ge deviations of the mobilities from $T^{-1.5}$-dependence, which is due to the acoustic phonon scattering, are large. These deviations are ascribed to the optical phonon scattering and the intervalley scattering.

	electron	hole
Ge[41]	$\mu_n = 4.90 \times 10^7\, T^{-1.66}$	$\mu_p = 1.05 \times 10^9\, T^{-2.3}$
Si[42]	$\mu_n = 4.0 \times 10^9\, T^{-2.6}$	$\mu_p = 2.5 \times 10^8\, T^{-2.3}$

Table 7.2 Mobilities of Ge and Si in the phonon scattering region. (μ is measured in cm^2/volt sec)

As discussed already, the inter valley scattering does not play a major role in n-Ge. Then, we must consider the optical phonon scattering. Herring-Vogt formulae (7.44) and (7.47) indicate that scattering anisotropy is small. Then, we can put

$\tau_A \doteqdot \tau_\perp \doteqdot \tau_\parallel$. Mean free path l_A is defined by

$$\begin{cases} \tau_A(E) = \left(\dfrac{m_\perp}{2E}\right)^{1/2} l_A , \quad l_A = \dfrac{\pi \hbar^4 d v_e^2}{\Xi^2 m_\perp^{3/2} m_\parallel^{1/2} k_0 T} , \\ \\ \Xi^2 = \dfrac{3}{4} \Xi_u^2 \left[1.31 (\Xi_d/\Xi_u)^2 + 1.61 (\Xi_d/\Xi_u) + 1.01 \right]. \end{cases} \tag{7.80}$$

A factor 3/4 comes from the average $\langle \cdots \rangle$ in (6.91) and (6.92).

Assuming (7.77) as the relaxation time due to the optical phonon scattering and combining it with (7.80), we get the total relaxation rate $1/\tau = 1/\tau_A + 1/\tau_{op}$ as

$$\frac{1}{\tau} = \frac{1}{\tau_A} \left[1 + \frac{l_A}{l_{op}} \frac{1}{(e^{x_{op}} - 1)} \left\{ \left(1 + \frac{\hbar\omega_0}{E}\right)^{1/2} + e^{x_{op}} \left(1 - \frac{\hbar\omega_0}{E}\right)^{1/2} \right\} \right], \tag{7.81}$$

$$\text{where} \quad x_{op} = \frac{\hbar\omega_0}{k_0 T}, \quad l_{op} = \frac{2\pi \hbar^3 d \omega_0}{D^2 m_\perp^{3/2} m_\parallel^{1/2}} . \tag{7.82}$$

Ratio of l_A to l_{op} is

$$\frac{l_A}{l_{op}} = \frac{D^2 \hbar^2 v_e^2}{2 \Xi^2 k_0 T \hbar\omega_0} \equiv \frac{x_{op}}{k_0 T} b. \tag{7.83}$$

Calculated mobility using (7.81) is compared with the observed value and we obtain $b = 0.4$. Consequently, we have 40)

$$\frac{D^2 v_e^2}{\Xi^2 \omega_0^2} = 0.4, \tag{7.84}$$

Inserting $\omega_0 = 5.65 \times 10^{13}$ sec^{-1} and $v_e = 5.4 \times 10^5$ cm/sec,

we obtain

$$D/\Xi = 6.6\times10^{7}\,\mathrm{cm}^{-1}. \qquad (7.85)$$

By using

$$\Xi_u = 19.3\,\mathrm{eV},\quad \Xi_d = -9.07\,\mathrm{eV},^{43)} \qquad (7.86)$$

the optical deformation potential constant is obtained as

$$D = 8\times10^{8}\,\mathrm{eV/cm}. \qquad (7.87)$$

On the other hand, from the analysis of the energy relaxation measurement in warm electron problem a different value from (7.87)

$$D = 4\times10^{8}\,\mathrm{eV/cm} \qquad (7.88)$$

is obtained.43) In getting (7.88) the electron distribution is assumed to be the Boltzmann distribution. Calculation based on the variation method leads to (7.87).43)

As is shown in Fig. 7.3, in n-Si there are the two types of the intervalley transition : [100] → [$\bar{1}$00] and [100] → [010]. The former is called "g-scattering" and the latter "f-scattering."44) Fig. 7.4 indicates the cross section of the [110] plane of the Brillouin zone in Si. g and f phonons participate in the scattering process through the U-process.

Δk represents an electron momentum change. Magnitude of q_g is equal to 0.3 times of the maximum wave vector along [100], and q_f is exactly equal to the maximum wave vector along its direction. $q_g/(q_{100})_{max} = 0.3$ is due to the fact that the band edge is located at the 0.85 position along [100] direction.

Since the angle between q_f and q_g is 10°, they are nearly parallel.

In Fig. 7.5 the lattice vibrational spectrum of Si which is determined from neutron scattering experiment, is shown. Fig. 7.5 indicates that the intervalley phonons fall within two ranges of energy which are rather widely separated.

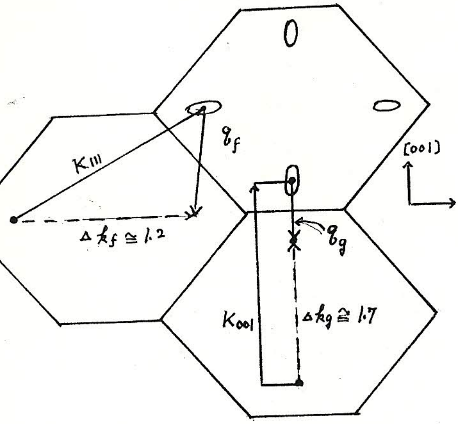


Fig. 7.4 Momentum Conservations in the intervalley scattering processes. K_{111} and K_{001} are principal vectors of the reciprocal lattice. • denotes the band edge points. 44)

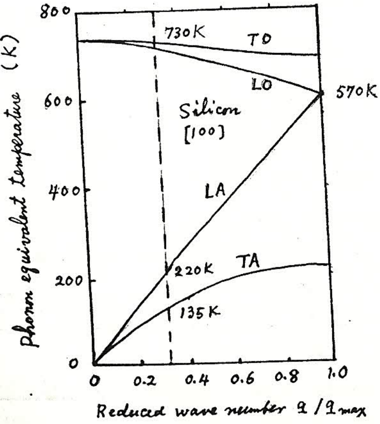


Fig. 7.5 Lattice vibration spectrum of silicon for [100] directed phonons. 45) The symbols TO, LO, LA, and TA indicate, respectively, transverse, optical, longitudinal optical, longitudinal acoustic, and transverse acoustic branches.

In terms of equivalent temperature, these ranges are from about 135 to 220K and from about 570 to 730K.

The combined relaxation time τ_α for the intra- and intervalley scatterings is given by [14)]

$$1/\tau_\alpha = \left\{ w_{A\alpha} \left(\frac{E}{k_0 T_0} \right)^{1/2} \left(\frac{T}{T_0} \right) + \sum_i w_i \left(\frac{\Theta_i}{T_0} \right)^{3/2} \left[\frac{(E/k_0\Theta_i + 1)^{1/2}}{e^{\Theta_i/T} - 1} + \frac{(E/k_0\Theta_i - 1)^{1/2} \text{ or } 0}{1 - e^{-\Theta_i/T}} \right] \right\}, \quad (7.89)$$

where α denotes $\parallel$ or $\perp$ corresponding to (7.48). $w_{A\alpha}$ and w_i measure the strength of coupling to acoustic and to intervalley phonons, respectively, and the subscript i ranges over all the intervalley phonons of different energies. The temperatures Θ_i and T_0 are, respectively, the characteristic temperature of the i-th phonon, and a reference temperature chosen to fix the magnitude of τ.

As the temperature is lowered to 30 K, the lattice scattering mobility μ_L approaches the $T^{-1.5}$ behavior expected from the acoustic phonon scattering alone (see (7.32)), where μ_L is obtained from the observed mobility by subtracting out the impurity scattering contributions. To do this, the following formula is employed.[46)]

$$\mu = \mu_L \left[1 + x^2 \left\{ C_i(x) + S_i(x) \sin x - \frac{1}{2}\pi \sin x \right\} \right], \quad (7.90)$$

$x^2 = 6\mu_L / \mu_I$, μ_I : mobility due to the ionized impurity scattering,

$Ci(x)$ and $Si(x)$ are cosine integral and sine integral, respectively.

According to Herring and Vogt [15)], the mobility takes the form

$$\mu = \frac{e}{3\langle E \rangle}\left[\frac{2\langle E\tau_\perp\rangle}{m_\perp} + \frac{\langle E\tau_\parallel\rangle}{m_\parallel}\right], \quad \langle g(E)\rangle = \int_0^\infty g(E)\, e^{-E/k_0T}\sqrt{E}\, dE \Big/ \frac{\sqrt{\pi}}{2}(k_0T)^{3/2}. \qquad (7.91)$$

By using the value $w_{A\perp}/w_{A\parallel} = 2/3$ the adjustable parameters $w_{A\perp}$, w_1, and w_2 are determined so as to make (7.91) fit with the experimental results. Here, the energies of the intervalley phonons are chosen as 630 K and 190 K. These values are lying in the region indicated in Fig. 7.5. w_1 corresponds to the phonon with energy 630 K and w_2 to 190 K. Finally, we get

$$w_1/w_{A\perp} = 2.0, \qquad w_2/w_{A\perp} = 0.15. \qquad (7.92)$$

These values also explain the Hall effect factor $\gamma = \mu_H/\mu_d$ and the magnetoresistance.[44] In n-Si effect of the intravalley transition due to the optical phonon scattering is small.[47]

7.8 Ionized Impurity Scattering

At the temperature well below the phonon scattering region the mobility is mainly controlled by the ionized impurity scattering. Since the slowly moving electrons are more strongly scattered than the fast ones, this mechanism becomes more important with decreasing temperatures.

At first the Conwell-Weisskopf theory[48] and in the next more refined theory due to Brooks-Hearing[49] are treated.

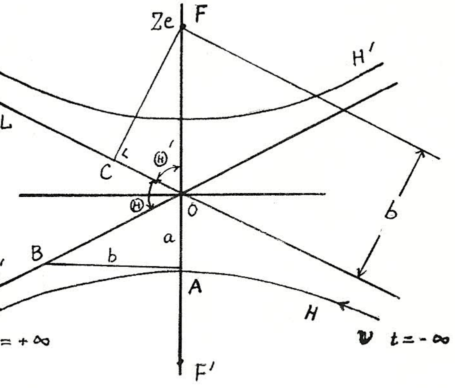


Fig. 7.6 Scattering of a carrier e by a charged ion Ze. FC⊥OL and AB⊥OF'.

In Fig. 7.6 the scattering of a carrier (e) by the repulsive potential due to a change Ze, is shown.

The following discussion is applicable to the case of the attractive potential.. In this case the carrier (e) moves along the orbit H' instead of H.

F and F' are the foci of the hyperbola H, H' and L and L' are the asymptotes.. Ze is located at the forcus F. It is well known that the following relations are satisfied:

$$\overline{OA} = \overline{OC} = a, \quad \overline{AB} = \overline{FC} = b. \qquad (7.93)$$

b is called the impact parameter. From (7.93) we have

$$OF \equiv \varepsilon = \sqrt{a^2+b^2}, \quad AF \equiv l - a + \varepsilon. \qquad (7.94)$$

By use of $a = \varepsilon \cos\Theta'$ and $b = \varepsilon \sin\Theta'$, l is rewritten

$$l = \varepsilon(1+\cos\Theta') = \frac{b(1+\cos\Theta')}{\sin\Theta'} = b\cot\frac{\Theta'}{2}. \qquad (7.95)$$

From the energy and angular momentum conservation laws,

$$\frac{1}{2} m^* v^2 = \frac{1}{2} m^* v_A{}^2 + \frac{Ze^2}{\kappa l}, \quad m^* v b = m^* v_A l, \qquad (7.96)$$

where v_A is the velocity at A and $\varkappa$ the dielectric constant. Eliminating l and v_A in (7.95) and (7.96) and using $\Theta' = (\pi - \Theta)/2$, we get

$$b = \frac{Ze^2}{\varkappa m^* v^2} \tan\Theta' = \frac{Ze^2}{\varkappa m^* v^2} \cot\frac{\Theta}{2} . \qquad (7.97)$$

Thus, we can obtain the differential scattering cross section $\sigma(\Theta)$:

$$\sigma(\Theta) = \frac{1}{\sin\Theta}\, b(\Theta) \frac{db(\Theta)}{d\Theta} = \left(\frac{Ze^2}{2m^* v^2 \varkappa}\right)^2 \frac{1}{\sin^4(\Theta/2)} . \qquad (7.98)$$

This is the Rutherford formula. The factor $\sin^4(\Theta/2)$ makes the total cross section $\sigma = 2\pi \int \sigma(\Theta) \sin\Theta \, d\Theta$ diverge. This is due to the long range character of the Coulomb potential. To avoid this difficulty, Conwell-Weisskopf took the maximum b value as ½ of the mean inter-ion distance. This determines the lower limit of Θ being finite. The Boltzmann equation is given by

$$\left(\frac{\partial f}{\partial t}\right)_{drift} + \left(\frac{\partial f}{\partial t}\right)_{coll} = 0, \qquad (7.99)$$

$$\left(\frac{\partial f}{\partial t}\right)_{drift} = \frac{\mathcal{E}_z e}{m^*} \frac{\partial f}{\partial v_z} , \quad \left(\frac{\partial f}{\partial t}\right)_{coll} = b - a, \qquad (7.100)$$

where an electric field is applied to the z-axis, b denotes the number of particles which enter into the phase space element $d\tau$ in unit time due to collisions, and a represents the number of particles leaving from $d\tau$.

Let specify the electron states at $t = -\infty$ and $+\infty$ by

(v, θ, φ) and (v, θ', φ'), respectively. Scattering angle Θ in (7.98) corresponds to $(\theta' - \theta)$. By putting $b_{max} = d$ ($2d$: mean interimpurity distance) in (7.97), one obtains

$$(\theta' - \theta)_{min} = 2 \arctan \left[Ze^2 / (\varkappa m^* v^2 d) \right]. \qquad (7.101)$$

Since the differential cross section $\sigma(\theta, \theta')$ is a function of $(\theta' - \theta)$, we can put the intial angle $\theta = 0$. The change of the distrubution f due to the collision with the ionized impurities, is

$$b - a = N_I \, v \int_{\theta' = \theta'_{min}} \int_{\varphi' = 0}^{2\pi} \left[f(v, \theta', \varphi') - f(v, \theta, \varphi) \right] \sigma(\theta') \, d\Omega', \qquad (7.102)$$

where N_I is the impurity concentration. Assuming f as

$$\begin{cases} f = f_0 - v_z \chi(v) = f_0 - v \cos\theta \, \chi(v), \\ f_0 = A e^{-m^* v^2 / 2k_0 T}, \; A = n \left(m^* / 2\pi k_0 T \right)^{3/2}, \end{cases} \qquad (7.103)$$

and inserting f into (7.99) and (7.102), we obtain

$$\begin{cases} \chi(v) = \dfrac{\varkappa^2 m^{*2} v^3 A \, \mathcal{E}_z \exp(-m^* v^2 / 2k_0 T)}{\pi N_I e^3 k_0 T \ln G}, \\ G = 1 + \varkappa^2 m^{*2} v^4 d^2 e^{-4} \end{cases} \qquad (7.104)$$

The relaxation time τ is related to χ by $\chi = -\tau e \mathcal{E}_z (\partial f_0 / \partial E)$. Therefore,

$$\tau = \varkappa^2 m^{*2} v^3 / \pi N_I e^4 \ln G, \qquad (7.105)$$

After carring out the integration over θ', φ' of the current density j_z:

$$j_z = \sigma_{zz}\,\mathcal{E}_z = e\int_{v=0}^{\infty}\int_{\theta'=0}^{\pi}\int_{\varphi'=0}^{2\pi} v^4 \chi \cos^2\theta' \sin\theta'\, dv\, d\theta'\, d\varphi', \qquad (7.106)$$

the conductivity takes the form

$$\sigma_{zz} = \frac{2\varkappa^2 m^{*2} A}{3 N_I e^2 k_0 T}\int_{v=0}^{\infty}\frac{v^7 \exp(-m^* v^2/2k_0T)\,dv}{\ln(1+\varkappa^2 m^{*2} v^4 d^2 e^{-4})} \qquad (7.107)$$

Since the denominator in the integrand is a slowly varying function of v, it is approximated by inserting the value of v which makes the numerator maximum. If we take $x \equiv m^* v^2/2k_0T$ as the integration variable, the numerator becomes maximum for

$$v^2 = 6k_0T/m^*. \qquad (7.108)$$

Thus, the mobility becomes

$$\mu = \frac{2^{7/2}\varkappa^2 (k_0T)^{3/2}}{N_I \pi^{3/2} e^3 m^{*1/2}}\left\{\ln(1+\beta^2)\right\}^{-1}, \quad \beta = 6\varkappa d\, k_0T/e^2. \qquad (7.109)$$

A similar result to (7.109) is obtained by introducing the screened Coulomb potential (see (2.70)),

$$U(r) = \frac{Ze^2}{\varkappa r}\, e^{-q_0 r} = \frac{4\pi Z e^2}{\Omega\varkappa}\sum_q \frac{e^{iqr}}{q^2 + q_D^2}. \qquad (7.110)$$

Matrix element between $\psi_k = e^{ikr}/\sqrt{\Omega}$ and $\psi_{k'} = e^{ik'r}/\sqrt{\Omega}$ is given by

$$U_{k'k} = \frac{4\pi Z e^2}{\Omega \varkappa} \frac{1}{|k'-k|^2 + q_D^2} = \frac{\pi Z e^2}{\Omega \varkappa k^2} \frac{1}{\sin^2(\theta/2) + (q_D/2k)^2}, \qquad (7.111)$$

where θ is the angle between k and k'.
Generally, there is the following relation between $U_{k'k}$ and $\sigma(\theta)$:

$$\sigma(\theta) = \left\{ \left(\frac{\Omega m^*}{2\pi \hbar^2}\right)^2 |U_{k'k}|^2 \right\}. \qquad (7.112)$$

Proof : The transition probability $W_{k'k}$ and $\sigma(\theta)$ is related by

$$W_{k'k} = N_I \, v \, \sigma(\theta) d\Omega_{k'}, \qquad (7.113)$$

and $W_{k'k}$ is given by

$$W_{k'k} = \Omega N_I \frac{2\pi}{\hbar} \frac{\Omega}{(2\pi)^3} \int dk' k'^2 d\Omega_{k'} |U_{k'k}|^2 \delta(E_{k'} - E_k)$$
$$= \frac{\Omega^2 N_I}{(2\pi)^2 \hbar} \frac{m^*}{\hbar^2} k |U_{k'k}|^2 d\Omega_{k'} = \frac{\Omega^2 N_I}{(2\pi)^2 \hbar^4} m^{*2} v |U_{k'k}|^2 d\Omega_{k'}. \qquad (7.114)$$

Comparing (7.113) with (7.114), we get (7.112).
Therefore, the differential scattering cross section becomes

$$\sigma(\theta) = \left(\frac{Z e^2}{2 m^* v^2 \varkappa}\right)^2 \frac{1}{\{\sin^2(\theta/2) + (q_D/2k)^2\}^2}. \qquad (7.115)$$

With $q_D \to 0$, (7.115) represents the Rutherford formula. The result due to quantum mechanical treatment is exactly equivalent to the one obtained by classical mechanics. This property is peculiar to the Coulomb potential.

The relaxation rate $1/\tau$ is connected with σ as follows:

$$\frac{1}{\tau} = 2\pi N_I v \int_0^{\pi} \sigma(\theta)(1-\cos\theta)\sin\theta d\theta$$

$$= \frac{\pi N_I}{\sqrt{2m^*}\, E^{3/2}} \left(\frac{e^2}{\varkappa}\right)^2 \left\{ \ln\left[1+\left(\frac{2k}{q_D}\right)^2\right] - \left[1+\left(\frac{q_D}{2k}\right)^2\right]^{-1} \right\}, \qquad (7.116)$$

where we put $Z=1$. From (6.91) the mobility is given by

$$\mu = \frac{e}{m^*} \frac{\sqrt{2m^*}}{\pi N_I} \left(\frac{\varkappa}{e^2}\right)^2 (k_0T)^{3/2} \frac{4}{3\sqrt{\pi}} \int_0^{\infty} dx \frac{x^3 e^{-x}}{\ln(1+\beta^2) - (1+\beta^{-2})^{-1}}, \qquad (7.117)$$

where $\beta \equiv 2k/q_D$ and $x \equiv \hbar^2k^2/2m^*k_0T$. Except the case in which k is small ($2k < q_D$) the denominator in the integrand is a slowly varying function, then in the similar way to (7.109) the mobility becomes

$$\mu = \frac{2^{7/2} e (k_0T)^{3/2}}{\varkappa^{3/2} N_I m^{*1/2}} \left(\frac{\varkappa}{e^2}\right)^2 \left\{ \ln(1+\beta_m^2) - (1+\beta_m^{-2})^{-1} \right\}^{-1}, \qquad (7.118)$$

where β_m is the value of β for $E = 3k_0T$.

According to the Debye-Hückel theory the screening length l_D (Debye length) is given by

$$l_D^{-2} = q_D^2 = \frac{4\pi n e^2}{\varkappa k_0 T}. \qquad (7.119)$$

Now, let estimate β_m. Using the parameters: $n = 10^{16}$ cm^{-3}, $T = 77$K, $\varkappa = 16$, $m^* = 0.22 m_0$ (n-Ge), we obtain

$q_D = 4.13 \times 10^5\ \mathrm{cm}^{-1}$, $2k_m = 3.39 \times 10^6\ \mathrm{cm}^{-1}$ and $\beta_m^2 = 270 \gg 1$. Then, the assumption used in deriving (7.118) is justified.

In the following we derive the Brooks-Herring formula. To be specific, we consider a n-type semiconductor with N_D donors and N_A acceptors. At the temperature below the exhaustion range shielding of an ionized center is due to the free electrons and also the rearrangement of the localized centers. Accordingly, we must replace n in (7.119) by n' which is larger than n.

If $N_A = 0$, n' should be replaced by

$$n' = n + n\left(1 - \frac{n}{N_D}\right), \qquad (7.120)$$

where $1 - n/N_D$ is the occupancy ratio of the neutral donors. In the case of $N_A \neq 0$ n in the right hand side of (7.120) is replaced by $n + N_A^-$ and n' becomes

$$n' = n + (N_D - n - N_A^-)(n + N_A^-)/N_D, \qquad (7.121)$$

where $N_A \cong N_A^-$ is assumed. Thus, we obtain the Brooks-Herring formula:

$$\mu = \frac{2^{7/2} e (k_0 T)^{3/2}}{\pi^{3/2} N_I\, m^{*\,1/2}} \left(\frac{\varkappa}{e^2}\right)^2 \left\{ \ln\left[1 + \frac{6m^*(k_0T)^2\varkappa}{\pi\hbar^2 e^2 n'}\right] - \left[1 + \frac{\pi\hbar^2 e^2 n'}{6m^*(k_0T)^2\varkappa}\right]^{-1} \right\}^{-1}, \qquad (7.122)$$

where $N_I = N_D^+ + N_A^-$. Except at low temperatures the second term in the curly bracket of (7.122) can be disregarded.

It should be noticed that n' remains finite even if $n = 0$.

This means that the Coulomb potential of an ionized center is shielded by the repopulation of the neighboring localized centers.

Relation of $\beta \equiv \beta_{cw}$ in Conwell-Weiskopf formula and $\beta_m \equiv \beta_{BH}$ in Brooks-Herring formula is as follows:

$$\beta_{cw} = \frac{k_0 T}{(e^2/6\pi\varepsilon d)}, \quad \beta_{BH} = \beta_{cw}^{1/2} \left\{ \frac{k_0 T}{(3\hbar^2/m)(d/d'^3)} \right\}, \qquad (7.123)$$

where $n' = \left(\frac{4\pi}{3} d'^3 \right)^{-1}$.

Long and Myers obtained curves of the temperature dependence of the electron mobility in a set of n-Si samples of varying impurity content N_D and compensation $K = N_A/N_D$ between 30K and 100K by combining data from electrical resistivity and Hall effect measurements.[50) The curves were used in an experimental test of the applicability of the Brooks-Herring formula.

7.9 Coulomb Scattering and Validity of the Born Approximation

In deriving Brooks-Herring formula (7.112) is employed. This relation corresponds to the first Born approximation. In this Section validity of this approximation and its relation to Rutherford formula are discussed.

Let consider the screened Coulomb potential (7.110). If the Born approximation is applicable, the condition of

$$Ua/\hbar v \ll 1 \qquad (7.124)$$

should be satisfied, where U is the average magnitude of the scattering potential and a the force range of the potential. (7.124) means that the Born approximation is applicable, if a/v which represents the time passing through the force field is enough shorter the force duration time $\hbar/U$.

From (7.119), we obtain

$$U \cong U(l_D) = \frac{Ze^2}{\varkappa l_D} e^{-1} \approx \frac{Ze^2}{\varkappa l_D}, \quad a \cong l_D = q_D^{-1}. \qquad (7.125)$$

By choosing a set of parameters for n-Si :

$m^* v^2/2 = k_0 T$, $T = 50K$. $Z = 1$, $\varkappa = 11.7$, $m^* = (m_\parallel m_\perp^2)^{1/3} = 0.3\ m_0$,

we obtain

$$Ua/\hbar v = 2.7. \qquad (7.126)$$

(7.126) violates the condition of the Born approximation. None the less, Conwell-Weisskopf and Brooks-Herring formulae qualitatively explain the observed results (see ref. 50)). This is due to the special situation of the Coulomb potential. Namely the condition of

$$e^2/\varkappa\hbar v \gg 1, \qquad (7.127)$$

which corresponds to the inapplicability of the Born approximation, just provides the condition of the classical theory being valid.

It is important to point out that in the Coulomb scattering. the classical theory, the Born approximation, and the rigorous treatment based on the quantum mechanics all give a same scattering cross section. We do not present a derivation of the rigorous formula.(51) In the following we prove (7.126).(52)

Classical particle is represented by a wave packet with an appropriate extension. The scattering angle related to an orbit is roughly determined by the magnitude of the scattering potential when the particle approaches closely to the scattering center. In Fig. 7.6 the impact parameter b roughly gives the closet distance to the scatterer.

If the wave packet moves along a classical orbit, the representative wave length λ of the wave packet must satisfy the condition of $\lambda < b$, or in other words the wave packet should be composed of a superposition of the waves with the momenta $\gg p \cong \hbar/2b$.

Accordingly, the uncertainty of the momenta is considerably larger than $\delta p \cong \hbar/2b$, and the uncertainty of the scattering angle becomes much larger than $\delta\theta \cong \delta p/p$.

If the classical description is valid, scattering angle must be much larger than $\delta\theta$. Namely, momentum change Δp due to the scattering process considerably exceeds δp:

$$\frac{\delta p}{\Delta p} \cong \frac{\hbar}{2b\Delta p} \ll 1, \qquad (7.128)$$

where Δp may be calculated from the classical mechanics. Let consider a particle moving along the x-axis at $t=-\infty$ with a momentum p. The scattering angle θ is given by

$$\sin\theta = \frac{p_y}{p}, \tag{7.129}$$

where p_y is calculated by

$$p_y = \int_{-\infty}^{\infty} K_y \, dt = \int_{-\infty}^{\infty} y \frac{K(r)}{r} \, dt. \tag{7.130}$$

$K(\mathbf{r})$ denotes the central force due to a scatterer exerted on the particle. If K is weak, the scattering angle becomes small and we obtain

$$y \cong b, \quad x \cong vt, \quad r \cong \sqrt{b^2 + v^2 t^2}. \tag{7.131}$$

Thus, $\Delta p = p_y$ is given by

$$\Delta p \cong b \int_{-\infty}^{\infty} \frac{K(r)}{r} \, dt \cong \frac{b}{v} \int_{-\infty}^{\infty} \frac{K(r)}{r} \, dx, \quad (r = \sqrt{b^2 + x^2}). \tag{7.132}$$

(7.128) is rewritten as

$$\frac{2b\Delta p}{\hbar} \cong \frac{2b^2}{\hbar v} \int_{-\infty}^{\infty} \frac{K(r)}{r} \, dx \gg 1. \tag{7.133}$$

Substituting $K(r) = e^2/\varkappa r^2$, one gets

$$\frac{4e^2}{\varkappa \hbar v} \gg 1. \tag{7.134}$$

[illegible] see Mahan, Polarons in Ionic Crystals and Semicon. (197[illegible])
p. 553-657

7.10 Piezoelectric Scattering

III - V compounds such as InSb and GaAs have the zincblende crystal lattice, while II - VI compounds, for example ZnO and CdS crystallizes in the wurzite structure. These structures are the simplest crystals lacking a center of symmetry and, hence, capable of exhibiting piezoelectric and related effects depending on polar symmetry.

Ionic characters f_i in covalent bonded crystals InSb and GaAs are estimated to be ~ 30%.[53] On the other hand, II - VI compounds have more stronger ionic character than III - V group. f_i in ZnO is 0.62 and 0.69 in CdS.[53] This situation is reflected in the magnitudes of the piezoelectric coefficients.

Piezoelectric crystals form layered structure along a certain direction. Since one type of layer is composed of A-atoms and the other layers includes only B-atoms, the lattice strain along a special direction induces the electric dipole moment and it causes electron scattering.

By choosing the strain tensor u_{ik} and electric field $\mathcal{E}$ as the independent variables, the free energy $\tilde{F}$ of a dielectrics is expressed as follows;[54]

$$\tilde{F} = F_0 + \frac{1}{2}\lambda_{iklm} u_{ik} u_{lm} - \frac{1}{8\pi}\varepsilon_{ik}\mathcal{E}_i\mathcal{E}_k - \frac{1}{4\pi}\mathcal{E}_i D_{i0} - e_{i,kl}\mathcal{E}_i u_{kl}, \tag{7.135}$$

where ε_{ik} denotes the dielectric constant tensor.

Landau-Lifshitz [illegible]

The last term represents the piezoelectric interaction. Crystals with finite $\mathbb{D}_0$ exhibit the spontaneous polarization without an external field. In this Section, we assume $\mathbb{D}_0 = 0$.

The piezoelectric interaction is effective only in highly purified crystals. In these crystals we can put div $\mathbb{D} = 0$, then $\mathbb{D}$ becomes a constant or zero. From $D_i = -4\pi\left(\partial\tilde{F}/\partial\mathcal{E}_i\right)$ and div $D = 0$, we obtain

$$\varepsilon_{ik}\frac{\partial \mathcal{E}_k}{\partial x_i} + 4\pi\, e_{i,kl}\frac{\partial u_{kl}}{\partial x_i} = 0. \tag{7.136}$$

Potential ϕ is introduced by $\phi = -\nabla\mathcal{E}$. The strain tensor u_{ik} is related to the lattice displacement $\xi(r)$:

$$u_{ik} = \frac{\partial \xi_i}{\partial x_k} + \frac{\partial \xi_k}{\partial x_i}, \quad k \neq i\,; \quad u_{ii} = \frac{\partial \xi_i}{\partial x_i}. \tag{7.137}$$

Consider a plane wave and put

$$\xi, \phi \propto e^{i(qr-\omega t)}. \tag{7.138}$$

Definition of the stress tensor s_{ik} and the equation of motion lead to

$$\left\{\begin{aligned} s_{ik} &= \frac{\partial\tilde{F}}{\partial u_{ik}} = \lambda_{ik,lm}\, u_{lm} - e_{l,ik}\,\mathcal{E}_l, \\ d\,\ddot{\xi}_i &= \frac{\partial s_{ik}}{\partial x_k} = \lambda_{ik,lm}\frac{\partial u_{lm}}{\partial x_k} - e_{l,ik}\frac{\partial \mathcal{E}_l}{\partial x_k}. \end{aligned}\right. \tag{7.139}$$

From (7.136) – (7.139) we obtain the following equations:

$$\begin{cases} \varepsilon_{ik} q_i q_k \phi - 4\pi e_{i,kl} q_i q_k \xi_l = 0 \\ d\omega^2 \xi_i = \lambda_{ik,lm} q_k q_l \xi_m + e_{l,ik} q_k q_l \phi . \end{cases} \tag{7.140}$$

By eliminating ϕ in (7.140), the equation giving the dispersion relation of sound wave is obtained and then the sound velocity is generally depends on the piezoelectric coefficients $e_{i,kl}$. The third rank tensor $e_{i,kl}$ which includes 18 independent components, is usually expressed by the contractions of the subscripts :

$$11 \to 1,\ 22 \to 2,\ 33 \to 3,\ 23 \to 4,\ 31 \to 5,\ 12 \to 6. \tag{7.141}$$

as follows

$$e = \begin{bmatrix} e_{11} & e_{12} & e_{13} & e_{14} & e_{15} & e_{16} \\ e_{21} & e_{22} & e_{23} & e_{24} & e_{25} & e_{26} \\ e_{31} & e_{32} & e_{33} & e_{34} & e_{35} & e_{36} \end{bmatrix} . \tag{7.142}$$

All components of e vanish in the crystals with inversion symmetry and the octahedral point group (O-symmetry). The piezoelectric crystals are classified into the following seven groups :[54)]

(1) triclinic system, C_1 ; (2) monoclinic system, C_s, C_2 ; (3) orthorhombic system, C_{2v}, D_2; (4) cubic system C_4, C_{4v}, D_4, D_{2d}, S_4 ; (5) rhombohedral system, C_3, C_{3v}, D_3 ; (6) hexagonal system, C_6, C_{6v}, D_6, C_{3h}, D_{3h} ; (7) trigonal system, T, T_d.

The zincblende lattice has the T_d-symmetry and the non-zero components are as follows:

$$e_{14} = e_{25} = e_{36} \,. \tag{7.143}$$

The situation is the same in the T-symmetry. The wurtzite lattice belongs to the C_{6v}-symmetry and the piezoelectric tensor $\boldsymbol{e}$ becomes

$$\boldsymbol{e} = \begin{bmatrix} 0 & 0 & 0 & 0 & e_{15} & 0 \\ 0 & 0 & 0 & e_{15} & 0 & 0 \\ e_{31} & e_{31} & e_{33} & 0 & 0 & 0 \end{bmatrix} . \tag{7.144}$$

Tables of $\boldsymbol{e}$ in other systems are listed in reference 54). Using (7.143) and $\varepsilon_{ik} = \delta_{ik}\,\varepsilon$ in the zincblende lattice, we get the piezoelectric interaction as follows:

$$\left\{ \begin{aligned} & H_{piezo} = -e \sum_q \phi_q e^{iqr}, \quad \phi_q = \frac{8\pi e_{14}}{\varepsilon} \left\{ \xi_x(q)\, n_y n_z + \text{cyclic terms} \right\}, \\ & \boldsymbol{n} = \boldsymbol{q}/q, \quad \boldsymbol{\xi}(r) = \sum_q \boldsymbol{\xi}(q)\, e^{iqr} . \end{aligned} \right. \tag{7.145}$$

Above expression was obtained by Meijer and Polder.[55) The order of magnitude of e_{ij} is expected from (7.140) to be

$$e_{ij} \sim e/a^2 \simeq 10^5 \sim 10^4, \ (\, a : \text{lattice constant}) . \tag{7.146}$$

On making use of (7.144) ϕ_q in the wurzite structure takes the form

$$\phi_q = \frac{4\pi}{\varepsilon} \left\{ n_z (n_x \xi_x + n_y \xi_y)(e_{31} + e_{15}) + n_z^2 \xi_z (e_{33} - e_{15}) + e_{15} \xi_z \right\} . \tag{7.147}$$

Bearing in mind of (7.3), we get

$$\phi_q \propto q^{-1/2}, \tag{7.148}$$

Detailed discussion on the scattering process in the wurzite crystals was given by Zook.56) In the following we calculate the relaxation time by using (7.145)55) Explicit form of the tensor λ is given by

$$\lambda \equiv \mathbf{C} = \begin{bmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{44} \end{bmatrix} \tag{7.149}$$

Secular equation for the sound velocity is obtained by eliminating ϕ in (7.140)

$$\left| d\omega^2 \delta_{ik} - \lambda_{il,km}\, q_l q_m - 4\pi (e_{l,mi}\, q_l q_m)(e_{r,sk}\, q_r q_s) / \varepsilon_{gh}\, q_g q_h \right| = 0, \tag{7.150}$$

Diagonal element (11) and non-diagonal element (12) of (7.150) are given by

$$\left\{ \begin{aligned} & d\omega^2 - (C_{11} - C_{44}) q_1^2 - C_{44} q^2 - 16\pi (e_{12}\, q_2 q_3)^2 / \varepsilon q^2, \\ & - q_1 q_2 (C_{12} + C_{44}) - 16\pi\, e_{14}^2\, q_1 q_2\, q_3^2 / \varepsilon q^2 , \end{aligned} \right. \tag{7.151}$$

and other elements are directly obtained by cyclic change of the indicies. It is difficult to solve (7.150) for a general direction of $\mathbf{q}$ and moreover, in this case the three solutions do not correspond to the pure longitudinal (l) and transverse (t) waves.

Instead of solving (7.150) for an arbitrary direction of q, we introduce a simplified treatment.

Sound velocities defined by $\omega^2/q^2 = v^2$ and ϕ_q corresponding to the three directions of q along [100], [110] and [111] are tabulated in Table 7.3.

Direction of propagation	Longitudinal wave		Transverse wave (1)		Transverse wave (2)	
	$d v_l^2$	ϕ_q	$d v_{t_1}^2$	ϕ_q	$d v_{t_2}^2$	ϕ_q
[100]	C_{11}	0	C_{44}	0	C_{44}	0
[110]	$\frac{1}{2}(C_{11}+C_{12}+2C_{44})$	0	$C_{44}+4\pi e_{14}^2/\varepsilon$	$A_q/2$	$\frac{1}{2}(C_{11}-C_{12})$	0
[111]	$\frac{C_{11}+2C_{12}+4C_{44}+16\pi e_{14}^2/\varepsilon}{2}$	$A_q/\sqrt{3}$	$\frac{C_{11}-C_{12}+C_{44}}{3}$	0	$\frac{C_{11}-C_{12}+C_{44}}{3}$	0

Table 7.3 Values of $d v^2$ and ϕ_q in the zincblende crystal for the three propagating vectors along [100], [110] and [111].$^{55)}$

In Table 7.3 A_q is given by

$$A_q = \frac{8\pi e_{14}}{\varepsilon}\sqrt{\frac{\hbar}{2d\Omega\omega}}\,(b_q + b_{-q}). \tag{7.152}$$

Table 7.3 indicates that if ϕ_q remains finite, the corresponding sound velocity depends on e_{14}. The relaxation rate due to (7.145) is given by

$$\frac{1}{\tau(E_k)} = \frac{2\pi}{\hbar}\sum_{k'}\sum_{\lambda}\Big\{\left|\langle k', n_{q\lambda}-1 \,|\, \mathcal{H}_{piezo} \,|\, k, n_{q\lambda}\rangle\right|^2 (1-\cos\theta')\,\delta(E_k - E_{k'} + \hbar\omega_{q\lambda})$$

$$+ \left|\langle k', n_{q\lambda}+1 \,|\, \mathcal{H}_{piezo} \,|\, k, n_{q\lambda}\rangle\right|^2 (1-\cos\theta')\,\delta(E_k - E_{k'} - \hbar\omega_{q\lambda})\Big\}, \tag{7.153}$$

where θ' denotes the angle between k and k' and λ represents the phonon modes. From Table 7.3 non-vanishing matrix elements $|\langle f|\mathcal{H}_{\text{piezo}}|i\rangle|^2$ are given by

$$\begin{cases} \dfrac{1}{3}\left(\dfrac{8\pi e e_{14}}{\varepsilon}\right)^2\left(\dfrac{\hbar}{2d\Omega v_l q}\right)\dfrac{k_0 T}{\hbar v_l q} & : \ l\text{-wave}, \ \mathbf{q} \parallel [111], \\ \dfrac{1}{4}\left(\dfrac{8\pi e e_{14}}{\varepsilon}\right)^2\left(\dfrac{\hbar}{2d\Omega v_{t_1} q}\right)\dfrac{k_0 T}{\hbar v_{t_1} q} & : \ t_1\text{-wave}, \ \mathbf{q} \parallel [110], \end{cases} \tag{7.154}$$

where the phonon distribution is approximated by the classical one, namely, $n_{q\lambda} \cong n_{q\lambda} + 1 \cong k_0 T/\hbar\omega_{q\lambda}$.

After carring out the integral over $|k'|$ or $E_{k'}$, the relaxation rate becomes

$$\frac{1}{\tau(E_k)} = \frac{\Omega m^* k}{2\pi^2\hbar^3}\int_0^{2\pi} d\varphi' \int_0^{\pi} d\theta' (1-\cos\theta')\sin\theta' \left\{ \left(|\langle k'|\mathcal{H}_{\text{piezo}}|k\rangle|^2\right)_l \right.$$

$$\left. + \left(|\langle k'|\mathcal{H}_{\text{piezo}}|k\rangle|^2\right)_t \right\}, \tag{7.155}$$

where the scattering processes are assumed to be elastic. $(\cdots)_l$ and $(\cdots)_t$ denote the weighted average over $\mathbf{q}/q$ shown in Table 7.3. Explicitly, $(\cdots)_l + (\cdots)_t$ is given by

$$\left\{ 6 \times |\mathcal{H}_{\text{piezo}}|^2_{[100]} + 12 \times |\mathcal{H}_{\text{piezo}}|^2_{[110]} + 8 \times |\mathcal{H}_{\text{piezo}}|^2_{[111]} \right\} /26, \tag{7.156}$$

Thus, the relaxation rate takes the following form:

$$\frac{1}{\tau(E)} = \frac{4\pi\sqrt{2}\, e^2 \sqrt{m^*}\, e_{14}^2 k_0 T}{\hbar^2 \varepsilon^2 \sqrt{E}} \left\{ \frac{16}{13\,(C_{11} + 2C_{12} + 4C_{44} + 16\pi e_{14}^2/\varepsilon)} + \frac{6}{13\,(C_{44} + 4\pi e_{14}^2/\varepsilon)} \right\}. \tag{7.157}$$

This is the expression obtained by Meijer-Polder.[55)] Similar calculation can be easily performed in the wurzite crystals. By substituting (7.157) into (6.91) the mobility is obtained as

$$\mu_{piezo} = \frac{\sqrt{2}\,\hbar^2 \varepsilon^2}{3\pi^{3/2} e\,(m^*)^{3/2} e_{14}^2 \sqrt{k_0 T}} \left[\frac{16}{13\,(C_{11} + 2C_{12} + 4C_{44} + 16\pi e_{14}^2/\varepsilon)} + \frac{6}{13\,(C_{44} + 4\pi e_{14}^2/\varepsilon)} \right]^{-1}. \tag{7.158}$$

Let estimate μ_{piezo} for InSb and GaAs at 77K. On making use of the following parameters

	ε	m^*/m_0	e_{14} (Coulomb/m^2)	C_{11} (10^{12} dyn/cm^2)	C_{12}	C_{44}
InSb	17.64	0.014	0.071	0.672	0.367	0.302
GaAs	10.82	0.07	0.16	1.188	0.538	0.594

(7.159)

we obtain

$$\mu_{piezo} = \begin{cases} 4.76 \times 10^{7}\ \text{cm}^2/\text{volt sec.} & : \text{InSb} \\ 6.29 \times 10^{5}\ \text{cm}^2/\text{volt sec} & : \text{GaAs}. \end{cases} \tag{7.160}$$

On the other hand, the mobility of InSb due to the acoustic phonon scattering is

$$\mu_{ac} = 3.08\times 10^{7}\, \mathrm{cm}^2/\mathrm{volt\ sec}, \qquad (7.161)$$

where we employ

$$d = 5.775, \quad v_s = 3.7\times 10^{5}\, \mathrm{cm/sec}, \quad D = 7.2\, \mathrm{eV} \qquad (7.162)$$

In the highly purified crystals the mobility at low temperatures is mainly controlled by the piezoelectric scattering because of $\mu_{piezo} \propto T^{-1/2}$ and $\mu_{ac} \propto T^{-3/2}$.

In Table 7.4 values of e_{ij} for several materials are shown.

	e_{31}	e_{33}	e_{15}	$e_{33}-e_{31}$
CdS	-0.244	$+0.440$	-0.210	
CdSe	-0.616	$+0.347$	-0.318	
ZnO	-0.5			1.8

Table 7.4 a. Piezoelectric coefficients in the wurzite crystals.57) e_{ij} is measured in unit of C/m^2.

	ZnS 57)	GaAs 58)	InSb 58)	InAs 58)
e_{14}	0.15	0.16	0.07	0.04

Table 7.4 b. Piezoelectric coefficients in the zincblende crystals.

It is worthy of note that substantial amplification of ultrasonic waves and non-ohmic behavior in CdS and ZnO are caused by the piezoelectric interaction.59)

7.11 Polar Optical Phonon Scattering

In Section 1.7 we have derived the electron-LO phonon interaction after the lengthy calculation along the procedures due to Born-Huang, and obtained

$$\begin{cases} H_{e\text{-}LO} = 2i\sqrt{\dfrac{\pi\alpha}{\Omega}}\,\hbar\omega_l\left(\dfrac{\hbar}{2m^*\omega_l}\right)^{1/4}\displaystyle\sum_q \frac{1}{q}\left(b_q e^{iqr} - b_q^+ e^{-iqr}\right), \\ \alpha = \dfrac{1}{2}\left(\dfrac{1}{\varepsilon_\infty} - \dfrac{1}{\varepsilon_0}\right)\dfrac{e^2}{\hbar\omega_l}\left(\dfrac{2m^*\omega_l}{\hbar}\right)^{1/2}. \end{cases} \qquad (7.163)$$

In the following the same interaction is derived by a different approach.60)

Out of phase oscillation of positive and negative ions induces the polarization $\mathbf{P}$,

$$P = E_0 \sum_q \mathbf{e}_q\left(b_q e^{iqr} + b_q^+ e^{-iqr}\right), \quad (\mathbf{e}_q = \mathbf{q}/q). \qquad (7.164)$$

The static potential $\varphi(r)$ associated with $\mathbf{P}$ is defined by

$$\varphi(r) = \sum_q \left(\varphi_q e^{iqr} + \varphi_q^+ e^{-iqr}\right). \qquad (7.165)$$

From the equations of $\mathcal{E} = -\nabla\varphi$, $\operatorname{div} D = 0$ or $\mathcal{E} + 4\pi\mathbf{P} = 0$,

we obtain

$$\varphi_q = -i\,4\pi E_0 b_q / q. \qquad (7.166)$$

Potential energies of two electrons located at $\mathbf{r}_1$ and $\mathbf{r}_2$ are

$$U(\mathbf{r}_1, \mathbf{r}_2) = -e\left[\varphi(\mathbf{r}_1) + \varphi(\mathbf{r}_2)\right]. \qquad (7.167)$$

Electron-electron interaction resulting from the second order perturbation on $U(\mathbf{r}_1, \mathbf{r}_2)$ takes the form:

$$\mathcal{H}'(r_1, r_2) = -2e^2 \sum_q \langle n_q=0 \,|\, \varphi(r_1) \,|\, n_q=1\rangle \langle n_q=1 \,|\, \varphi(r_2) \,|\, n_q=0\rangle (\hbar\omega_\ell)^{-1}$$

$$= -\frac{2e^2(4\pi E_0)^2}{\hbar\omega_\ell} \sum_q \frac{1}{q^2} e^{iq(r_1-r_2)} . \qquad (7.168)$$

Since $4\pi \sum_q e^{iqr}/q^2 = \Omega/r$, (7.168) becomes

$$\mathcal{H}'(r_1, r_2) = -\frac{8\pi E_0^2}{\hbar\omega_\ell} \frac{\Omega e^2}{|r_1-r_2|} . \qquad (7.169)$$

This is the Coulomb attractive potential via the LO-phonon exchange and it corresponds to the ionic polarizability. Therefore, (7.169) should be equal to $e^2/\varepsilon_0 r - e^2/\varepsilon_\infty r$, and we have

$$\frac{1}{\varepsilon_0} - \frac{1}{\varepsilon_\infty} = -\frac{8\pi E_0^2}{\hbar\omega_\ell}\Omega , \quad E_0 = \sqrt{\frac{\hbar\omega_\ell}{8\pi\Omega}\left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0}\right)} . \qquad (7.170)$$

This leads to the Fröhlich interaction (7.164).

As has been shown in Table 1.1, values of α in III-V compounds are usually much smaller than unity, then the perturbational calculation is applicable.. However, the scattering process is essentially inelastic except at the high temperatures as $\hbar\omega_\ell/k_0 \sim 300$K (264 K in InSb, 408 K in GaAs), and so it is not easy to solve the Boltzmann equation. One of the method getting an approximate solution is the variation method which will be discussed later.$^{61)}$

Using (7.163), one obtains the relaxation rate due to the

LO-phonon scattering as follows:

$$\frac{1}{\tau_{LO}} = \frac{e^2\omega_\ell}{\hbar}\sqrt{\frac{m^*}{E}}\left\{ n \ln\left|\frac{a+1}{a-1}\right| + (n+1)\ln\left|\frac{1+b}{1-b}\right|\right\}, \qquad (7.171)$$

where $n = (e^{\hbar\omega_e/k_0T} - 1)^{-1}$ $a = \sqrt{1+\hbar\omega_e/E}$, $b = \mathrm{Re}\sqrt{1-\hbar\omega_e/E}$.

In this case the relaxation time can not be defined, but $1/\tau_{LO}$ provides a measure of the relaxation process. In the case of $E \ll \hbar\omega_e$ τ_{LO} becomes independent on E. Phonon emitting process which is active for $E > \hbar\omega_e$ makes τ_{LO} short. With further increase of E ($E \gg \hbar\omega_e$), τ_{LO} is approximately proportional to $E^{1/2}$ because the logarithmic terms are weakly dependent on E. In the region of $E \simeq 2\hbar\omega_e, 3\hbar\omega_e$ τ_{LO} is roughly proportional to $E^{1/4}$ in consideration of the logarithmic terms. Since the transition probability from k to k' is proportional to $q^{-2} = |k-k'|^{-2}$, the small angle scatterings are very important. Therefore, the high energy electrons with $E \gg \hbar\omega_e$ exhibit strongly focussing effect in the presence of a strong electric field.[62] As is shown in Fig. 7.7,

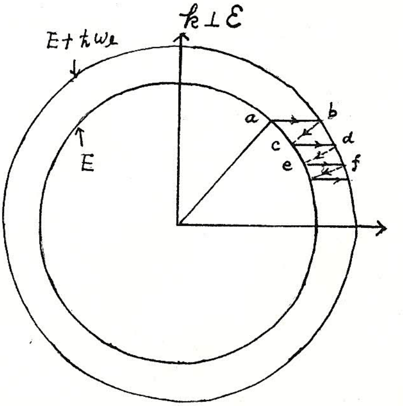


Fig. 7.7. Focussing effect due to the LO-phonon scattering.

An electron with energy E starting from a, reaches b by accerlation of the electric field and rapidly makes transition to c by emitting a LO-phonon. After passing through c → d → e → f … electrons are focussed around the direction parallel to E. This corresponds to a highly anisotropic distribution and it play an important in the high field conduction.[62]

In Fig. 7.8 temperature dependence of the Hall mobility in n-GaAs is shown. At the temperature higher than 100K the optical phonon scattering plays a dominant role. The Boltzmann equation including the LO-phonon scattering is a difference equation.

Calculated curves shown in Fig. 7.8 are obtained by solving the difference equation neumerically.[63]

In the following section we discuss on the neutral impurity scattering.

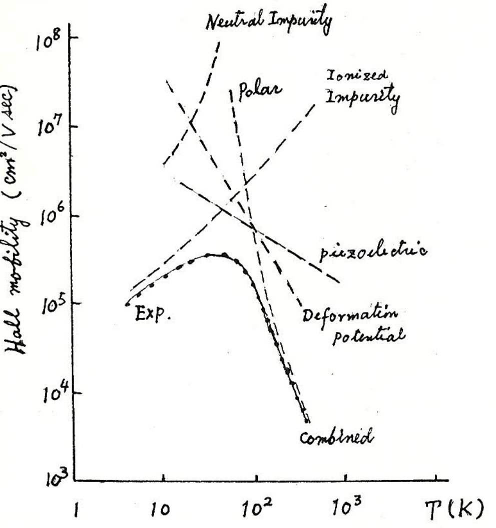


Fig. 7.8 Hall mobility of n-GaAs. Dotted lines denote the calculation due to Fletcher and Butcher.[63]

In Table 7.5 relative contributions from the various scattering mechanisms for Ⅲ-Ⅴ compounds are listed.[64]

Scattering Mechanism	InSb	InAs	InP	GaAs	GaP
LO-phonon scattering	75.1%	96.8%	94.1%	89.1%	21.4%
Acoustic phonon scattering	3.3	1.6	5.8	8.8	2.6
Piezoelectric scattering	0.6	0.2	0.1	2.1	0.3
Intervalley scattering	—	—	—	—	52.3
Electron-hole scattering	21.0	1.4	—	—	—
Hall Mobility ($cm^2/V sec$)	72,180	27,980	6,387	9,825	199

Table 7.5 Relative contributions to the Hall mobility from the various scattering processes for III-V semiconductors at 300K.64)

7.12 Neutral Impurity Scattering

If the concentration of the neutral impurity is comparable to that of the ionized centers, the neutral impurity scattering can not be disregarded as compared with the scattering due to the ionized centers and in a favorable condition the scattering probabilities due to the two processes are in same order of magnitude.

Electron-donor scattering and electron-acceptor scattering do not provide a same scattering cross section since in the former process electron exchange effect plays an important role.

At first we consider the electron-donor scattering. Consider a slowly moving electron. In this case the scattering process mainly comes from the s-wave scattering and the scattering cross section is given by

$$\sigma(\theta) = \frac{1}{k^2} \sin^2\eta_0 , \tag{7.172}$$

where η_0 is the phase shift in the zeroth order and k denotes the wave vector of the incident wave (See Appendix 1).

The incident electron exerts on the neutral center through the following two effects : (1) the electron exchange effect and (2) polarization effect of the neutral center. Among these two effects (1) is more important. Erginsoy calculated the scattering cross section of an electron by a hydrogen atom 65) by use of the Massey-Moiseiwitch theory. 66)

Let introduce the Bohr radius of a donor electron

$$a = \frac{\varepsilon \hbar^2}{4\pi m^* e^2} , \ (\varepsilon : \text{dielectric constant}). \tag{7.173}$$

In the range of $ka \leq 0.5$; the total scattering section becomes

$$4\pi \sin^2\eta_0 / k^2 = 20\, a/k . \tag{7.174}$$

Since the donor ionization energy is given by $E_I = \hbar^2/2a^2m^*$, the energy of the incident electron for $ka \leq 0.5$ corresponds to $E \leq \frac{1}{4} E_I$.

In order to obtain (7.174) it needs a lengthy calculation, then here we do not present the detail.

The relaxation time due to (7.174) is given by

$$\frac{1}{\tau_n} = N_n v \int \sigma(\theta)(1-\cos\theta)\, d\Omega = N_n v \left(\frac{4\pi}{k^2}\right) \sin^2\eta_0 = \frac{20\, \varepsilon N_n \hbar^3}{m^{*2} e^2} , \tag{7.175}$$

and the corresponding mobility becomes

$$\mu_n = \frac{e\langle\tau\rangle}{m^*} = \frac{m^* e^3}{20\,\varepsilon N_n \hbar^3}, \tag{7.176}$$

where N_n is the concentration of the neutral centers. Ratio of μ_n to the Conwell-Weisokopf mobility (7.109) is

$$\frac{\mu_{cw}}{\mu_n} = 160\sqrt{\frac{2}{\pi^3}}\,\frac{N_n}{N_I}\left(\frac{k_0 T}{m^*}\right)^{3/2}\left(\frac{\varepsilon\hbar}{e^2}\right)^3\left\{\ln\left(1+\beta_{cw}^2\right)\right\}^{-1}. \tag{7.177}$$

Let estimate it for n-InSb. Inserting $m^* = 0.014 m_0$, $\varepsilon = 17.64$ and $T = 10\,K$, we get

$$\frac{\mu_{cw}}{\mu_n} = \frac{24}{\ln(1+\beta_{cw}^2)}\left(\frac{N_n}{N_I}\right), \tag{7.178}$$

Erginsoy formula is not applicable to the electron-acceptor scattering since the electron exchange effect does not occur and the problem is formally the same as the case in a positron scattering by a hydrogen atom. According to Blagosklonskaya et al [67] the relaxation rate takes the form

$$\frac{1}{\tau(E)} = \frac{C(E/E_I)\,\hbar a}{m^*} N_A, \tag{7.179}$$

where N_A is the neutral acceptor concentration. $C(x)$ is a function represented in Fig. 7.9. If we put $N_I = N_A$ and use the comom values of a and m^*, we obtain the inequality (7.175) > (7.179).

The mobility μ calculated from (7.179) is a function of T

and it is compared with the line width of the cyclotron resonance.

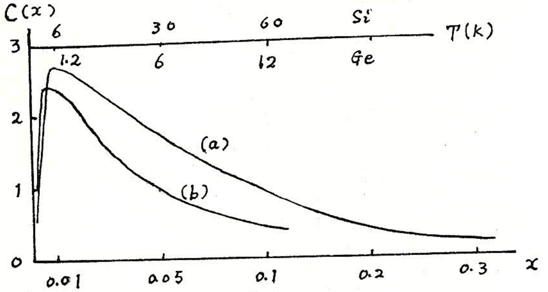


Fig. 7.9 C(x) versus x curve. In abscissa scale of x for $x > 0.1$ is enlarged by a factor of 2, where $x = E/E_I$ in (a) and $x = k_0T/E_I$ in (b). 67)

In deriving (7.179) Blagosklonskaya employed the theory due to Schwarz on the position scattering due to a hydrogen atom, 68) and (7.179) corresponds to the s-wave scattering.

In the energy range of $E/E_I \gtrsim 1/4$ the $l\,(\neq 0)$ wave scattering must be taken into consideration. In getting the relaxation time related to the mobility by $\mu = (e/m^*)\,\tau(T)$, $\tau(E)$ is inserted into (6.92) and we obtain

$$\frac{1}{\tau(T)} = \frac{C(k_0T/E_I)\,\hbar a}{m^*}\,N_A \qquad (7.180)$$

$C(k_0T/E_I)$ is shown in Fig. 7.9. In contrast with the neutral donor scattering the neutral acceptor scattering is temperature dependent.

13 Dipole Scattering due to the Ion Pairs in Compensated Semiconductors

In compensated semiconductors ionized donors (D^+) and acceptors (A^-) approach through the attractive Coulomb potentials and form the dipole moments. Usually, the contribution from the dipole scattering is negligible in comparison with the one from the ionized impurity scattering. However, if the number of ion pairs exceeds the isolated center concentration, the dipole scattering becomes important. Scattering Amplitude, which corresponds to the collision process $k(\parallel z) \rightarrow k'(\theta, \varphi)$ caused by the potential $V(r)$ is given by

$$f(\theta,\varphi) = -\frac{m^*}{2\pi\hbar^2}\int V(r)\exp(i\mathbf{K}\mathbf{r})\,d\mathbf{r}, \qquad (7.181)$$

(See Appendix 2).

Here,

$$\begin{cases} V(\mathbf{r}) = eM\cos(\hat{\mathbf{M}}\mathbf{r})/\varepsilon r^2, \\ \mathbf{K} = \mathbf{k} - \mathbf{k}', \quad K = 2k\sin(\theta/2), \end{cases} \qquad (7.182)$$

and $\mathbf{M}$ is the dipole moment of an ion-pair. Let denote the directions of $\mathbf{M}$ and $\mathbf{r}$ by (μ, ν) and (α, β).

Then,

$$\cos(\hat{\mathbf{M}}\mathbf{r}) = \cos\alpha\cos\mu + \sin\alpha\sin\mu\cos(\beta-\nu). \qquad (7.183)$$

After integration over β the term including $\cos(\beta-\nu)$ vanishes and $f(\theta,\varphi)$ becomes

$$f(\theta,\varphi) = \frac{m^* e}{\hbar^2}\,\frac{M}{\varepsilon}\cos\mu\int\exp(iKr\cos\alpha)\cos\alpha\sin\alpha\,d\alpha\,dr. \qquad (7.184)$$

Carrying out the integrations on α and r, one obtains

$$f(\theta,\varphi) = i\,\frac{2m^* e}{\hbar^2}\,\frac{M}{\varepsilon}\,\cos\mu \int_0^\infty \left\{ \frac{\cos Kr}{Kr} - \frac{\sin Kr}{(Kr)^2} \right\} dr$$

$$= -\frac{m^* e^2 L \cos\mu}{i\,\varepsilon \hbar^2 k \sin(\theta/2)}\,, \quad (M = Le). \tag{7.185}$$

Differential cross section becomes

$$\sigma_d(\theta,\varphi) = |f(\theta,\varphi)|^2 = \left(\frac{m^* e^2 L \cos\mu}{\varepsilon \hbar^2 k} \right)^2 \frac{1}{\sin^2(\theta/2)}\,. \tag{7.186}$$

As is shown in (7.98) the Rutherford formula contains $1/\sin^4(\theta/2)$, while in the dipole scattering case a factor $1/\sin^2(\theta/2)$ appears. Therefore, it is unnecessary to cut off the small angle region of θ in order to remove the divergence. Thus, the relaxation time is

$$\frac{1}{\tau_d} = \frac{\hbar k}{m^*} N_d \int \sigma_d(\theta)\,(1-\cos\theta)\,\sin\theta\, d\theta\, d\varphi\,, \tag{7.187}$$

where N_d denotes the dipole concentration.

If the carrier concentration is small enough, the screening effect is negligible and (7.187) is given by

$$\frac{1}{\tau_d} = \frac{2\pi}{3}(2kL)^2\,\frac{N_d \hbar k}{m^*}\left(\frac{e^2 m^*}{\varepsilon k^2 \hbar^2} \right)^2. \tag{7.188}$$

and the mobility becomes

$$\mu_d = \frac{2^{1/2}\,\hbar^2 \varepsilon^2 (k_0 T)^{1/2}}{\pi^{3/2} e^3 (m^*)^{3/2} N_d L^2} \propto T^{1/2}. \tag{7.189}$$

This is the expression obtained by Stratton.[69]

at high temperatures electron sees the scattering centers as the point charges since the de Broglie wave length λ is smaller than L. With decreasing temperature λ becomes longer than L and the dipole scattering becomes effective. Such examples are shown in Fig. 7.10, 70) Carrier densities n_0 at room temperature in 3, 4 and 8 samples are $10^{15} \sim 10^{16}$ cm^{-3} and they are non-degenerate even at $T \simeq 2$K, while n_0 in $18 \sim 20$ ranges from $10^{17} \sim 10^{18}$ cm^{-3} and these carriers are degenerate at helium temperature.

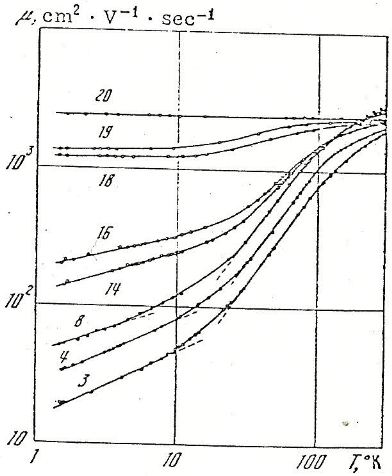


Fig. 7.10 mobility of n-GaAs. Compensation degrees K in 3.4 and 8 are larger than 90%. 70)

Mobilities of the samples with $n_0 \lesssim 10^{16}$ cm^{-3} exhibit $T^{1.5}$-dependence at $20K \lesssim T \lesssim 100K$. At the temperatures below 10K $\mu \propto T^{1/2}$ is observed. This corresponds to the dipole scattering.

Chapter 8 Band Structures of Semiconductors and Fermi Surfaces of Semimetals

8.1 Kane Model

Conduction band minima and valence band maxima of the III-V compounds such as InSb, InAs and GaAs are located at the Γ-point (0,0,0), and the conduction band at $k=0$ is s-like, while the valence band has p-character. Since the band gaps of these materials are usually small, then at the finite value of k s- and p-functions are admixed due to the $k\cdot p$-perturbation and spin-orbit interaction. Coupled secular equations was solved by Kane.71) A brief explanation on the Kane model is given in the following.

Substituting the Bloch function $\psi_k = e^{ikr}u_k(r)$ into the Schrödinger equation including the spin-orbit interaction, we obtain the equation

$$\left\{ \frac{p^2}{2m} + V + \frac{\hbar}{m}\boldsymbol{k}\cdot\boldsymbol{p} + \frac{\hbar}{4m^2c^2}[\nabla V\times\boldsymbol{p}]\cdot\boldsymbol{\sigma} + \frac{\hbar^2}{4m^2c^2}[\nabla V\times\boldsymbol{k}]\cdot\boldsymbol{\sigma} \right\} u_k = E_k' u_k, \tag{8.1}$$

where $E_k' = E_k - \frac{\hbar^2}{2m}k^2$ and $\boldsymbol{\sigma}$ denotes the Pauli spin matrix. The fourth and fifth terms in (8.1) come from the spin-orbit interaction

$$\frac{\hbar}{4m^2c^2}\left\{[\nabla V(r)\times\boldsymbol{p}]\cdot\boldsymbol{\sigma}\right\} e^{ikr}u_k(r), \tag{8.2}$$

and the fifth term is negligible as compared with the fourth term since we are interested in the small k region. The third term is the so called the $k \cdot P$ perturbation. The solution of the unperturbed equation

$$\left\{ \frac{p^2}{2m} + V(r) \right\} U_i = E_i U_i \quad , \tag{8.3}$$

must of course be known, where U_i is the wave function for the unperturbed case $k=0$ without the spin-orbit interaction.

In the zincblende structure from group theory the functions for the conduction band are singly degenerate and for the valence band are triply degenerate. The functions describing the conduction band have the symmety properties of s-function (designated S), whereas the valence band is made of p-functions x, y, z (designated X, Y, Z). Spin degeneracy gives doubly degenerate functions for the conduction band ($S\uparrow$, $S\downarrow$) and six fold degeneracy for the valence band ($X\uparrow, Y\uparrow, Z\uparrow, X\downarrow, Y\downarrow, Z\downarrow$).

In solving the secular equation two parameters P and Δ appear:

$$P = -i \frac{\hbar}{m} \langle S | p_z | Z \rangle, \quad \Delta = \frac{3\hbar i}{4m^2C^2} \langle X | \frac{\partial V}{\partial x} p_y - \frac{\partial V}{\partial y} p_x | Y \rangle , \tag{8.4}$$

where P is real and $\Delta (>0)$ denotes the spin-orbit splitting. It is convenient to choose the following unperturbed wave functions.

$$\left\{ \begin{array}{l} (A) : |iS\downarrow\rangle, |(X-iY)\uparrow/\sqrt{2}\rangle, |Z\downarrow\rangle, |(X+iY)\uparrow/\sqrt{2}\rangle, \\ \\ (B) : |iS\uparrow\rangle, |-(X+iY)\downarrow/\sqrt{2}\rangle, |Z\uparrow\rangle, |(X-iY)\downarrow/\sqrt{2}\rangle. \end{array} \right. \tag{8.5}$$

The four functions which belong to (A), are degenerate with the (B) functions. The 8×8 interaction matrix may be written

$$\begin{bmatrix} H & 0 \\ 0 & H \end{bmatrix}, \qquad H = \begin{bmatrix} E_s & 0 & kP & 0 \\ 0 & E_p - \Delta/3 & \sqrt{2}\,\Delta/3 & 0 \\ kP & \sqrt{2}\,\Delta/3 & E_p & 0 \\ 0 & 0 & 0 & E_p + \Delta/3 \end{bmatrix}, \qquad (8.6)$$

where we assume $k \parallel z$. Order of the row of H is the same as (A) or (B). E_s and E_p refer to the eigenvalues of (8.3). E_s corresponds to the conduction band E_p to the valence band. If the k is not in the z-direction, the Hamiltonian is more complicated but it can be transformed to the form of (8.6) by a rotation of the basis functions.

$$\begin{bmatrix} \uparrow' \\ \downarrow' \end{bmatrix} = \begin{bmatrix} e^{-i\phi/2}\cos\theta/2 & e^{i\phi/2}\sin\theta/2 \\ -e^{-i\phi/2}\sin\theta/2 & e^{i\phi/2}\cos\theta/2 \end{bmatrix} \begin{bmatrix} \uparrow \\ \downarrow \end{bmatrix}, \qquad (8.7)$$

$$\begin{bmatrix} X' \\ Y' \\ Z' \end{bmatrix} = \begin{bmatrix} \cos\theta\cos\phi & \cos\theta\sin\phi & -\sin\theta \\ -\sin\phi & \cos\phi & 0 \\ \sin\theta\cos\phi & \sin\theta\sin\phi & \cos\theta \end{bmatrix} \begin{bmatrix} X \\ Y \\ Z \end{bmatrix}, \qquad S' = S \qquad (8.8)$$

The angles θ, ϕ are the polar angles of the k vector refered to the crystal symmetry axes x, y and z with θ measured from z and ϕ measured from x.

The four double roots of the secular equation corresponding to

(8.6) can be written

$$E' = 0 , \quad E'(E' - E_G)(E' + \Delta) - k^2 P^2 (E' + 2\Delta/3) = 0 , \qquad (8.9)$$

where $E_s = E_G$, $E_p = -\Delta/3$, E' is defined by $E' = E - (\hbar^2/2m)k^2$ and E_G is the band gap at $k = 0$.

The solutions of (8.9) for 1) $k \approx 0$ and 2) $\Delta \gg kP$, E_G are tabulated in Table 8.1.

	1) $k \approx 0$	2) $\Delta \gg kP$, E_G
Heavy hole (v_1)	$\frac{\hbar^2 k^2}{2m}$	$\frac{\hbar^2 k^2}{2m}$
Spin-orbit split valence band (v_3)	$-\Delta + \frac{\hbar^2 k^2}{2m} - \frac{k^2 P^2}{3(E_G + \Delta)}$	$-\Delta + \frac{\hbar^2 k^2}{2m} - \frac{k^2 P^2}{3(E_G + \Delta)}$
Light hole (v_2)	$\frac{\hbar^2 k^2}{2m} - \frac{2k^2 P^2}{3E_G}$	$\frac{\hbar^2 k^2}{2m} + \frac{1}{2}E_G - \frac{1}{2}(E_G^2 + \frac{8}{3}k^2P^2)^{1/2}$
Conduction band (c_1)	$\frac{\hbar^2 k^2}{2m} + \frac{k^2 P^2}{3}\left(\frac{2}{E_G} + \frac{1}{E_G + \Delta}\right) + E_G$	$\frac{\hbar^2 k^2}{2m} + \frac{1}{2}E_G + \frac{1}{2}(E_G^2 + \frac{8}{3}k^2P^2)^{1/2}$

Table 8.1 Energy expressions for the bands from the $k.P$ perturbation. Energies are measured from the valence band edge.

The perturbing effects of higher and lower bands on the conduction and valence bands can be taken into account by second order perturbation theory. This makes the heavy hole mass reduce from m to $0.4 \sim 0.5\,m$

Since $\Delta \cong 0.8\,\text{eV}$ and $E_G \cong 0.2\,\text{eV}$ in InSb the approximation 2) is valid, whereas $\Delta \cong 0.35\,\text{eV}$ and $E_G \cong 1.54\,\text{eV}$ in GaAs.

The solutions of (8.9) for $\Delta \ll E_G$ and $kP \ll \Delta$ are

$$\begin{cases} E_c = E_G + \dfrac{\hbar^2 k^2}{2m} + \dfrac{E_G}{2}\left[\left(1+\dfrac{4k^2P^2}{E_G^2}\right)^{1/2} - 1\right], \\ E_{v_1} = \dfrac{\hbar^2}{2m}k^2 \\ E_{v_2} = \dfrac{\hbar^2 k^2}{2m} - \dfrac{2k^2p^2}{2E_G}, \\ E_{v_3} = -\Delta + \dfrac{\hbar^2 k^2}{2m} - \dfrac{k^2p^2}{3E_G}. \end{cases} \qquad (8.10)$$

(8.9) gives the energy expressions for the small k region. Qualitative feature of the energies including the Brillouin zone boundaries are shown for III − V semiconductors in Fig. 8.1.

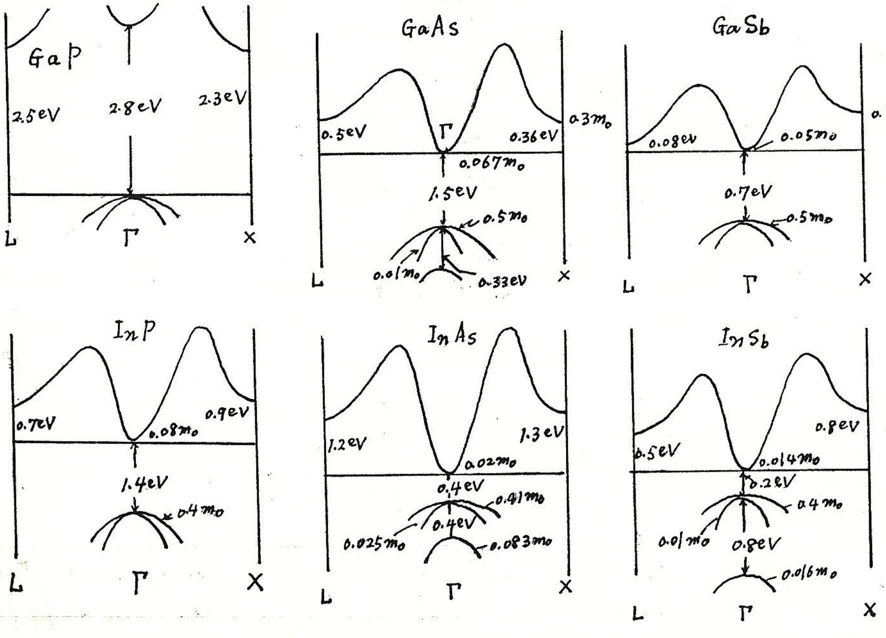


Fig. 8.1 Band structures of the III − V compounds. Spin-orbit splitting levels are shown in GaAs, InAs and InSb.

The Brillouin zone which is common to the face centered cubic, diamond lattice and zincblende structures is shown in Fig. 8.2. X- and L-points in Fig. 8.1, respectively correspond to the boundary points along [100] and [111] directions.

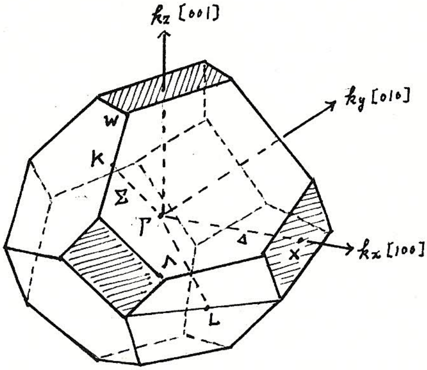


Fig. 8.2 Brillouin zone of the face-centered cubic lattice.

8.2 Band Structures and Mobilities of p-type Germanium and Silicon

The structures of the valence band edges of germanium and silicon are qualitatively similar. The band edge lies at the center of the Brillouin zone ($k=0$), at which point the band edge states have a three fold orbital degeneracy if the spin-orbit interaction is not included. We discuss briefly the band edge states in terms of a tight-binding model. Tight-binding functions are not a good approximation to the actual wave functions, but they provide a correct information on the symmetry properties of the exact solutions.

Crystal structures of Ge and Si are the diamond structure. Diamond structure is composed of the two interpenetrating fcc lattices displaced from the other by the vector $\mathbf{t} = \frac{1}{4}a(1.1.1)$, where a is the side of the cube.

At $k=0$ the tight-binding wave functions have the form

$$\Phi_i^{(\pm)}(r) = (2N)^{-1/2}\sum_n\left[\varphi_i(r-R_n) \pm \varphi_i(r-R_n-\mathbf{t})\right], \qquad (8.11)$$

where R_n runs over all the lattice points of one fcc lattice and φ_i are atomic functions with $i = s, p_x, p_y$, or p_z. By examining the transformation properties one may readily show that Φ_s^+ forms a representation of Γ_1; Φ_s^- of Γ_2'; $\Phi_{x,y,z}^-$ of Γ_{25}'; and $\Phi_{x,y,z}^+$ of Γ_{15}. Energy bands in germanium along [100] and [111] axes are shown in Fig. 8.3.72) Γ_{15} and Γ_{25}' are the threefold levels. We expect Γ_{25}' to lie below Γ_{15}.

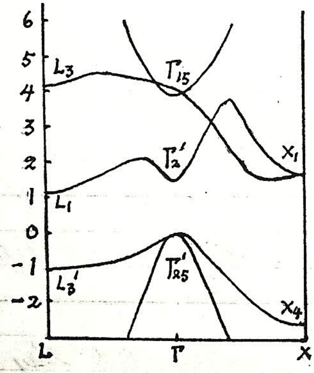
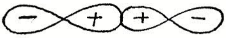


Fig. 8.3 Energy Bands of germanium.72)

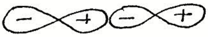
ΓL ∥ [111], ΓX ∥ [100] (See Fig. 8.2).

p-orbital for Γ_{25}' along the line joining the nearest two atoms is even under inversion at the center of the line and schematically as:



(Bonding p-orbitals),

while for Γ_{15} it is odd under inversion operation:



(antibonding p-orbitals).

We make an arbitrary choice of a basis for the representation Γ_{25}' at $k=0$, taking the three degenerate states to transform as $\varepsilon_1' \sim yz$, $\varepsilon_2' \sim zx$, $\varepsilon_3' \sim xy$.36) Since the diamond lattice has the inversion symmetry, the terms linear in k of the Hamiltonian matrix vanish. This is the essential difference between the zinc-blend lattice and the diamond lattice (See (8.6)).

The perturbation matrix has the form

$$\langle \varepsilon_r' | \mathcal{H}' | \varepsilon_s' \rangle = \frac{\hbar^2}{m^2} \sum_t{}' \frac{\langle r | k P | t \rangle \langle t | k P | s \rangle}{E_s - E_t}, \qquad (8.12)$$

where the matrix elements of p among ε_r' $(r=1.2.3)$ are all zero. We can determine the dependence of $\langle \varepsilon_r' | \mathcal{H}' | \varepsilon_s' \rangle$ on the components of k by a simple observation. If all energy denominators are equal, the sum above could be carried out, giving

$$\langle \varepsilon_r' | \mathcal{H}' | \varepsilon_s' \rangle \propto \langle \varepsilon_r' | (k.P)^2 | \varepsilon_s' \rangle .$$

Namely, we have

$$\langle 1 | \mathcal{H}' | 2 \rangle \propto k_x k_y \langle 1 | p_y p_x | 2 \rangle, \qquad (8.13)$$

with similar relations for other matrix elements.

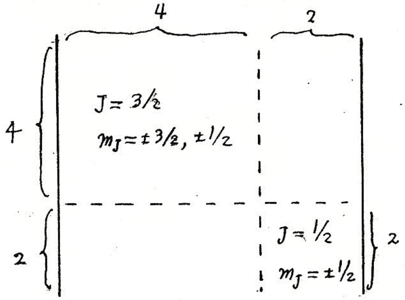
The perturbation matrix is then of the form 36)

$$\begin{vmatrix} Lk_x^2+M(k_y^2+k_z^2)-E' & Nk_xk_y & Nk_xk_z \\ Nk_xk_y & Lk_y^2+M(k_z^2+k_x^2)-E' & Nk_yk_z \\ Nk_xk_z & Nk_yk_z & Lk_z^2+M(k_x^2+k_y^2)-E' \end{vmatrix} = 0, \tag{8.14}$$

The energy eigenvalue E_k is related to root E' by $E_k = (\hbar^2/2m)k^2 + E'$. As the next step we include the spin-orbit interaction in the perturbation,

$$\mathcal{H}_{so} = \frac{\hbar}{4m^2c^2}[\nabla V \times \mathbf{P}] \cdot \boldsymbol{\sigma}, \tag{8.15}$$

and then to diagonalize the energy matrix with respect to H_{so}; the Jm_J representation is diagonal in the spin-orbit interaction. Thus, we have the new 6×6 Hamiltonian matrix:



(8.16)

The elements in the two 2×4 strips affect the roots only in the order k^4/Δ, where Δ denotes the spin-orbit splitting. Neglecting these blocks, we obtain the approximate eigenvalues of the 6×6 secular equation

$$E_{\pm}(k) = Ak^2 \pm \left[B^2k^4 + C^2(k_x^2k_y^2 + k_y^2k_z^2 + k_z^2k_x^2) \right]^{1/2}, \tag{8.17}$$

where

$$A = \frac{1}{3}(L+M) + \frac{\hbar^2}{2m}, \quad B = \frac{1}{3}(L-M), \quad C = \frac{1}{3}[N^2 - (L-M)^2], \tag{8.18}$$

Each root occurs twice, so that each of the two bands is double; this degeneracy results from the inversion symmetry of the diamond structure.

The roots of 2×2 block in (8.16) are

$$E(k) = -\Delta + Ak^2, \tag{8.19}$$

where the constant A is identical with that in (8.18) if the spin-orbit splitting Δ may be neglected in comparison with the forbidden energy gap. This approximation is valid in Si, where Δ may be of the order of 0.04 eV but in Ge Δ is thought to be about 0.3 eV.

It should be noted that if Δ in Si is of the order of 0.04 eV, the approximation neglecting the 2×4 strips in (8.16) and accordingly (8.17), (8.19) may not be an adequate approximation to describe carriers at room temperature.

The constants A, B, C are determined by analyzing the cyclotron resonance experiments. From (6.164) the cyclotron frequency $\omega_c = eH/m^*c$ is

$$\frac{2\pi}{\omega_c} = \frac{\hbar c}{eH}\oint \frac{dk}{v_\perp} = \frac{\hbar^2 c}{eH}\oint \frac{\rho\, d\phi}{(\partial E/\partial \rho)}, \tag{8.20}$$

where a cylindrical coordinate (ρ, ϕ, k_ζ), with k_ζ parallel to the magnetic field, is introduced. Then the cyclotron mass m^* becomes

$$m^* = \frac{\hbar^2}{2\pi} \oint \frac{\rho \, d\phi}{(\partial E/\partial \rho)} . \tag{8.21}$$

This is the expression of the tube mass introduced by Shockley.73) The tube mass is a function of k_ζ, but m^* with $k_\zeta \cong 0$ plays an important role in the cyclotron resonance since it remains stationary around $k_\zeta \cong 0$.

In the configuration of H parallel to a (110) plane we can easily obtain an explicit expression of (8.21). Putting $k_\zeta = 0$, we get

$$m^* = -\frac{\hbar^2}{2\pi} \int_0^{\pi/2} \frac{d\phi}{A \pm \{ B^2 + \frac{1}{4} C^2 [1 + g(\phi)] \}^{1/2}} , \tag{8.22}$$

$$g(\phi) = -(3\cos^2\theta - 1)\left[(\cos^2\theta - 3)\cos 4\phi + 2\cos 2\phi\right] , \tag{8.23}$$

where θ is the angle between H and [100] direction.

An expression in power of $g(\phi)$ gives

$$m^* = \frac{\hbar^2}{2} \frac{1}{A \pm [B^2 + (C/2)^2]^{1/2}} \left\{ 1 \pm \frac{C^2 (1 - 3\cos^2\theta)^2}{64 [B^2 + (C/2)^2]^{1/2} \{ A \pm [B^2 + (C/2)^2]^{1/2} \}} + \cdots \right\} . \tag{8.24}$$

The above expression is exact for the [111] direction ; in other directions the contribution of the next term in the expression is not greater than about 1 percent in Ge and Si

In Fig. 8.4 we give the experimental points for holes in Ge at 4K and the theoretical curves obtained from (8.24). Similar results are obtained for p-Si. The band parameters are determined as follows.

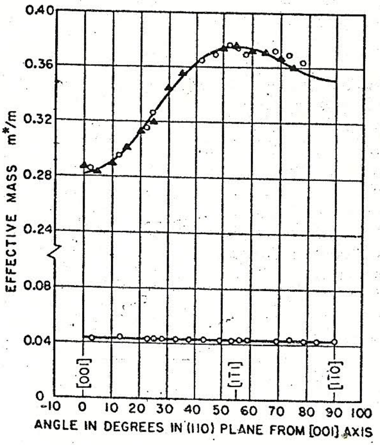


Fig. 8.4 Effective mass of holes in Ge at 4K for magnetic field directions in a (110) plane. (Dresselhaus, Kip and Kittel[36])

	Ge	Si
A	-13.27	-4.1
|B|	8.62	1.6
|C|	12.4	3.3

Table 8.2 The band paramters A, B, C for holes in Ge and Si. (Unit is measured in $\hbar^2/2m$.)

As shown in Fig. 8.4 the light hole has an isotropic mass $m^* \cong 0.04\, m_0$ while the heavy hole mass is anisotropic and nearly equal to $0.3\, m_0$. Such a large difference between these effective masses makes the Hall effect and magnetoresistance strongly field-dependent.[74)] Let designate carrier densities and mobilities for the heavy and light holes by n_h, n_ℓ and μ_h, μ_ℓ. In weak magnetic field limit the Hall coefficient and magnetoresistance are given by

$$R_{H\to 0} = \frac{3\pi}{8|e|n_h} \frac{1+(n_l/n_h)(\mu_l/\mu_h)^2}{[1+(n_l/n_h)(\mu_l/\mu_h)]^2}, \tag{8.25}$$

$$\lim_{H\to 0} \frac{1}{H^2}\left(\frac{\Delta\rho}{\rho_H}\right) = \frac{9\pi}{16}(\mu_h)^2\left[\frac{1+(n_l/n_h)(\mu_l/\mu_h)^3}{1+(n_l/n_h)(\mu_l/\mu_h)} - \frac{\pi}{4}\left\{\frac{1+(n_l/n_h)(\mu_l/\mu_h)^2}{1+(n_l/n_h)(\mu_l/\mu_h)}\right\}^2\right]. \tag{8.26}$$

Transition probability is proportional to the density of states of the final state. Therefore, the transitions to the light hole band $l \to l$, $h \to l$ are neglected as compared with the transitions $l \to h$, $h \to h$. Since the relaxation times of the heavy and light holes are nearly equal, we have

$$\mu_l/\mu_h \cong m_h/m_l \tag{8.27}$$

Using the relation

$$n_l/n_h = (m_l/m_h)^{3/2}, \tag{8.28}$$

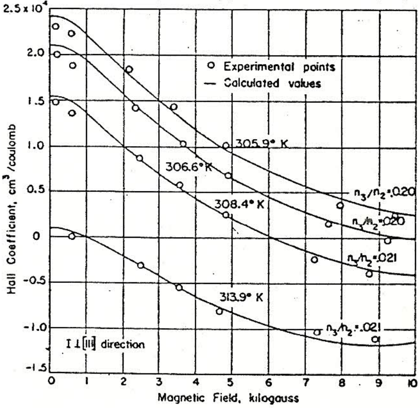
we can estimate $R_{H\to 0}$ and $\lim_{H\to 0}(\Delta\rho/H^2\rho_H)$ from (8.25) and (8.26),

$$R_{H\to 0} = \frac{3\pi}{8|e|n_h} \times 2.0, \quad \lim_{H\to 0}\frac{1}{H^2}\left(\frac{\Delta\rho}{\rho_H}\right) = \frac{9\pi}{16}(\mu_h)^2 \times 10. \tag{8.29}$$

This result indicates that contribution of the light holes to the Hall and magnetoresistance effects are very important in spite of its small concentration ($n_l/n_h \sim 0.04$). Especially, it is more important in the magnetoresistance effect.

In a finite field strength at which the condition of $\omega_l \tau > 1$

is satisfied ($\omega_l = eH/m_l c$), the light hole contribution decreases and as the result R and $\Delta\rho/H^2\rho_H$ become very small. Though (6.125) and (6.126) are the expressions for the degenerate system, they give the qualitative feature of R and $\Delta\rho/H^2\rho_H$. In Figs. 8.5 and 8.6 we can see the observed results on R and $\Delta\rho/H^2\rho_H$ due to Willardson et al.[74] By choosing appropriate values of n and μ, the good agreement with the experimental results is obtained.



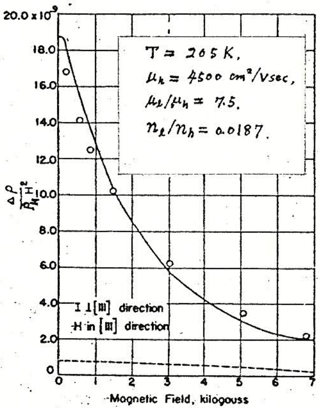


Fig. 8.5 R versus H curves for a p-type Ge specimen, where n_2 denotes the heavy hole concentration and n_3 the light hole density. Contribution from the conduction band electrons is included.

Fig. 8.6 $\Delta\rho/H^2\rho_H$ versus H curve. for a p-type Ge specimen. ‧ ‧ ‧ indicates the contribution from the heavy holes only.

To calculate the mobility of p-type germanium in consideration of the band structure is a laborius task. Here, we present a simple treatment due to Brown-Bray.[75)] Their calculation is based on the two assumptions: (1) Phonon scattering relaxation times are equal for the light and heavy holes. This is due to the large density of states of the heavy hole. (2) Cross section of the ionized impurity scattering is given by the Brooks-Herring formula and the transitions are limited to the intra-band scattering. Because the scattering matrix element includes a factor $|k-k'|^2$ in the denominator.

Below 70K the mobility of p-Ge with small impurity concentration is expressed by

$$\mu_{ac} = 3.37 \times 10^7 \, T^{-3/2} \ \mathrm{cm^2/V\,sec}. \qquad (8.30)$$

Introducing an adjustable parameter A, we write

$$\tau_{ac} = A T^{-1} E^{-1/2} . \qquad (8.31)$$

(See (7.15)). At the temperatures above 70K the optical phonon scattering becomes important and the relaxation rate is given by

$$\frac{1}{\tau_{op}} = \frac{1}{\tau_{ac}} \frac{B}{A} \frac{\Theta_0}{T} \left\{ n\left(1+\frac{k\Theta_0}{E}\right)^{1/2} + (n+1)\,\mathrm{Re}\left(1-\frac{k\Theta_0}{E}\right)^{1/2} \right\}, \qquad (8.32)$$

, where $\Theta_0 = 430\,K$ (See (7.77)). B/A value is determined in comparison with the observed mobility $\mu_p = 1.05 \times 10^9 \, T^{-2.3}$ for $120K < T < 300K$, and B/A is obtained to be 1.9.

At low temperatures where the ionized impurity scattering is important, we can estimate $N_A - N_D$ by using (8.31) and the

Brooks – Herring formula.

8.3 Fermi Surfaces of Bismuth, Antimony and Arsenic

These three crystals are semimetallic and they have a similar rhombohedral crystal structure which is formed from the simple cubic structure by a small distortion. Point group belongs to $R\bar{3}m$ (D^5_{3d}) with two atoms in unit cell. Angle α between two fundamental vectors in fcc lattice is 60°, while in the arsenic structure α is slightly smaller than 60°. The two atoms in unit cell are located at $(0,0,0)$ and $(2u, 2u, 2u)$. Values of α, u and lattice constant a are given in Table 8.3. The crystal structure and Brillouin zone are shown in Figs. 8.7 and 8.8.

	α	u	a (Å)
Bi	57° 14.2′	0.237	4.746
Sb	57° 6.5′	0.233	4.507
As	54° 10′	0.226	4.131

Table 8.3 Lattice parameters of Bi, Sb and As. u is equal to 0.25 for fcc structure.

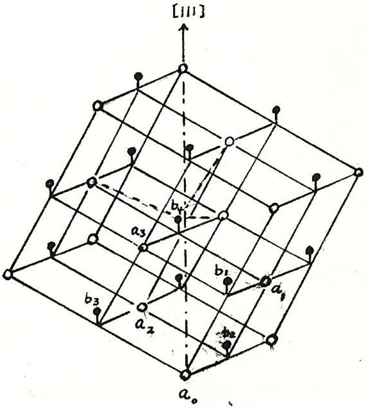


Fig. 8.7 Arsenic structure.

$\alpha = (\widehat{a_0 a_1, a_0 a_2})$. $a_0 a_1 = a$.

Three white atoms connected to b_4 by dotted lines are the nearest neighbor atoms of b_4 atom.

Little differences in the shape of the Brillouin zone occurs between Bi, Sb and As due to the small differences in the lattice parameters given in Table 8.3, but the general shape is the same. L point in the Brillouin zone of the fcc structure (see Fig. 8.2) has higher symmetry, whereas in the arsenic structure L corresponds to a lower symmetry point.

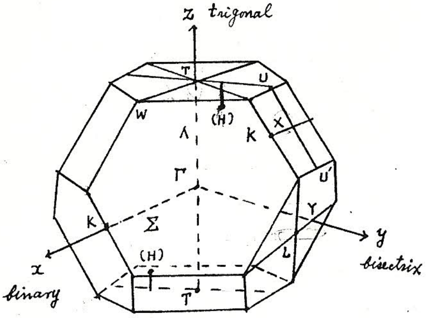


Fig. 8.8 Brillouin zone for Bi. Sb and As. H point indicates the position of hole in Sb.

ΓT-axis is a trigonal axis. There are three binary axes TW which are perpendicular to the mirror plane and three bisectrix axes TU which lie in the mirror plane.

Bi, Sb and As have two atoms per unit cell and five electrons per atom ($((S)^2(P)^3)$). Then, there are sufficient valence electrons to fill completely five bands. Small lattice distortion makes the bands at the L points lower and them at the T points raise. Hence, electron pockets should appear at the L points and hole pockets at the T points. This is just the case corresponding to Bi and Sb. In the case of As electron pockets locate at the L points but the hole Fermi surface extends over a wide region in the Brillouin zone.

Deviation of u from 2.5 and α from 60° is a measure of the distortion and the trend of increase of band overlap from Bi through Sb to As is consistent with the magnitudes of the lattice distortion.

The hole Fermi surfaces in Bi are located at the T point and its shape is an elongated ellipsoid along the trigonal axis.

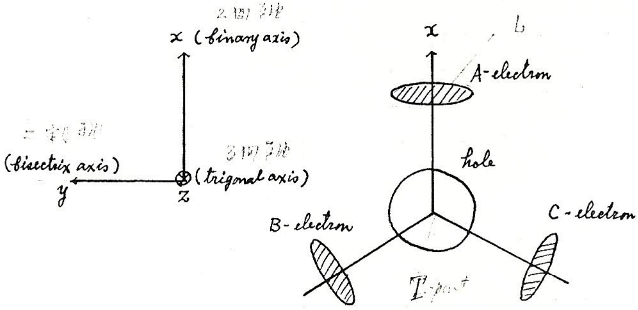


Fig. 8.9 Electron and hole Fermi surfaces in Bi.

There are three electron ellipsoids near the L points. Axis of the ellipsoid is slightly tipped from the bisectrix axis to the trigonal axis. Rotations of 120° and 240° about the trigonal axis transform the A-ellipsoid into the B- and C- ellipsoids (See Fig. 8.9).

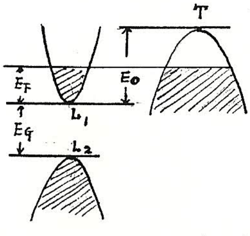


Fig. 8.10 Band structure of Bi.

The Fermi energy and overlapping energy of Bi are

$$E_F = 27.6 \text{ meV}, \quad E_0 = 38.5 \text{ meV}.$$

L_2 band is located at 15 meV below the electron L_1 band and we should solve the secular equation of the coupled bands L_1 and L_2 in order to obtain the electron energy.76.77)

Let denote the time reversal degeneracy (spin degeneracy) by 1, 2 and specify the L_1- and L_2-bands by c and v. There are, therefore, four band edge wave functions at the L-point,

$$\phi_i = e^{ik_0 r} u_i , \qquad (8.33)$$

where k_0 is the wave vector at the L-point and $U_1 = U_{c1}$, $U_2 = U_{c2}$, $U_3 = U_{v1}$, $U_4 = U_{v2}$. (8.33) are eigenfunctions of the one-electron Hamiltonian

$$H = \frac{p^2}{2m} + V + \frac{\hbar}{4m^2c^2} [\nabla V \times P] \cdot \sigma . \qquad (8.34)$$

To calculate the wave function, Φ_k of an electron with k near k_0 in the Brillouin zone we write

$$\Phi_k(r) = e^{ikr} u_k(r) \qquad (8.35)$$

and expand u in terms of the four periodic band-edge functions u_i. We may then write

$$u_k(r) = \sum_{i=1}^{4} \varphi_k^{(i)} u_i \qquad (8.36)$$

Perturbation comes from the third and fifth terms in (8.1). By using the notation of $\Delta k = k - k_0$ and the velocity operator v, the perturbation is expressed by

$$\mathcal{H}' = \hbar \Delta k \cdot v , \quad v = \frac{p}{m} + \frac{\hbar}{4m^2c^2}\left[\sigma \times \nabla V\right]. \tag{8.37}$$

(8.36) is now substituted into the Schrödinger equation and the secular equation becomes

$$\begin{array}{cccc} u_1 & u_2 & u_3 & u_4 \\ \end{array}$$

$$\begin{vmatrix} -E' & 0 & \hbar\Delta k\langle 1|v|3\rangle & \hbar\Delta k\langle 1|v|4\rangle \\ 0 & -E' & \hbar\Delta k\langle 2|v|3\rangle & \hbar\Delta k\langle 2|v|4\rangle \\ \hbar\Delta k\langle 3|v|1\rangle & \hbar\Delta k\langle 3|v|2\rangle & -E_G-E' & 0 \\ \hbar\Delta k\langle 4|v|1\rangle & \hbar\Delta k\langle 4|v|2\rangle & 0 & -E_G-E' \end{vmatrix} = 0, \tag{8.38}$$

where $E' + (\hbar\Delta k)^2/2m = E$. Cohen and Blount[78)] use the notation

$$t = \langle 1|v|3\rangle, \quad u = \langle 1|v|4\rangle \tag{8.39}$$

Due to time reversal and inversion symmetry, we obtain

$$t = \langle 4|v|2\rangle, \quad u = -\langle 3|v|2\rangle. \tag{8.40}$$

Explanation on the time reversal operator and the proof of (8.40) are given in Appendix 3.

A straightforward calculation shows that there are two doubly degenerate roots whose values are determined by

$$E'^2 + E_G E' - \hbar^2|\Delta k.t|^2 - \hbar^2|\Delta k.u|^2 = 0. \tag{8.41}$$

Energy of the conduction band is

$$E = \frac{\hbar^2(\Delta k)^2}{2m} + \frac{1}{2}\left\{-E_G + \sqrt{E_G^2 + 4\hbar^2\left[|\Delta k.t|^2 + |\Delta k.u|^2\right]}\right\}. \tag{8.42}$$

If the second term under the square root is small compared to the first, we obtain the following approximate expression for the conduction band energy

$$\left\{ \begin{aligned} E &\cong \frac{\hbar^2(\Delta k)^2}{2m} + \frac{\hbar^2}{2m}(\Delta k.\alpha.\Delta k), \\ \alpha_{ij} &= \frac{2m}{E_G}\left(t_i t_j^* + u_i u_j^* \right). \end{aligned} \right. \tag{8.43}$$

Rewriting (8.41) in terms of α, we obtain

$$E'(1+E'/E_G) = \frac{\hbar^2}{2m}(\Delta k \, \alpha \, \Delta k), \tag{8.44}$$

where α/m corresponds to the inverse mass tensor. From (8.43) energy of the A electron pocket becomes

$$E = \frac{\hbar^2}{2m}\left(\alpha_1 k_x^2 + \alpha_2 k_y^2 + \alpha_3 k_z^2 + 2\alpha_4 k_y k_z\right), \tag{8.45}$$

where α is related to the mass tensor $\tilde{m}$ by

$$\alpha^{-1} = \frac{\tilde{m}}{m} = \frac{1}{m}\begin{bmatrix} m_1 & 0 & 0 \\ 0 & m_2 & m_4 \\ 0 & m_4 & m_3 \end{bmatrix}, \tag{8.46}$$

and

$$\left\{ \begin{aligned} &\frac{m_1}{m} = \frac{1}{\alpha_1}, \quad \frac{m_2}{m} = \frac{\alpha_3}{\alpha_2\alpha_3 - \alpha_4^2}, \quad \frac{m_3}{m} = \frac{\alpha_2}{\alpha_2\alpha_3 - \alpha_4^2}, \\ &\frac{m_4}{m} = -\frac{\alpha_4}{\alpha_2\alpha_3 - \alpha_4^2}. \end{aligned} \right. \tag{8.47}$$

Here it should be emphasized that the tensor α defined by (8.43) refers to curvatures at the bottom of the conduction band and will not yield the masses at the Fermi surfaces. These differences are quite large. One may easily show from (8.44) that the mass tensor at the Fermi surface is related to that at the band minimum by

$$\alpha_{F.S.} \cong \frac{E_G}{E_G + E_F}\,\alpha, \tag{8.48}$$

where the term of $\hbar(\Delta k)^2/2m$ is neglected. The Fermi surface of holes is expressed by the equation

$$E_0 - E_F = \frac{\hbar^2}{2m}\left\{\beta_1(k_x^2 + k_y^2) + \beta_3 k_z^2\right\}, \tag{8.49}$$

where E_0 is the overlap energy between the conduction band and the valence band. The effective mass tensor $\tilde{M}$ is diagonal and has a form

$$\beta^{-1} = \frac{\tilde{M}}{m} = \frac{1}{m}\begin{bmatrix} M_1 & 0 & 0 \\ 0 & M_1 & 0 \\ 0 & 0 & M_3 \end{bmatrix}. \tag{8.50}$$

Values of $\tilde{m}$ and $\tilde{M}$ obtained by various experiments do not provide consistent results. Putting together these results, we obtain

$$-\left\{\begin{array}{l} m_1 = 0.0067,\quad m_2 = 1.34,\quad m_3 = 0.0263,\quad m_4 = 0.142, \\ M_1 = 0.0700,\quad M_3 = 0.630, \end{array}\right. \tag{8.51}$$

and the electron and hole densities are

$$n \doteqdot p \doteqdot 2.90 \times 10^{17}\ \mathrm{cm}^{-3}. \tag{8.52}$$

Since m_2 is the same order of magnitude as the free electron mass value, the validity of the two-band model may be questionable in the heavy mass direction and the coupling of the two bands under considerations (L_1 and L_2) with another lower or higher lying bands may be important.

Electron pockets in antimony are located at the L points and the Fermi surfaces have non-ellipsoidal shape with the major axis slightly tipped from the bisectrix axis to the triad one.

Holes are located at the six equivalent H points in the vicinity of the T points and the Fermi surfaces are banana shape largely inclined from the bisectrix axis (See Figs. 8.11 and 8.12).

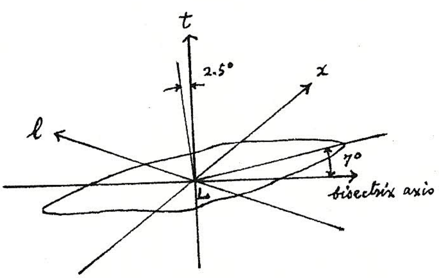


Fig. 8.11 Electron Fermi surface in Sb.

$x = \overrightarrow{\Gamma X}$, $t = \overrightarrow{\Gamma T}$, $\ell = \overrightarrow{\Gamma L}$.

Bisectrix axis – ΓT plane is the minor plane.

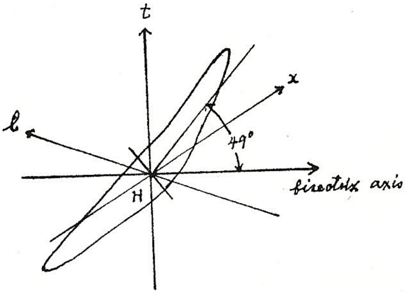


Fig. 8.12 Hole Fermi surface in Sb.

$x = \overrightarrow{\Gamma X}$, $t = \overrightarrow{\Gamma T}$, $\ell = \overrightarrow{\Gamma L}$

It is more difficult to determine the number of ellipsoids for the carriers in the cases of Sb and As since the Fermi surfaces exhibit strong departures from an ellipsoidal shape. It was clearly determined that there were twice as many carriers pockets of one carrier sign as of the other. Carrier signs in Sb were identified by Ishizawa and Tanuma.79) In their experiments the Fermi level was changed by the doping of pure antimony with very small amounts of either the electron acceptor tin or the electron donor tellurium.

The effect of this on the size of the pockets of each carrier was determined by observing the changes in the de Haas-van Alphen periods. (Detail discussions on the de Haas-van Alphen effect will be given in Chapter 11.) In this way they determined that number of the electron pockets is three and that of the hole pockets are six.

Carrier concentration was found to be

$$n \doteqdot p \doteqdot 5.5\times 10^{19}\ \mathrm{cm}^{-3}, \tag{8.53}$$

which is two order larger than the concentration in Bi.

Approximating the Fermi surfaces by ellipsoids, we obtain80)

	$10^{-7} k_1$	$10^{-7} k_2$	$10^{-7} k_3$ (cm^{-1})
Electron	0.42	0.50	2.7
Hole	0.42	0.45	1.4

(8.54)

where k_i is (1/2) × principal axis along the i-direction.

Electron Fermi surfaces in arsenic are located at the L points, while the energy surfaces for the holes are multiply connected.81)

They are given in Figs. 8.13 and 8.14. Arsenic has four times as many carriers as does antimony and so has a large Fermi surface than that of antimony.

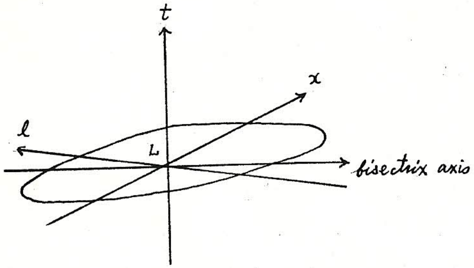


Fig. 8.13 Electron Fermi surface in As.
$t = \overrightarrow{\Gamma T}$, $l = \overrightarrow{\Gamma L}$, $x = \overrightarrow{\Gamma X}$

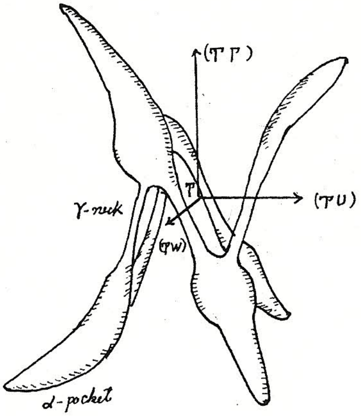


Fig. 8.14 Hole Fermi surface in As. α-pockets are connected by six thin γ-necks.

Carrier concentration in As is

$$n \doteqdot p \doteqdot 2.12 \times 10^{20}\ \mathrm{cm}^{-3} \tag{8.55}$$

Effective masses approximated by the ellipsoid model and the Fermi energies in Sb and As are shown in Table 8.4.[82)]

	antimony		Arsenic		
	electron	hole	electron	α-hole	γ-hole
m_1'	0.093	0.068	0.135	0.106	0.046
m_2'	1.14	0.92	1.52	1.56	0.016
m_3'	0.088	0.050	0.127	0.089	-1.82
E_F (meV)	96	104	190.5	177	10.6

Table 8.4 Effective masses of electrons and holes and Fermi energies for Sb and As.

8.4 Band Structure and Fermi Surface of Graphite

Graphite is a typical semimetal with layer structure and the band structure, Fermi surface and electronic properties have been extensively investigated.

The crystal structure and Brillouin zone are shown in Figs. 8.15 and 8.16.

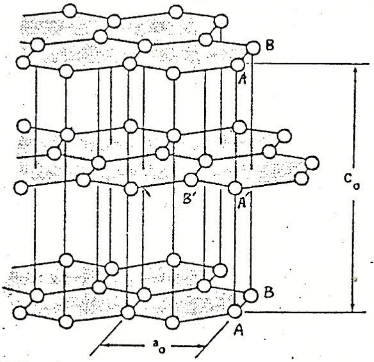


Fig. 8.15 Crystal structure of graphite. $C_o/2 = 3.354$ Å, $a_o = 2.46$ Å. unit cell volume is $\sqrt{3}\,a_o^2\,C_o/2$.

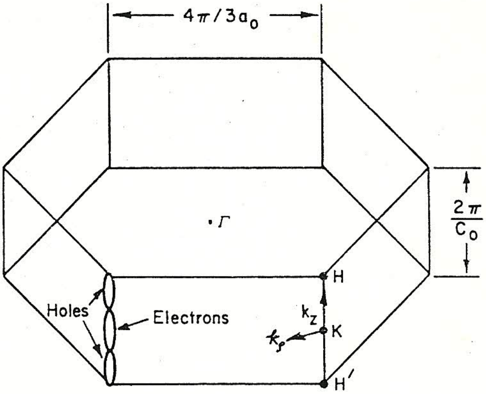


Fig. 8.16 Brillouin zone and Fermi surface of graphite. Brillouin zone volume is $16\pi^3/(\sqrt{3}\,a_o^2\,C_o)$.

Fermi surface is located along the edge HKH' and the Hamiltonian near HKH' is well described by the Slonczewski-Weiss[8-3)] and McClure[84] model.

Fig. 8.15 shows the stacking sequences 1212⋯. A and A' type atoms have neighbors directly above and below in adjacent planes, while B and B′ atoms have no corresponding neighbors. The unit cell contains four atoms (labeled A B A′B′ in Fig. 8.15).

As shown in Fig. 8.15, the spacing between adjacent layers is large and as a first approximation a single two-dimensional model which neglects any interaction between adjacent layers, will provide a qualitative feature of the energy band structure.

Therefore, to describe the properties along the c-direction the calculation based on the LCAO model is employed. On the other hand in the basal plane electrons can move freely, then it is not a good approximation to describe these electrons in terms of the tight binding approximation. As far as we are concerned with the symmetrical properties, the tight binding calculation is useful if we consider the resonance integrals as parameters to be determined in comparison with the experiments.

Consider the $2p_z$ orbitals localized at A, A′, B and B′ sites and denote the corresponding Bloch sums for $k_x = k_y = 0$ by a, a′, b and b′ We choose the following four basis:

$$\psi_1 = \frac{1}{\sqrt{2}}(a+a'),\quad \psi_2 = \frac{1}{\sqrt{2}}(a-a'),\quad \psi_3 = b,\quad \psi_3' = b'. \tag{8.56}$$

(8.56) are the functions along the vertical edge HKH′.

Introducing the $\mathbf{k}.\mathbf{p}$-perturbation, where $k \equiv (k_\rho, 0)$, $k_\rho \equiv (k_x, k_y)$

we obtain the Hamiltonian matrix

$$\mathcal{H} = \left(\begin{array}{cccc} E_1 & 0 & H_{13} & H_{13}^* \\ 0 & E_2 & H_{23} & -H_{23} \\ H_{13}^* & H_{23}^* & E_3 & H_{33} \\ H_{13} & -H_{23}^* & H_{33}^* & E_3 \end{array}\right) \begin{array}{c} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_3' \end{array} , \qquad (8.57)$$

where

$k_\rho e^{i\alpha} = k_y + i k_x$

$$\left\{\begin{array}{l} E_{1(2)} = \Delta \pm 2\gamma_1 \cos\varphi + 2\gamma_5 \cos^2\varphi , \\ E_3 = 2\gamma_2 \cos^2\varphi , \\ H_{13} = -\eta_0 (1-\nu) k_\rho e^{i\alpha}/\sqrt{2} , \quad H_{23} = \eta_0 (1+\nu) k_\rho e^{i\alpha}/\sqrt{2} , \\ H_{33} = 2\eta_3 k_\rho \cos\varphi \, e^{i\alpha} , \end{array}\right. \qquad (8.58)$$

$$\left\{\begin{array}{l} \varphi = k_z c_0/2 , \quad \eta_0 = \sqrt{3}\,\gamma_0 a/2 , \quad \eta_3 = \sqrt{3}\,\gamma_3 a/2 , \\ \nu = 2\cos\varphi \, \gamma_4/\gamma_0 . \end{array}\right. \qquad (8.59)$$

α is the angle between $\mathbf{k}_\rho$ and k_y axis. Physical meanings of the band parameters and their magnitudes are listed in Table 8.5.

γ_0	γ_1	γ_2	γ_3	γ_4	γ_5	Δ
In-plane nearest neighbor (AB) interaction.	nearest layer interaction between A and A'. atoms.	next nearest layer interaction between B and B atoms	Interlayer interaction between A and B' atoms.	Interlayer interaction producing differences in valence and conduction band	Next nearest layer interaction between A and A atoms.	Shift resulting from differences in A and B atom sites
3.16 eV	0.39	−0.020	0.30	0.044	0.038	−0.008

Table 8.5 Band parameters of Graphite

The secular equation of the Hamiltonian (8.57) are factorized into two second order solutions, if the parameter γ_3 is neglected,

$$\begin{cases} E_1^{\pm} = (E_1 + E_3)/2 \pm \left[(E_1 - E_3)^2/4 + \eta_0^2 (1-\nu)^2 k_\rho^2 \right]^{1/2}, \\ E_2^{\pm} = (E_2 + E_3)/2 \pm \left[(E_2 - E_3)^2/4 + \eta_0^2 (1+\nu)^2 k_\rho^2 \right]^{1/2}. \end{cases} \tag{8.60}$$

Variations of E_1, E_2 and E_3 along the zone edge HKH' and $E_1^{\pm}$, $E_2^{\pm}$ vs k_ρ curves for a fixed φ-value are shown in Fig. 8.17. The Fermi surface with the trigonal warping introduced by the parameter γ_3 is depicted in Fig. 8.18.

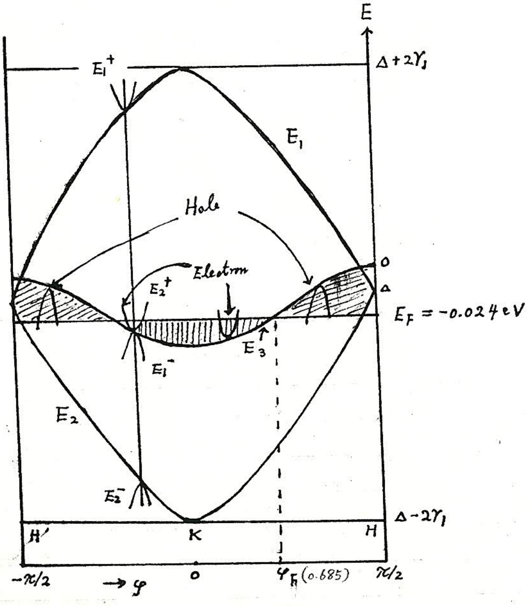


Fig. 8.17 Dispersion relation of π-bands of graphite

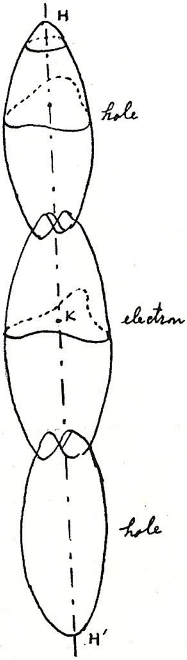


Fig. 8.18 Fermi surface of graphite

If the parameter $\gamma_3 \neq 0$, deviation from the circular cross section becomes important in the vicinity of the K-point ($\varphi = 0$), and the cross section perpendicular to k_z-axis is trigonally symmetric. The trigonal warping of the bands has important effects on the diamagnetic susceptibility and transport properties. For simplicity, we assume $\gamma_3 = 0$.

In the region except $\varphi \cong \pm\pi/2$ the first term under the square root in (8.60) is larger than the second. Expanding the square root, we get the approximate expressions:

$$\left\{\begin{aligned} E_1^{\pm} &\doteqdot \begin{pmatrix} E_1 \\ E_3 \end{pmatrix} \pm \frac{\eta_0^2(1-\nu)^2 k_\rho^2}{E_1 - E_3}, \\ E_2^{\pm} &\doteqdot \begin{pmatrix} E_3 \\ E_2 \end{pmatrix} \pm \frac{\eta_0^2(1+\nu)^2 k_\rho^2}{E_3 - E_2}. \end{aligned}\right. \qquad (8.61)$$

At the temperatures $T \ll T_F = E_F/k_0$ carriers participating in the conduction phenomena are E_2^+-electrons and E_1^--holes (see Fig. 8.17), and their effective masses in the basal plane are given by

$$\frac{1}{m^*(E_1^-)} = \frac{2}{\hbar^2}\,\frac{\eta_0^2(1-\nu)^2}{E_1 - E_3}, \qquad \frac{1}{m^*(E_2^+)} = \frac{2}{\hbar^2}\,\frac{\eta_0^2(1+\nu)^2}{E_3 - E_2}. \qquad (8.62)$$

$m^*(E_1^-)$ and $m^*(E_2^+)$ are functions of φ and become very small in the vicinity of $\varphi = \pm\pi/2$. These behaviors are shown in Fig. 8.19.

As is expected from the highly anisotropic crystal structure, many physical properties exhibit marked anisotropy. For example the resistivity ρ_c along the c-axis is higher than the basal plane resistivity ρ_a and its ratio ρ_c/ρ_a takes the values $10^2 \sim 10^3$. Such a large anisotropy stems from the effective mass difference along the two directions. In Figs. 8.19 and 8.20 m_a^* and m_z^* vs k_z curves are shown.85) These curves show that $m_a^* \approx 10^{-2} m_z^*$. Ratio of the major axis to the minor one in the electron Fermi surface is found to be 17:1, while in the hole Fermi surface the corresponding ratio is 12:1.

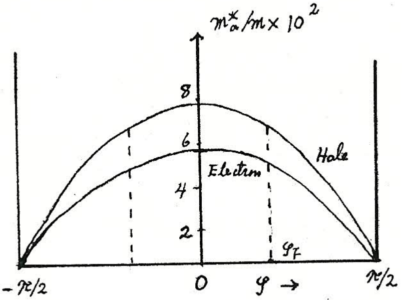


Fig. 8.19 k_z- dependences of the effective masses in the basal plane. 85)

Total carrier concentration at 0°K is

$$n + p \doteqdot 5 \times 10^{18}\ \mathrm{cm}^{-3}. \qquad (8.63)$$

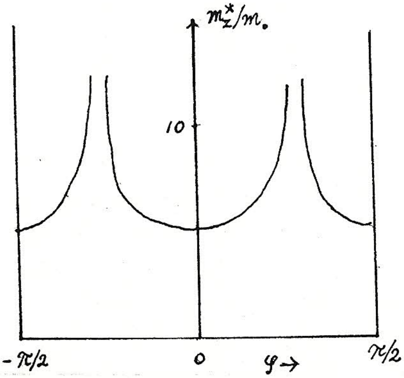


Fig. 8.20 k_z – dependence of the effective mass along the c- axis. 85)

Chapter 9 Boltzmann-Bloch Equation

9.1 Conductivity of Monovalent Metals with an isotropic Effective Mass

The Boltzmann-Bloch equation (6.7) is explicitly written down in terms of the electron-phonon interaction (7.4)

$$\left(\frac{\partial f(k)}{\partial t}\right)_{coll} = \frac{2\pi}{\hbar} D^2 \sum_q \left(\frac{\hbar q^2}{2d\Omega\omega_q}\right)\Big\{ \big[n_q f(k-q)(1-f(k)) - (n_q+1) f(k)(1-f(k-q))$$

$$\times\, \delta(E_k - E_{k-q} - \hbar\omega_q) + \big[(n_q+1) f(k+q)(1-f(k)) - n_q f(k)(1-f(k+q))\big]$$

$$\times\, \delta(E_k - E_{k+q} + \hbar\omega_q) \Big\}. \qquad (9.1)$$

Throughout this Section we assume that the phonon system is in thermal equilibrium, and then $n_q = n_{-q} = (e^{\beta\hbar\omega_q} - 1)^{-1}$. Rewriting the first term in the curly bracket by putting $q \to -q$, we obtain

$$\left(\frac{\partial f(k)}{\partial t}\right)_{coll} = \frac{2\pi}{\hbar} D^2 \sum_q \left(\frac{\hbar q^2}{2d\Omega\,\omega_q}\right)\Big\{ \big[n_q f(k+q)(1-f(k)) - (n_q+1) f(k)(1-f(k+q))\big]$$

$$\times\, \delta(E_k - E_{k+q} - \hbar\omega_q) + \big[(n_q+1) f(k+q)(1-f(k)) - n_q f(k)(1-f(k+q))\big]$$

$$\times\, \delta(E_k - E_{k+q} + \hbar\omega_q) \Big\}. \qquad (9.2)$$

In general the phonon distribution is deviated from the thermal equilibrium and in this case $n_q \neq n_{-q}$. The case in which the deviation from the thermal equilibrium plays an important role, is treated in Chapter 14. It is easily shown that (9.1) and (9.2) become zero if the electron and phonon distribution functions are in thermal equilibrium.

We seek the solution of (9.2) in the form

$$f(k) = f_0(k) - \Phi(k)\,\frac{\partial f_0}{\partial E}. \tag{9.3}$$

By making use of the identities :

$$\begin{aligned} & n_q f_0(k+q)(1-f_0(k))\,\delta(E_k - E_{k+q} - \hbar\omega_q) \\ & = (n_q+1) f_0(k)(1-f_0(k+q))\,\delta(E_k - E_{k+q} - \hbar\omega_q), \end{aligned} \tag{9.4}$$

$$\begin{aligned} & (n_q+1) f_0(k+q)(1-f_0(k))\,\delta(E_k - E_{k+q} + \hbar\omega_q) \\ & = n_q f_0(k)(1-f_0(k+q))\,\delta(E_k - E_{k+q} + \hbar\omega_q), \end{aligned} \tag{9.5}$$

(9.2) is transformed into

$$\begin{aligned} \left(\frac{\partial f}{\partial t}\right)_{coll} = & \frac{2\pi}{\hbar k_0 T} D^2 \sum_q \left(\frac{\hbar q^2}{2 d \Omega \omega_q}\right) n_q \Big\{ f_0(k+q)(1-f_0(k))\,\delta(E_k - E_{k+q} - \hbar\omega_q) \\ & + f_0(k)(1-f_0(k+q))\,\delta(E_k - E_{k+q} + \hbar\omega_q)\Big\}\,[\Phi(k+q) - \Phi(k)]. \end{aligned} \tag{9.6}$$

(9.6) is also written in the form :

$$\left(\frac{\partial f}{\partial t}\right)_{coll} = \frac{1}{k_0 T} \sum_{k'} V(k.k')\,[\Phi(k') - \Phi(k)], \tag{9.7}$$

where

$$V(k.k') = \frac{2\pi}{\hbar} D^2 \frac{\hbar |k - k'|}{2 d \Omega\, \omega_{|k-k'|}} \frac{f_0(k) f_0(k')}{\left| e^{-\beta(E-\zeta)} - e^{-\beta(E'-\zeta)} \right|}$$

$$\times \left\{ \delta\left(E_k - E_{k'} - \hbar\omega_{|k-k'|}\right) + \delta\left(E_k - E_{k'} + \hbar\omega_{|k-k'|}\right) \right\}. \qquad (9.8)$$

(9.7) and (9.8) are the explicit expressions for (6.7) and (6.9) and the symmetry relation

$$V(k, k') = V(k', k), \qquad (9.9)$$

is satisfied.

We consider the case in which an electric field and/or temperature gradient are applied along the 1-direction, and assume $\Phi(k)$ as

$$\Phi(k) = k_1\, C(E). \qquad (9.10)$$

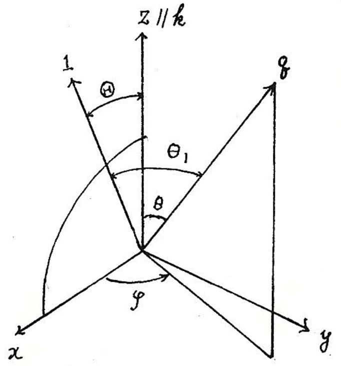


Fig. 1. 1-axis lies in the zx-plane.
($\mathcal{E} \parallel \nabla T \parallel$ 1-axis)

Configurations of k and q are shown in Fig. 9.1. From (9.10) $\Phi(k+q)$ becomes

$$\Phi(k+q) = (k_1 + q_1)\, C(E'). \qquad (9.11)$$

arguments of the δ-functions in (9.6) are

$$\frac{\hbar^2}{2m^*}\left(2kq\cos\theta + q^2\right) \pm \hbar v_s q, \qquad (9.12)$$

where $E_k = (\hbar^2/2m^*)k^2$ is assumed.

$\vec{q} = q(\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta)$

From Fig. 9.1, q_1 is given by

$$q_1 = q\cos\theta_1 = q(\sin\Theta\sin\theta\cos\varphi + \cos\Theta\cos\theta), \tag{9.13}$$

In the integration over q ($\int dq \cdots = \int dq\, q^2 \sin\theta\, d\theta\, d\varphi \cdots$) in (9.6) only $\Phi(k+q)$ depends on φ through q_1. From (9.13) and (9.12) we have

$$\int_0^{2\pi} q_1 d\varphi = 2\pi q\cos\theta\cos\Theta = 2\pi q\cos\theta\left(\frac{k_1}{k}\right), \tag{9.14}$$

$$\left\{\begin{aligned} &\int_0^{\pi} \delta(E_k - E_{k+q} \mp \hbar\omega_q)\sin\theta\, d\theta = \frac{m^*}{\hbar^2 k q}\int_0^{\pi} \delta(\cos\theta - \cos\theta_0)\sin\theta\, d\theta = \frac{m^*}{\hbar^2 k q}, \\ &\cos\theta_0 = \frac{-q \mp \frac{2m^* v_s}{\hbar}}{2k}, \quad \left| q \pm \frac{2m^* v_s}{\hbar}\right| < 2k. \end{aligned}\right. \tag{9.15}$$

Since we are interested in the electrons near the Fermi surface, we can approximate $\hbar k/m^* \simeq v_F$ (v_F : Fermi velocity). Therefore, (9.15) becomes

$$-1 \pm \frac{v_s}{v_F} < \frac{q}{2k} < 1 \pm \frac{v_s}{v_F}. \tag{9.16}$$

In monovalent metals $v_s/v_F \sim 10^{-3}$ and substantially (9.16) becomes

$$0 < q < 2k \cong 2k_F. \tag{9.17}$$

At a glance we might consider that the integration over q should be performed in the region $0 < q < 2k_F$. This is not the case because in the Debye model q is smaller than q_D. It is necessary to know which of $2k_F$ and q_D is smaller.

q_D and k_F are related to the electron concentration per unit volume :

$$\frac{1}{(2\pi)^3}\,\frac{4\pi}{3}\,q_D{}^3 = N\,. \tag{9.18}$$

$$\frac{2}{(2\pi)^3}\,\frac{4\pi}{3}\,k_F{}^3 = N\,. \tag{9.19}$$

Accordingly,

$$2k_F = 2^{2/3}\,q_D > q_D\,. \tag{9.20}$$

Namely, the integration limit for q is

$$0 < q < q_D\,. \tag{9.21}$$

On the other hand, in semiconductors or semimetals with small carrier concentration $2k$ is smaller than q_D and (9.17) should be used.

By substituting (9.15) into (9.14), we get

$$\int_0^{2\pi} q_1\,d\varphi = -\pi k_1\left(\frac{q^2}{k^2} \pm \frac{\hbar\omega_q}{2E_k}\right). \tag{9.22}$$

Thus, (9.6) is given by

$$\left(\frac{\partial f}{\partial t}\right)_{coll} = -\frac{D^2 m^* k_1}{4\pi d\hbar^2 k v_s}\,\frac{\partial f_0}{\partial E_k}\int_0^{q_D} n_q\left\{\left[\left(1+\frac{\hbar\omega_q}{E_k}-\frac{q^2}{2k^2}\right)c(E+\hbar\omega_q)-C(E)\right]\right.$$
$$\left.\times\,\frac{f_0(E+\hbar\omega_q)}{f_0(E)}\,e^{\beta\hbar\omega_q}+\left[\left(1-\frac{\hbar\omega_q}{E_k}-\frac{q^2}{2k^2}\right)c(E-\hbar\omega_q)-c(E)\right]\frac{f_0(E-\hbar\omega_q)}{f_0(E)}\right\}q^2dq. \tag{9.23}$$

If we write $\eta = (E - \zeta)/k_0 T$, $z = \hbar\omega_q / k_0 T$ and allows z to take negative as well as positive values, we obtain

$$\left(\frac{\partial f}{\partial t}\right)_{coll} = - k_1 \mathcal{L}(c) , \qquad (9.24)$$

$$\mathcal{L}(c) = - \frac{D^2 (m^*/2)^{1/2} q_D{}^3}{4\pi d \hbar v_s E_k{}^{3/2}} \left(\frac{T}{\Theta_D}\right)^3 \frac{\partial f_0}{\partial E_K} \int_{-\Theta_D/T}^{\Theta_D/T} \left\{ E_k c(\eta) - c(\eta + z) \left[E_k + \frac{1}{2} k_0 T z - E_D \left(\frac{T}{\Theta_D}\right)^2 z^2 \right] \right\}$$

$$\times \frac{e^{\eta} + 1}{e^{\eta + z} + 1} \cdot \frac{z^2 dz}{|1 - e^{-z}|} , \left(E_D \equiv \frac{\hbar^2}{4 m^*} q_D{}^2 \right) . \qquad (9.25)$$

$\mathcal{L}$ is called the collision operator. The Boltzmann-Bloch equation for $H = 0$, $\mathcal{E} \parallel \nabla T \parallel x$ takes the form

$$\mathcal{L}(c) = \frac{\hbar}{m^*} \frac{\partial f_0}{\partial E_k} \left\{ e\mathcal{E} + T \frac{\partial}{\partial x}\left(\frac{\zeta}{T}\right) + \frac{E}{T}\frac{\partial T}{\partial x} \right\} . \qquad (9.26)$$

For large values of T/Θ_D, the integrand in (9.25) is expanded in powers of z. Retaining the most important term, we obtain

$$\mathcal{L}(c) \doteqdot - \frac{D^2 (m^*/2)^{1/2} q_D{}^3 E_D}{8\pi d \hbar v_s E_k{}^{3/2}} \left(\frac{T}{\Theta_D}\right) c(\eta) \frac{\partial f_0}{\partial E_k} , \qquad (9.27)$$

and the relaxation time is given by

$$\tau = \frac{8\pi d \hbar v_s E_k{}^{3/2}}{D^2 (m^*/2)^{1/2} q_D{}^2 E_D} \left(\frac{\Theta_D}{T}\right) , \quad (T \gg \Theta_D) \qquad (9.28)$$

If E_k is replaced by $E_F\ (= \zeta)$, (9.28) is just the same as (7.20).

At very low temperatures ($T \ll \Theta_D$) we can find a simple solution of the integral solution which is sufficiently accurate to determine the electrical conductivity, but not the second-order phenomena.

If only an electric field is applied, (9.26) is rewritten as

$$E_k \frac{\partial f_0}{\partial E_k} \int_{-\Theta_D/T}^{\Theta_D/T} \left\{ c(\eta+z) - c(\eta) \right\} \frac{e^{\eta}+1}{e^{\eta+z}+1} \frac{z^2 dz}{|1-e^{-z}|} = A E_k^{3/2} \left(\frac{\Theta_D}{T}\right)^3 \frac{\hbar}{m^*} \frac{\partial f_0}{\partial E_k} e\mathcal{E}$$

$$+ \frac{\partial f_0}{\partial E_k} \int_{-\Theta_D/T}^{\Theta_D/T} c(\eta+z) \left\{ E_D \left(\frac{T}{\Theta_D}\right)^2 z^2 - \frac{1}{2} k_0 T z \right\} \frac{e^{\eta}+1}{e^{\eta+z}+1} \frac{z^2 dz}{|1-e^{-z}|}, \qquad (9.29)$$

where

$$\frac{1}{A} \equiv \frac{D^2 (m^*/2)^{1/2} q_D^3}{4\pi d \hbar v_s}.$$

At sufficiently low temperatures it is permissible to put $\Theta_D/T = \infty$. By changing the integration variable from z to $\xi = \eta + z$ in the left hand side of (9.29), (9.29) takes the form

$$c(\eta)\lambda(\eta) + \int_{-\infty}^{\infty} K(\eta, \xi)\, c(\xi)\, d\xi = F(\eta). \qquad (9.30)$$

The transposed homogeneous equation corresponding to (9.30) is given by

$$\psi(\eta)\lambda(\eta) + \int_{-\infty}^{\infty} K(\xi, \eta)\, \psi(\xi)\, d\xi = 0. \qquad (9.31)$$

Let carry out the integration $\int_{-\infty}^{\infty} d\eta\, \psi(\eta) \times (9.30)$. It is permitted to perform the integration over $(-\infty, +\infty)$, since $\zeta / k_0T \gg 1$ at very low temperatures.

Thus, we obtain

$$\int d\eta\, c(\eta)\, \psi(\eta)\, \lambda(\eta) + \iint d\eta\, d\xi\, K(\eta, \xi)\, c(\xi)\, \psi(\eta) = \int d\eta\, F(\eta)\, \psi(\eta). \quad (9.32)$$

Transforming the variables by $\xi \rightleftarrows \eta$ in the second term of the left hand side and taking into account (9.31), we obtain

$$\int d\eta\, c(\eta) \left\{ \psi(\eta)\lambda(\eta) + \int K(\xi, \eta)\, \psi(\xi)\, d\xi \right\} = \int d\eta\, F(\eta)\, \psi(\eta). \quad (9.33)$$

Accordingly,

$$\int d\eta\, F(\eta)\, \psi(\eta) = 0. \quad (9.34)$$

It is verified that the transposed homogeneous equation of (9.30) is orthogonal to the right hand side. Now let return to (9.29). We obtain a simple solution of the transposed homogeneous equation of (9.29) $c(\eta) = \text{constant} = c_0$ and c_0 is determined by

$$-A \left(\frac{\Theta_D}{T} \right)^3 \frac{\hbar}{m^*} e \mathcal{E} \int_{-\infty}^{\infty} d\eta\, E_k^{3/2} \frac{\partial f_0}{\partial E_k} = c_0 \int_{-\infty}^{\infty} d\eta\, \frac{\partial f_0}{\partial \eta} \int_{-\Theta_D/T}^{\Theta_D/T} \left\{ E_D \left(\frac{T}{\Theta_D} \right)^2 z^2 - \frac{1}{2} k_0 T z \right\}$$

$$\times \frac{e^{\eta} + 1}{e^{\eta + z} + 1} \frac{z^2\, dz}{|1 - e^{-z}|}. \quad (9.35)$$

The integration over η can be performed by use of the formula:

$$-\int_{\infty}^{\infty} d\eta\, \frac{\partial f_0}{\partial \eta}\, \frac{e^{\eta}+1}{e^{\eta+z}+1} = \int_{-\infty}^{\infty} \frac{d\eta}{(e^{\eta+z}+1)(e^{-\eta}+1)} = \frac{1}{e^{z}-1}\int_{-\infty}^{\infty}\left(\frac{1}{e^{\eta}+1} - \frac{1}{e^{\eta+z}+1}\right) d\eta$$

$$= \frac{z}{e^{z}-1}. \qquad (9.36)$$

In obtaining (9.36) we employed the following relation

$$\left\{ \begin{aligned} &\int_{-A}^{\infty} \frac{dx}{e^{x}+1} = \int_{e^{-A}}^{\infty} \frac{du}{u(u+1)} = \left| \ln \frac{u}{u+1} \right|_{e^{-A}}^{\infty} = A, \\ &\int_{-A}^{\infty} \frac{dx}{e^{x+z}+1} = \int_{e^{-A+z}}^{\infty} \frac{du}{u(u+1)} = A - z. \end{aligned} \right. \qquad (9.37)$$

Since the first term in curly bracket of (9.35) is much larger than the second term, (9.35) becomes

$$A\left(\frac{\Theta_D}{T}\right)^3 \frac{\hbar}{m^*} e\mathcal{E}\zeta^{3/2} = -c_0 E_D \left(\frac{T}{\Theta_D}\right)^2 2 \int_0^{\Theta_D/T} \frac{z^5\, dz}{(e^{z}-1)(1-e^{-z})}. \qquad (9.38)$$

Then, we have

$$c_0 = -\frac{A\zeta^{3/2}\hbar e}{2E_D m^* J_5}\left(\frac{\Theta_D}{T}\right)^5 \mathcal{E}, \quad J_n\left(\frac{\Theta_D}{T}\right) = \int_0^{\Theta_D/T} \frac{z^n\, dz}{(e^{z}-1)(1-e^{-z})}, \qquad (9.39)$$

$$\sigma = -\frac{e}{\mathcal{E}}\sum_k v_1 f_1 = \frac{e}{\mathcal{E}}\sum_K \frac{\hbar k_1}{m^*} k_1 c_0 \frac{\partial f_0}{\partial E}$$

$$= \frac{A e^2 \zeta^3}{6\pi^2 E_D m^* J_5}\left(\frac{2m^*}{\hbar^2}\right)^{3/2}\left(\frac{\Theta_D}{T}\right)^5 \quad \text{(Bloch formula)}. \qquad (9.40)$$

The specific resistivity is then expressed by

$$\rho = B\,T^5 J_5 (\Theta_D/T). \tag{9.41}$$

This is called Grüneisen formula. Reduced function defined by $f(x) = \rho(T)/\rho(\Theta_D)$ $(x = \Theta_D/T)$ is a universal function which does not include any material constants.

The limiting forms of the integral $J_5(x)$ at low and high temperatures can readily be obtained.

$$J_n(x) = \int_0^x \frac{z^n\,dz}{(e^z-1)(1-e^{-z})} = -\frac{x^n}{e^x-1} + n\int_0^x \frac{z^{n-1}}{e^z-1}\,dz. \tag{9.42}$$

For small values of x,

$$J_5(x) = \int_0^x \left(z^3 - \frac{1}{12}z^5 + \dots\right)dz = \frac{1}{4}x^4 - \frac{1}{72}x^6 + \cdots,$$

while

$$J_5(\infty) = 5\int_0^\infty \frac{z^4\,dz}{e^z-1} = 5!\sum_{n=1}^{\infty}\frac{1}{n^5} = 124.4\cdots. \tag{9.43}$$

Therefore, at low temperatures

$$\sigma \propto T^{-5}. \tag{9.44}$$

Above results are derived on the following assumptions 1) ~ 5).

1) Energy dispersion relation is assumed to be isotropic. The relation of $E_k \propto k^2$ is unnessary. 2) Phonon spectrum

is approximated by the Debye model. 3) Electrons interact only with the longitudinal acoustic phonons. 4) U-processes can be disregarded. 5) Phonon system is in thermal equilibrium.

The conditions 1) ~ 3) are not necessarily satisfied in actual metals. Here, we pay attentions to the Peierls remarks related to 4) and 5).[87)]

Peierls pointed out that in the absence of an electric field the quantity

$$S = \sum_{k} f(k)\,k + \sum_{q} n(q)\,q , \qquad (9.45)$$

is conserved as a consequence of the interference conditions $k' = k \pm q$. Now, if we have an electric field $\mathcal{E}_x$ acting on the metal, S_x changes according to $dS_x/dt = -ne\mathcal{E}_x/\hbar$. Continual supply of the crystal momentum from an electric field makes S_x infinite large unless there are other processes tending to reduce S_x. As a result the conductivity becomes infinite. Bloch theory implicitly assumed that phonon-phonon interaction due to the anharmonic terms or phonon-imperfection interaction can restore the thermal equilibrium distribution of the phonon system. If the sample is very pure the restoring process to the thermal equilibrium are ineffective at low temperatures.

In order to remove the above mentioned difficulty Peierls introduced the electron-phonon collision process called the Umklapp-process, which we have neglected so far (See (2.24)):

$$k' = k \pm q + G \quad (G : \text{reciprocal vector}), \qquad (9.46)$$

and he showed that if these more general interference conditions are included, it is possible to set up a steady state and that many of the preceding results can be re-established. Let consider these problems in detail in the following.

1. In Fig. 9.2 electron-phonon U-process in the repeated zone scheme is depicted. H is the point on the Brillouin zone boundary which is closest to the Fermi surface.

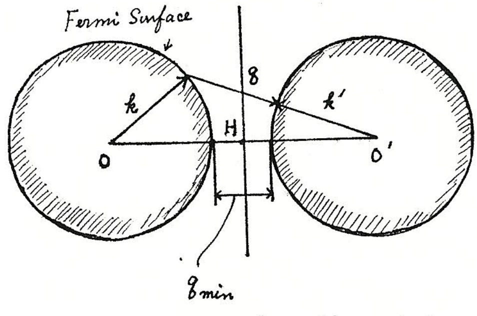


Fig. 9.2 Electron-phonon U-process in the repeated zone scheme.
$k' = k + q + G$, $G = \overrightarrow{O'O}$

minimum q value in U-process is

$$q_{min} = 2(k_H - k_F), \qquad (9.47)$$

where $k_H = OH$.

Inserting $k_F = (3/4\pi)^{1/3}(2\pi/a)$
$= 0.620\,(2\pi/a)$

and $k_H = (2\pi/a)\sqrt{(1/2)^2 + (1/2)^2 + 0} = 0.707\,(2\pi/a)$ (alkali metals)

$$q_{min} = \frac{0.547}{a}, \tag{9.48}$$

where a denotes the lattice parameter. At low temperatures when only small q phonons are excited, U-processes are "frozen out." In monovalent metals "frozen out" temperature of U-processes T_U is estimated to be

$$T_U \sim \alpha \hbar v_s q_{min}/k_0, \quad \alpha \simeq 1 \tag{9.49}$$

In sodium T_U is estimated to be 20 ~ 30K, while experimentally T^5-law is satisfied far below 20K.

2. Phonon relaxation time due to the phonon-phonon scattering is proportional to T^{-4} (See Appendix 4) and then at low temperatures it becomes less effective than the relaxation process due to electron scattering in which the relaxation time is proportional to T^{-1}. Thus, the phonon-phonon scattering processes are also "frozen out" at low temperatures. How can we explain the observed T^5-dependence at low temperatures?. Bailyn and Brooks presented a following explanation to this problem.[88)]
In alkali metals the transverse phonon velocity is about 0.4 times the longitudinal phonon velocity. Therefore, U-processes associated with the transverse phonons are active at the helium temperatures

where the longitudinal phonons no longer participate in U-processes.. Complex calculation of U-process belongs to a pure geometrical problem. Detailed calculation is given in Ziman's text book.89)

T^5-dependence of the resistivity can be easily derived from a qualitative consideration. The resistivity due to the phonon scattering is given by (See (7.12))

$$\rho = \langle | M_{kk'} |^2 n_q (1-\cos\theta) \rangle , \tag{9.50}$$

where $M_{kk'}$ denotes the remaining part of H_{e-p} (See (7.4)) excluding the phonon operators and $|M_{kk'}|^2 \propto |k'-k| = q$ and θ is the angle between k and k'. Most of the phonons excited at low temperatures have wave vectors $q \approx k_0 T/\hbar v_s$. Since the scattering processes are limited in the vicinity of the Fermi surface, we have $(1-\cos\theta) \fallingdotseq q^2/2k_F^2$. Then, $|M_{kk'}|^2 (1-\cos\theta) \propto q^3 \propto T^3$. Integration on q is performed over the shaded area which is surrounded by a circle formed by crossing between the Fermi surface and the small sphere with radius q. This area is roughly given by $\pi q^2 \propto T^2$. In combining

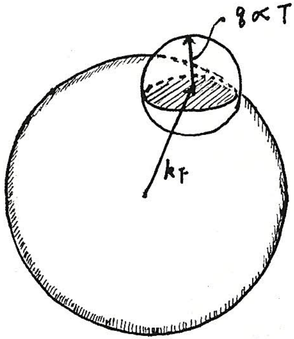


Fig. 9.3 Electron-phonon scattering at low temperatures.

with $|M_{kk'}|^2(1-\cos\theta)$, we obtain T^5-dependence of the resistivity. Above considerations show that T^5-dependence at low temperatures is a general law not restricted to the metals with spherical Fermi surface. If the shaded region is entirely on the Fermi surface, T^3-dependence is expected.

As already shown in Section 8.3, bismuth and antimony have highly anisotropic Fermi pockets. In these materials there is a temperature region in which the relation $(k_F)_{major} > k_0T/\hbar v_s > (k_F)_{minor}$ is satisfied, where $(k_F)_{major}$ and $(k_F)_{minor}$ respectively, denote the long and short axes of the Fermi pocket. In this region the observed resistivity is not proportional to T^5 but to T^2.[90] Detailed considerations will be given in Section 9.6.

The electron-phonon coupling constant D is assumed to be a constant in the Bloch theory. Actually, it is not the case. Resistivity calculation by use of the Bardeen's formula (6.29) was performed.[91] However, obtained result is similar to that based on the Bloch theory.

9.2 Thermal Conductivity of Metals

Consider an electron which reaches to the local equilibrium with the lattice system specified by a local temperature $T+\delta T$ through the scattering by lattice vibrations. When the electron arrives at the place with a temperature T after a time interval τ, δT is given by

$$\delta T = \tau\, \mathbf{v}_k \cdot (-\nabla T)\,, \tag{9.51}$$

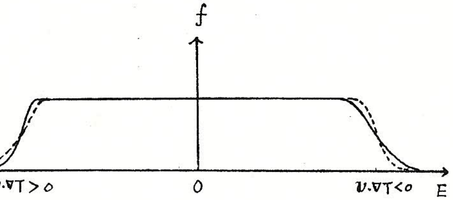
where $\mathbf{v}_k$ denotes the electron velocity. (9.51) means that the temperature of the electrons moving from the high (low) temperature side to the low (high) temperature side is δT higher (lower) than the average temperature. Accordingly, the electron distribution in the presence of a temperature gradient is given by

$$f_k = f_0\,(T - \tau\, \mathbf{v}_k \cdot \nabla T) = f_0 - (\tau\, \mathbf{v}_k \cdot \nabla T)\,\frac{\partial f_0}{\partial T}\,. \tag{9.52}$$

As $\nabla \zeta$ is included in the observed electric field, (9.52) becomes

$$f_k - f_0 = f_1 = \frac{(E-\zeta)}{T}\,(\nabla T \cdot \mathbf{v}_k)\,\tau\,\frac{\partial f_0}{\partial E}\,, \tag{9.53}$$

(See (6.17)). (9.53) is schematically represented in Figs. 9.4 and 9.5. Deviation f_1 in the region $\mathbf{v}\cdot\nabla T<0$ is larger than that in the region $\mathbf{v}\cdot\nabla T>0$. Thermal conductivity is measured under the condition of no electric current. Hot electrons drift to the cold side and simultaneously cold electrons to the hot side. As a result,



ig. 9.4 Fermi distribution in the presence of he temperature gradient. dotted line indicate the thermal equilibrium distribution.

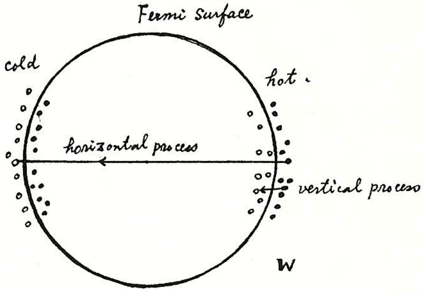


Fig. 9.5 Scattering processes in the thermal conduction. W denotes the heat flux.

e heat current flows. Relaxation processes in the thermal conduction are classified into two kinds as shown in Fig. 9.5. Hot electrons n the right hand side of the Fermi surface make transitions to the old part with large momentum change. This process is the elastic scattering and called the horizontal process. In the presence of an lectric field this process effectively contributes to the electrical resistance and therefore, the Wiedemann-Franz law is satisfied in this process. On the other hand, the vertical process which hardly changes the crystal **momentum**, is an effective relaxation mechanism in the thermal resistance but an ineffective process in the electrical resistance. As is shown in Fig. 9.5 this is the inelastic scattering process.

At sufficiently low temperatures the horizontal process accompanied by large momentum change is induced by the impurity scattering, And at high temperatures $T \gg \Theta_D$ scattering processes are quasi elastic and the horinzontal process is also possible. Then, the Wiedemann-Franz law holds.

From (6.27), we have

$$\varkappa \propto \begin{cases} T : \text{Impurity scattering}, \\ \text{constant} : \text{Phonon Scattering at } T \gg \Theta_D, \end{cases} \tag{9.54}$$

where we emplog the relations of $\sigma =$ constant at low temperatures and $\sigma \propto T^{-1}$ at $T \gg \Theta_D$.

In the temperature region where the vertical process is effective more detailed considerations are needed.

The relaxation time associated with the thermal conduction does not include a factor $(1-\cos\theta)$ (See (7.12)). $(1-\cos\theta)$ is a factor representing the randomization of the initial velocity after collision. In the vertical process $(1-\cos\theta)$ is nearly equal to zero. However, it contributes to the thermal resistance as the large angle scattering does. Therefore, we have

$$1/\tau \propto T^3. \tag{9.55}$$

From the kinetic theory of gases we find the following expression for the thermal conductivity:

$$\varkappa = \frac{1}{3} C_e l v_F, \tag{9.56}$$

where C_e is the electronic heat capacity per unit volume, l is the mean free path of an electron and v_F is the Fermi velocity. C_e is given by $C_e = \gamma T$ $(\gamma = \pi^2 k_0^2 n / 2\zeta)$ and $l = v_F \tau \propto T^{-3}$.

Then, we have

$$\kappa \propto T^{-2}. \tag{9.57}$$

The Lorentz ratio $\kappa / \sigma T$ becomes

$$\kappa / \sigma T \propto T^2. \tag{9.58}$$

Namely, in this case the Wiedemann-Franz law is not satisfied. In order to consider the effect of U-process, it needs a complicated calculation,89) but the discussions until now are sufficient to understand the qualitative feature of the thermal conduction.

9.3 Application of the Variation Principle to Conduction Phenomena

In the previous Chapters and in this Chapter the Boltzmann equation was solved in certain special cases, but all the solutions obtained have limited range of validity. We now present a more powerful and systematic method of solving the integral equation, which is based on the variation method.86)

If the distribution function is written as

$$f = f_0 - \Phi \frac{\partial f_0}{\partial E}, \quad \Phi = \sum_{i=1}^{3} \left[\left(e\mathcal{E}_i + T \frac{\partial}{\partial x_i} \frac{\zeta}{T} \right) \phi_i + \frac{1}{T} \frac{\partial T}{\partial x_i} \psi_i \right]. \tag{9.59}$$

the Boltzmann equation ($H = 0$) can be replaced by

$$\mathcal{L}(\phi_i) = v_i \frac{\partial f_0}{\partial E}, \quad \mathcal{L}(\psi_i) = v_i E \frac{\partial f_0}{\partial E}, \tag{9.60}$$

where $\mathcal{L}$ is the collision operator defined by

$$\mathcal{L}(F) \equiv \frac{1}{k_0 T} \int V(k.k') \{ F(k) - F(k') \} dk'. \tag{9.61}$$

The variation method is based on the following theorem :

Let F be the solution of the equation

$$\mathcal{L}(F) = v_i E^n \frac{\partial f_0}{\partial E}, \tag{9.62}$$

and let G be any function satisfying the relation

$$(G.G) \equiv \frac{1}{4\pi^3} \int G \mathcal{L}(G) dk = \frac{1}{4\pi^3} \int G v_i E^n \frac{\partial f_0}{\partial E} dk . \tag{9.63}$$

Then, among the functions G satisfying (9.63), F is the one which makes $(G.G)$ maximum.

[Proof]

Define the expression

$$(F.G) \equiv \frac{1}{4\pi^3 k_0 T} \iint V(k.k') F(k) \{ G(k) - G(k') \} dk dk'. \tag{9.64}$$

Since $V(k.k') = V(k'.k)$ (see (9.9)), (9.64) is rewritten as

$$(F.G) = \frac{1}{4\pi^3 k_0 T}\iint V(k.k')F(k')\{G(k')-G(k)\}\,dk\,dk'. \qquad (9.65)$$

Hence, by addition,

$$(F.G) = \frac{1}{8\pi^3 k_0 T}\iint V(k.k')\{F(k)-F(k')\}\{G(k)-G(k')\}\,dk\,dk'. \qquad (9.66)$$

Then,

$$(F.G) = (G.F), \quad (G.G) \geqq 0. \qquad (9.67)$$

Since G satisfies (9.63) and F is the solution of (9.62), we have

$$(G.F) = \frac{1}{4\pi^3}\int G v_i E^n \frac{\partial f_0}{\partial E}\,dk = (G.G). \qquad (9.68)$$

Now $(F-G)(F-G) \geqq 0$ and so $(F-G)(F-G) = (F.F) - (F.G)$ $- (G.F) + (G.G) = (F.F) - 2(G.F) + (G.G) = (F.F) - (G.G) \geqq 0$.

$$\therefore (F.F) \geqq (G.G), \qquad (9.69)$$

which proves the maximum theorem.

An alternative expression of the variation principle is as follows:

Let G be any function for which (G,G) exists. Then, among such functions, the solution F which satisfies (9.62) is the one which makes

$$(G.G)\Big/\left[\frac{1}{4\pi^3}\int G v_i E^n \frac{\partial f_0}{\partial E}\,dk\right]^2, \qquad (9.70)$$

minimum.

[Proof]

From (9.67), we have for any real λ and μ

$$(\lambda F + \mu G, \lambda F + \mu G) = \lambda^2 (F.F) + 2\lambda\mu (F.G) + \mu^2 (G.G) \geqq 0 . \qquad (9.71)$$

Since the discrimant is negative, i.e.

$$(F.F)(G.G) \geqq (F.G)^2 . \qquad (9.72)$$

From (9.62),

$$(F.F) = \frac{1}{4\pi^3}\int F v_i E^n \frac{\partial f_0}{\partial E} dk, \quad (G.F) = \frac{1}{4\pi^3}\int G v_i E^n \frac{\partial f_0}{\partial E} dk. \qquad (9.73)$$

Dividing the left and right hand sides of (9.72) by $(F.F)(F.G)^2$, we have

$$(G.G)/(F.G)^2 \geqq 1/(F.F) . \qquad (9.74)$$

By inserting (9.73), (9.74) gives the relation

$$(G.G)\Big/\Big[\frac{1}{4\pi^3}\int G v_i E^n \frac{\partial f_0}{\partial E} dk\Big]^2 \geqq (F.F)\Big/\Big[\frac{1}{4\pi^3}\int F v_i E^n \frac{\partial f_0}{\partial E} dk\Big], \qquad (9.75)$$

which proves the minimum principle.

In the following we calculate the transport coefficients of the simple metals with an isotropic effective mass by making use of the variation method. We follow quite closely the procedures in Wilson's book.[91)]

In the absence of a magnetic field, the Boltzmann equation may be written in the form

$$\left\{\begin{aligned} & f = f_0 - k_1 C(E) \frac{\partial f_0}{\partial E} , \\ & \left(\frac{\partial f}{\partial t}\right)_{\mathrm{coll}} = - k_1 \mathcal{L}(c) = - k_1 \frac{\hbar}{m^*} \frac{\partial f_0}{\partial E} \left(e\mathcal{E} + T \frac{\partial}{\partial x} \frac{\zeta}{T} + \frac{E}{T} \frac{\partial T}{\partial x} \right) . \end{aligned}\right. \tag{9.76}$$

$$\mathcal{L}(c) = - \left(\frac{2}{m^*}\right)^{1/2} \frac{E^{1/2}}{l_r} \frac{\partial f_0}{\partial E} C(E) - \frac{1}{A E^{3/2}} \frac{\partial f_0}{\partial E} \left(\frac{T}{\Theta_D}\right)^3 \int_{-\Theta_D/T}^{\Theta_D/T} \Big\{ E\, C(\eta) - C(\eta+z) \Big[E + \tfrac{1}{2} k_0 T z$$
$$- E_D \left(\frac{T}{\Theta_D}\right)^2 z^2 \Big] \Big\} \frac{e^{\eta}+1}{e^{\eta+z}+1} \frac{z^2 dz}{|1-e^{-z}|} . \tag{9.77}$$

The first term in the right hand side of (9.77) represents the impurity scattering process and l_r is the mean free path, and the second term corresponds to the phonon scattering which is already derived in (9.25).

Let $C^{(n)}(E)$ be the solution of the equation

$$\mathcal{L}(C^{(n)}) = E^{n-3/2} \frac{\partial f_0}{\partial E} . \tag{9.78}$$

$C(E)$ in (9.76) is written in terms of $C^{(n)}(E)$ as

$$C(E) = \frac{\hbar}{m^*} \left(e\mathcal{E} + T \frac{\partial}{\partial x} \frac{\zeta}{T} \right) C^{(3/2)}(E) + \frac{\hbar}{m^*} \frac{1}{T} \frac{\partial T}{\partial x} C^{(5/2)}(E) . \tag{9.79}$$

Now, the statement of the variation principle is as follows:
Under the subsidiary condition

$$k_0 T \int_{-\infty}^{\infty} E^{3/2} C^{(n)} \mathcal{L}(C^{(n)}) d\eta = \int_{-\infty}^{\infty} E^{n} C^{(n)} \frac{\partial f_0}{\partial \eta} d\eta , \quad (\eta = (E-\zeta)/k_0 T) , \tag{9.80}$$

$C^{(n)}$ is the function which maximizes the integral

$$(c^{(n)}, c^{(n)}) = k_0T\int_{-\infty}^{\infty} E^{3/2} c^{(n)} \mathcal{L}(c^{(n)})d\eta . \qquad (9.81)$$

To prove this, it is needed to verify the relations of $(c^{(n)}, d^{(n)}) = (d^{(n)}, c^{(n)})$ and $(c^{(n)}, c^{(n)}) \geqq 0$.

Concrete proof is given in Appendix 5.

Ziman related the inequality $(G.G) \geqq 0$ to the entropy production associated with the irreversible process.[92)] A brief introduction of the Ziman's theory is given in Appendix 6.

To solve (9.78), $c^{(n)}(E)$ is developed in terms of the functions ϕ_r of a complete set :

$$c^{(n)} = \sum_{r=0}^{\infty} C_r^{(n)} \phi_r . \qquad (9.82)$$

It is convenient to choose ϕ_r as

$$c^{(n)}(\eta) = \sum_{r=0}^{\infty} C_r^{(n)} \eta^r \quad : \text{degenerate system.} \qquad (9.83)$$

$$c^{(n)}(\eta) = \sum_{r=0}^{\infty} C_r^{(n)} E^r \quad : \text{non-degenerate system} \qquad (9.84)$$

Since we are interested in metals, we assume (9.83). Let define the quantities

$$\alpha_r^{(n)} = \int_{-\infty}^{\infty} E^n \eta^r \frac{\partial f_0}{\partial \eta} d\eta , \quad d_{rs} \equiv (\eta^r, \eta^s) = k_0T\int_{-\infty}^{\infty} E^{3/2} \eta^r \mathcal{L}(\eta^s) d\eta . \qquad (9.85)$$

The coefficients $C_r^{(n)}$ are determined so as to maximize the quantity

$$(c^{(n)}, c^{(n)}) = \sum_{r=0}^{\infty} \sum_{s=0}^{\infty} d_{rs} C_r^{(n)} C_s^{(n)}, \tag{9.86}$$

under the subsidiary condition

$$C \equiv \sum_{r=0}^{\infty} \sum_{s=0}^{\infty} d_{rs} C_r^{(n)} C_s^{(n)} - \sum_{r=0}^{\infty} \alpha_r^{(n)} C_r^{(n)} = 0 . \tag{9.87}$$

For this purpose we make the quantity $(\lambda-1)(c^{(n)}, c^{(n)}) + C$ maximize, where λ is a Lagrange undetermined multiplier. By differentiating it on $C_s^{(n)}$ we obtain $2\lambda \sum_r d_{rs} C_r^{(n)} - \alpha_s^{(n)} = 0$, and if we multiply the equation by $C_s^{(n)}$, sum over s and use (9.87), we find $2\lambda = 1$, where we employ the relation of $d_{rs} = d_{sr}$ (See Appendix 5). Then, the coefficients $C_s^{(n)}$ satisfy the infinite set of linear equations

$$\sum_{s=0}^{\infty} d_{rs} C_s^{(n)} - \alpha_r^{(n)} = 0 , \quad (r = 0, 1, 2, \cdots). \tag{9.88}$$

The electric current density and heat current density are expressed by

$$j_x = -\frac{e}{4\pi^3} \int v_x f \, dk = \frac{(2m^*)^{3/2} e}{3\pi^2 \hbar^4} \int_{-\infty}^{\infty} E^{3/2} c(\eta) \frac{\partial f_0}{\partial \eta} d\eta .$$

$$= K_{3/2,3/2} \left(e^2 \mathcal{E} + eT \frac{\partial}{\partial x} \frac{\zeta}{T} \right) + K_{3/2,5/2} \frac{e}{T} \frac{\partial T}{\partial x} , \tag{9.89}$$

$$w_x = \frac{1}{4\pi^3} \int v_x (E - \zeta) f \, dk = \frac{\zeta}{e} j_x + K_{5/2,3/2} \left(-e\mathcal{E} - T \frac{\partial}{\partial x} \frac{\zeta}{T} \right)$$

$$- K_{5/2,5/2} \frac{1}{T} \frac{\partial T}{\partial x} , \tag{9.90}$$

where

$$K_{m.n} = \frac{2(2m^*)^{1/2}}{3\pi^2\hbar^3}\int_{-\infty}^{\infty} E^m c^{(n)}(\eta)\frac{\partial f_0}{\partial\eta}d\eta = \frac{2(2m^*)^{1/2}}{3\pi^2\hbar^3}\sum_{s=0}^{\infty}\alpha_s^{(m)}C_s^{(n)} = K_{n.m}. \tag{9.91}$$

$K_{m.n} = K_{n.m}$ is a direct consequence of the Onsager relation.

The main mathematical problem is the convergence of the formal series (9.91). The equations are, however, so complex that we are limited to find few terms.

Solving the infinite set of equations (9.88) and inserting them into (9.91), we obtain

$$K_{m.n} = -\frac{2(2m^*)^{1/2}}{3\pi^2\hbar^3}\frac{D_{m.n}}{D}, \tag{9.92}$$

where $D = |d_{rs}|$ is the determinant of the d_{rs}'s and D_{mn} is the determinant formed by bordering D with $0, \alpha_0^{(m)}, \alpha_1^{(m)} \dots$ and $0, \alpha_0^{(n)}, \alpha_1^{(n)}, \dots$, i.e.

$$D_{m.n} = \begin{vmatrix} 0 & \alpha_0^{(m)} & \alpha_1^{(m)} & \alpha_2^{(m)} & \cdots \\ \alpha_0^{(n)} & d_{00} & d_{01} & d_{02} & \cdots \\ \alpha_1^{(n)} & d_{10} & d_{11} & d_{12} & \cdots \\ \alpha_2^{(n)} & d_{20} & d_{21} & d_{22} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \end{vmatrix}. \tag{9.93}$$

In general, neither D nor D_{mn} is convergent, and we should consider the ratio D_{mn}/D. In the following Section we calculate

σ, $\mathcal{H}$ and S.

9.4 Calculation of the Transport Coefficients due to the Variation Principle

From (9.89) σ becomes

$$\sigma = e^2 K_{3/2,3/2} = -\frac{2(2m^*)^{1/2} e^2}{3\pi^2 \hbar^3} \frac{\mathcal{D}_{3/2,3/2}}{\mathcal{D}} . \qquad (9.94)$$

To rewrite (9.94) in a more convenient form, Jacobi's theorem is employed.

Jacobi's theorem : Let denote the determinant removing (i_1, i_2) columns and $(k_1. k_2)$ rows by $D\begin{pmatrix} i_1 & i_2 \\ k_1 & k_2 \end{pmatrix}$ and the original determinant by $D = |a_{ik}| = \sum a_{ik} A_{ik}$.

We have

$$\begin{vmatrix} A_{ii} & A_{ik} \\ A_{ki} & A_{kk} \end{vmatrix} = D . D \begin{pmatrix} i & k \\ i & k \end{pmatrix} . \qquad (9.95)$$

We now apply (9.95) to the case

$$D = \mathcal{D}^{(n)}_{\alpha\alpha} = \begin{vmatrix} d_{00} & \cdots & d_{0n-1} & \alpha_0^{(3/2)} \\ \vdots & & \vdots & \vdots \\ d_{n-1\,0} & \cdots & d_{n-1,n-1} & \alpha_{n-1}^{(3/2)} \\ \alpha_0^{(3/2)} & \cdots & \alpha_{n-1}^{(3/2)} & 0 \end{vmatrix} , \quad D\begin{pmatrix} i & k \\ i & k \end{pmatrix} = \mathcal{D}^{(n-1)} = \begin{vmatrix} d_{00} & \cdots & d_{0n-2} \\ \vdots & & \vdots \\ d_{n-2\,0} & \cdots & d_{n-2,n-2} \end{vmatrix} . \qquad (9.96)$$

In a similar way $\mathcal{D}_{\alpha\alpha}^{(n-1)}$ is defined, and moreover introduce

$$A_{ki} \equiv \mathcal{D}_{\alpha}^{(n-1)} \equiv \begin{vmatrix} d_{00} & \cdots & d_{0n-2} & \alpha_0^{(3/2)} \\ \vdots & & \vdots & \vdots \\ d_{n-1,0} & \cdots & d_{n-1,n-1} & \alpha_{n-1}^{(3/2)} \end{vmatrix} . \qquad (9.97)$$

The Jacobi's theorem leads to

$$\begin{vmatrix} \mathcal{D}_{\alpha\alpha}^{(n-1)} & \mathcal{D}_{\alpha}^{(n-1)} \\ \mathcal{D}_{\alpha}^{(n-1)} & \mathcal{D}^{(n)} \end{vmatrix} = \mathcal{D}_{\alpha\alpha}^{(n)} \mathcal{D}^{(n-1)} . \qquad (9.98)$$

From (9.98), we have

$$\left\{ \begin{aligned} & -\frac{\mathcal{D}_{\alpha\alpha}^{(n)}}{\mathcal{D}^{(n)}} + \frac{\mathcal{D}_{\alpha\alpha}^{(n-1)}}{\mathcal{D}^{(n-1)}} = \frac{(\mathcal{D}_{\alpha}^{(n-1)})^2}{\mathcal{D}^{(n-1)}\mathcal{D}^{(n)}} , \quad (n \geqq 2) \\ & -\frac{\mathcal{D}_{\alpha\alpha}^{(1)}}{\mathcal{D}^{(1)}} = \frac{(\alpha_0^{(3/2)})^2}{d_{00}} . \end{aligned} \right. \qquad (9.99)$$

In consideration of (9.94) and (9.99) the conductivity takes the form

$$\sigma = -\frac{2(2m^*)^{1/2}e^2}{3\pi^2\hbar^3} \lim_{n\to\infty} \frac{\mathcal{D}_{\alpha\alpha}^{(n)}}{\mathcal{D}^{(n)}} = \frac{2(2m^*)^{1/2}e^2}{3\pi^2\hbar^3}\left[\frac{(\alpha_0^{(3/2)})^2}{d_{00}} + \sum_{n=2}^{\infty} \frac{(\mathcal{D}_{\alpha}^{(n-1)})^2}{\mathcal{D}^{(n-1)}\mathcal{D}^{(n)}} \right] . \qquad (9.100)$$

The first approximation is obtained by estimating $\alpha_0^{(3/2)}$ and d_{00}, and it corresponds to the approximation for $(k_0T/\zeta)^0$.

From (9.85) and (9.77) we have

$$\left\{\begin{aligned} &\alpha_0^{(3/2)} = -\zeta^{3/2}, \\ &\alpha_{00} = -\sqrt{\frac{2}{m^*}}\,\frac{1}{l_r}\int_{-\infty}^{\infty} E^2 \frac{\partial f_0}{\partial \eta}\, d\eta + \frac{1}{A}\left(\frac{T}{\Theta_D}\right)^3 \int_{-\infty}^{\infty} d\eta \int_{-\Theta_D/T}^{\Theta_D/T} dZ \left[E_D\left(\frac{T}{\Theta_D}\right)^2 Z^2 - \frac{1}{2}k_0 T Z\right] \\ &\times \frac{Z^2}{|1-e^{-Z}|}\,\frac{1}{(e^{\eta+Z}+1)(e^{-\eta}+1)}, \end{aligned}\right. \qquad (9.101)$$

and then

$$\alpha_{00} = \sqrt{\frac{2}{-m^*}}\,\frac{\zeta^2}{l_r} + \frac{2E_D}{A}\left(\frac{T}{\Theta_D}\right)^5 J_5\left(\frac{\Theta_D}{T}\right) = \frac{2(2m^*)^{1/2}e^2\zeta^3}{3\pi^2\hbar^3}\left(\frac{1}{\sigma_r}+\frac{1}{\sigma_i}\right). \qquad (9.102)$$

$1/\sigma_r$ is the residual resistance and $1/\sigma_i$ denotes the ideal resistance due to the phonon scattering:

$$\frac{1}{\sigma_r} = \rho_r = \frac{3\pi^2\hbar^3}{2m^* e^2 l_r \zeta}. \qquad (9.103)$$

$$\frac{1}{\sigma_i} = \rho_i = \frac{6\pi^2\hbar^3 E_D}{4e^2 A\left(\frac{1}{2}m^*\right)^{1/2}\zeta^3}\left(\frac{T}{\Theta_D}\right)^5 J_5\left(\frac{\Theta_D}{T}\right). \qquad (9.104)$$

(9.104) is the same expression as (9.40). Further approximation can be obtained by the following formula:

$$\sigma = \sigma^{(0)} + \frac{2(2m^*)^{1/2}e^2}{3\pi^2\hbar^3}\sum_{n=2}^{\infty}\frac{\left(\mathscr{D}_\alpha^{(n-1)}\right)^2}{\mathscr{D}^{(n-1)}\mathscr{D}^{(n)}}, \quad \sigma^{(0)} = \left(1/\sigma_r + 1/\sigma_i\right)^{-1}. \qquad (9.105)$$

Expression of the thermal conductivity is obtained by putting $j_x = 0$

in (9.89) and (9.90). as follows :

$$\varkappa = \left(K_{3/2,3/2} K_{5/2,5/2} - K_{3/2,5/2}^{\,2} \right) / K_{3/2,3/2} T$$

$$= \frac{2(2m^*)^{1/2}}{3\pi^2\hbar^3 T} \left(- \frac{\mathcal{D}_{5/2,5/2}}{\mathcal{D}} + \frac{\mathcal{D}_{3/2,5/2}^{\,2}}{\mathcal{D}_{3/2,3/2}\,\mathcal{D}} \right) . \qquad (9.106)$$

Let $\mathcal{D}_{3/2,3/2,5/2,5/2}$ be the determinant formed by borderning $\mathcal{D}$ $= |d_{rs}|$ in (1.2) rows and (1.2) columns :

$$\mathcal{D}_{3/2,3/2,5/2,5/2} = \begin{vmatrix} 0 & 0 & \alpha_0^{(3/2)} & \alpha_1^{(3/2)} & \cdots \\ 0 & 0 & \alpha_0^{(5/2)} & \alpha_1^{(5/2)} & \cdots \\ \alpha_0^{(3/2)} & \alpha_0^{(5/2)} & d_{00} & d_{01} & \cdots \\ \alpha_1^{(3/2)} & \alpha_1^{(5/2)} & d_{10} & d_{11} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \end{vmatrix} . \qquad (9.107)$$

In a similar way to (9.98), we get

$$\begin{vmatrix} \mathcal{D}_{5/2,5/2} & \mathcal{D}_{3/2,5/2} \\ \mathcal{D}_{5/2,3/2} & \mathcal{D}_{3/2,3/2} \end{vmatrix} = \mathcal{D}\,\mathcal{D}_{3/2,3/2,5/2,5/2} . \qquad (9.108)$$

Then,

$$\varkappa = - \frac{2(2m^*)^{1/2}}{3\pi^2\hbar^3 T} \frac{\mathcal{D}_{3/2,3/2,5/2,5/2}}{\mathcal{D}_{3/2,3/2}} . \qquad (9.109)$$

Approximating $\mathcal{D}_{3/2,3/2,5/2,5/2}$ by the first 4-4 matrix and $\mathcal{D}_{3/2,3/2}$ by the first 3-3 matrix, we obtain the zero-th order approximation of $\varkappa$:

$$\varkappa^{(0)} = \frac{2(2m^*)^{1/2}}{3\pi^2\hbar^3\Theta_D}\left(\frac{\Theta_D}{T}\right)\frac{\left(\alpha_0^{(3/2)}\alpha_1^{(5/2)} - \alpha_0^{(5/2)}\alpha_1^{(3/2)}\right)^2}{(\alpha_0^{(3/2)})^2 d_{11} - 2\alpha_0^{(3/2)}\alpha_1^{(3/2)} d_{01} + (\alpha_1^{(3/2)})^2 d_{00}} . \qquad (9.110)$$

It is sufficient to estimate this to the smallest non-vanishing power of $(k_0T/\zeta)^2$. Detailed result is given in Wilson's text book.

The thermoelectric power is given by

$$S = \frac{\zeta K_{3/2,3/2} - K_{3/2,5/2}}{eTK_{3/2,3/2}} = \frac{\zeta D_{3/2,3/2} - D_{3/2,5/2}}{eTD_{3/2,3/2}} . \qquad (9.111)$$

On making use of the relation $\alpha_r^{(5/2)} - \zeta\alpha_r^{(5/2)} = k_0T\alpha_{r+1}^{(3/2)}$, (9,11) is rewritten as

$$S = -\frac{k_0}{e}\frac{E_{3/2,3/2}}{D_{3/2,3/2}} , \qquad (9.112)$$

where

$$E_{m,n} = \begin{vmatrix} 0 & \alpha_0^{(m)} & \alpha_1^{(m)} & \cdots \\ \alpha_1^{(n)} & d_{00} & d_{01} & \cdots \\ \alpha_2^{(n)} & d_{10} & d_{11} & \cdots \\ \vdots & \vdots & \vdots & \end{vmatrix} . \qquad (9.113)$$

In finishing this Section we mention several comments.

1) Higher order corrections on σ have been calculated by Sondheimer[93] and were found to be very small. The corrections give rise to a deviation from Matthiesen's rule, that is the total resistivity differs slightly from the value $\rho = \rho_r + \rho_i$.

The deviations obtained by Sondheimer are, however much too small to account for the experimental results.[91)]

2) Sondheimer[93)] has found that higher order corrections are considerably more important in the case of thermal conductivity than in that of the electrical conductivity.

The theoretical thermal conductivity is given by

$$\frac{1}{\varkappa} = \frac{\rho_r}{L_0 T} + \frac{4A}{L_0 T}\left(\frac{T}{\Theta_D}\right)^5 \left[\left\{1 + \frac{3}{2\pi^2}\frac{\zeta}{D}\left(\frac{\Theta_D}{T}\right)^2\right\} J_5\left(\frac{\Theta_D}{T}\right) - \frac{1}{2\pi^2} J_5\left(\frac{\Theta_D}{T}\right)\right], \quad (9.114)$$

where the first term is the residual thermal resistivity and the second term represents the electron-phonon scattering process due to the Bloch theory. Here, A is the parameter defined by (6.28) and $D = (\hbar^2/4m^*)\, q_D^2$.

At low temperatures, (9.114) becomes

$$\frac{1}{\varkappa} = \frac{a}{T} + b\,T^2. \qquad (9.115)$$

Sondheimer has shown that b should be multiplied by about 0.75 if higher order corrections are included. Klemens has carried out more detailed calculation[94)] and obtained the correction factor about 0.68. It should be noted these corrections are much larger than for the electrical conductivity, where σ_0 gives a good answer.

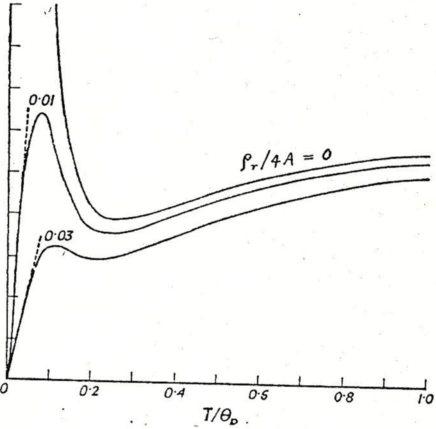


Fig. 9.6 Theoretical curves for thermal nductivity with different amounts of impurity esistance, calculated from the Bloch theory.93)

3) Fig. 9.6 indicates that unless the residual resistivity is fairly large, the theoretical curves exhibit a fairly pronounced minimum near $T = 0.25\,\Theta_D$. Such a minimum has never been observed experimentally. Even when corrected by higher order terms, this function is of the form shown in Fig. 9.6. This discrepancy is removed if we use an electron-phonon interaction that permits U-processes. The minimum is caused by the term related to the "vertical transitions" (See Fig. 9.5). Introduction of U-processes makes the weight of the vertical transitions reduce and the minimum disappears.90)

4) The variation principle has been given only for the case in the absence of a magnetic field. Attempts to extend the variation principle to the case for $H \neq 0$ have been proposed.95) However, this extension is not quite so powerful as the principle used in the case for $H = 0$.

9.5 Electrical Conductivity of Polar Semiconductors, Application of Variation Principle

As has been pointed out in Section 7.11, in polar semiconductors the scattering process due to the polar optical phonon is very important and at low temperatures ($\hbar\omega_l > k_0T$) it is impossible to define a unique time of relaxation for the scattering process. The Boltzmann equation is solved by means of the variation principle, and exact expressions for the electrical conductivity and the thermoelectric power are obtained in the form of ratios of infinite determinants.$^{61)}$

Assuming the phonon system being in thermal equilibrium, we have

$$\left(\frac{\partial f_K}{\partial t}\right)_{coll} = -\frac{e^2\omega_l}{2\pi\varepsilon^* k_0 T}\int\frac{d\mathbf{q}}{q^2} f_0(k+q)\left\{1-f_0(k)\right\}\left[(n_q+1)\,\delta(E_k-E_{k+q}+\hbar\omega_l)\right.$$

$$\left.+\,n_q\,\delta(E_K-E_{K+q}-\hbar\omega_l)\right]\left\{\Phi(k)-\Phi(k+q)\right\}, \qquad (9.116)$$

where $1/\varepsilon^* = 1/\varepsilon_\infty - 1/\varepsilon_0$, and $n_q = (e^{\hbar\omega_l/k_0T}-1)^{-1}$.

The integration over θ, φ may be performed on putting

$$\Phi(k) = k_x\,c(E), \qquad (9.117)$$

where we assume $E_k = \hbar^2k^2/2m^*$.

$$\left(\frac{\partial f_k}{\partial t}\right)_{coll} = -\frac{e^2\omega_\ell k_x m^*}{\varepsilon^* \hbar^2 k}\frac{\partial f_0}{\partial E}\left[\!\left[\int_{q_1^{(+)}}^{q_2^{(+)}}\left[(n_q+1)\frac{f_0(E+\hbar\omega_\ell)}{f_0(E)}\left\{\left(1+\frac{\hbar\omega_\ell}{2E}-\frac{q^2}{2k^2}\right)C(E+\hbar\omega_\ell)-C(E)\right\}\right]\frac{dq}{q}\right.\right.$$

$$\left.\left.+\int_{q_1^{(-)}}^{q_2^{(-)}}\left[n_q\frac{f_0(E-\hbar\omega_\ell)}{f_0(E)}\left\{\left(1-\frac{\hbar\omega_\ell}{2E}-\frac{q^2}{2k^2}\right)C(E-\hbar\omega_\ell)-C(E)\right\}\right]\frac{dq}{q}\right]\!\right], \qquad (9.118)$$

where

$$q_1^{(\pm)} = \pm\sqrt{\frac{2m^*}{\hbar^2}}\left\{\sqrt{E\pm\hbar\omega_\ell}-\sqrt{E}\right\},$$

$$q_2^{(\pm)} = \sqrt{\frac{2m^*}{\hbar^2}}\left\{\sqrt{E\pm\hbar\omega_L}+\sqrt{E}\right\}. \qquad (9.119)$$

After carrying out the integration over q, (9.118) becomes

$$\left(\frac{\partial f_K}{\partial t}\right)_{coll} = -\frac{e^2\omega_\ell m^*}{\varepsilon^* E\,\hbar^2 k}\frac{\partial f_0}{\partial E}\,\mathcal{L}(C). \qquad (9.120)$$

Collision operator $\mathcal{L}(C)$ takes the form

$$\mathcal{L}(C) = (n+1)\frac{f_0(E+\hbar\omega_\ell)}{f_0(E)}\left[C(E+\hbar\omega_\ell)\left\{(2E+\hbar\omega_\ell)\sinh^{-1}\sqrt{E/\hbar\omega_\ell}-\sqrt{E(E+\hbar\omega_\ell)}\right\}\right.$$

$$\left.-2E\,C(E)\sinh^{-1}\sqrt{E/\hbar\omega_\ell}\right]+h(E-\hbar\omega_\ell)\,n\,\frac{f_0(E-\hbar\omega_\ell)}{f_0(E)}\left[C(E-\hbar\omega_\ell)\right.$$

$$\left.\times\left\{(2E-\hbar\omega_\ell)\cosh^{-1}\sqrt{E/\hbar\omega_\ell}-\sqrt{E(E-\hbar\omega_\ell)}\right\}-2E\,C(E)\cosh^{-1}\sqrt{E/\hbar\omega_\ell}\right], \qquad (9.121)$$

where

$$h(x) = \begin{cases} 0 : & x<0, \\ 1 : & x>0. \end{cases} \qquad (9.122)$$

At high temperatures $\hbar\omega_l < k_0 T$ $\mathcal{L}(c)$ may be expanded in power series of $\hbar\omega_l / k_0 T$ and $\hbar\omega_l / E$:

$$\mathcal{L}(c) = -2 E k_0 T \, C(E) \hbar\omega_l \left\{ 1 + O\left(\frac{\hbar\omega_l}{k_0 T}\right) + O\left(\frac{\hbar\omega_l}{E}\right) \right\} . \qquad (9.123)$$

and (9.120) becomes

$$\left(\frac{\partial f_k}{\partial t}\right)_{\text{coll.}} = k_x \frac{\partial f_0}{\partial E} \frac{2 e^2 m^* k_0 T}{\varepsilon^* \hbar^3 k} C(E) = - \frac{f - f_0}{\tau} , \qquad (9.124)$$

where the relaxation is given by

$$\tau(E) = \frac{\varepsilon^* \hbar^2 E^{1/2}}{(2m^*)^{1/2} e^2 k_0 T} . \qquad (9.125)$$

The Boltzmann equation in the general case is

$$\frac{\sqrt{2}\, \hbar^2 \varepsilon^*}{e^2 \omega_l \, m^{*3/2}} E^{3/2} \left(e \mathcal{E} + T \frac{\partial}{\partial x} \frac{\zeta}{T} + \frac{E}{T} \frac{\partial T}{\partial x} \right) = \mathcal{L}(c) . \qquad (9.126)$$

This is a linear finite difference equation. There is the one to one correspondence between an energy interval $N\hbar\omega_l < E < (N+1)\hbar\omega_l$ and a difference equation. By solving numerically the infinite set of the difference equations a reliable result may be obtained. Especially, this method is powerful and convenient in the presence of a magnetic field, since in this case the variation method is not useful.

On making use of this procedure Fletcher and Butcher calculated the Hall mobility and the Hall factor and obtained a good agreement with the observed data.[63)]

Put

$$C(E) = \frac{\sqrt{2}\,\hbar^2\,\mathcal{E}^*}{e^2 \omega_\ell\, m^{*3/2}} \left\{ \left(e\mathcal{E} + T\frac{\partial}{\partial x}\frac{\zeta}{T} \right) C^{(3/2)} + \frac{1}{T}\frac{\partial T}{\partial x} C^{(5/2)} \right\}, \qquad (9.127)$$

then $C^{(n)}$ is the solution of

$$E^n = \mathcal{L}(C^{(n)}), \quad (n = 3/2,\ 5/2). \qquad (9.128)$$

The electric current and heat current densities are given by (9.89) and (9.90), where K_{mn} is

$$K_{mn} = \frac{4\mathcal{E}^*}{3\pi^2 e^2 \hbar \omega_\ell} \int_0^\infty E^m C^{(n)} \frac{\partial f_0}{\partial E}\, dE. \qquad (9.129)$$

Let c, d be any functions of E and define

$$(d.c) = \int_0^\infty d\ \mathcal{L}(c)\, \frac{\partial f_0}{\partial E}\, dE. \qquad (9.130)$$

To apply the variation principle, it needs to verify $(c.d) = (d.c)$ and $(c.c) \geq 0$. These relations may be proved in the similar way to Appendix 5. The solution $C^{(n)}(E)$ of (9.128) is such as to make $(C^{(n)}, C^{(n)})$ a maximum, subject to the subsidiary condition

$$\int_0^\infty C^{(n)} \mathcal{L}(C^{(n)}) \frac{\partial f_0}{\partial E}\, dE = \int_0^\infty E^n C^{(n)} \frac{\partial f_0}{\partial E}\, dE. \qquad (9.131)$$

Since we are interested in the non-degenerate semiconductors,

$C^{(n)}(E)$ is assumed to be

$$C^{(n)}(E) = \sum_{r=0}^{\infty} C_r^{(n)} \phi_r(E), \quad \phi_r(E) = E^r. \tag{9.132}$$

Combination (9.129) and (9.132) gives

$$K_{m.n} = K_{n.m} = \frac{4\mathcal{E}^*}{3\pi^2 e^2 \hbar^2 \omega_e} \sum_{r=0}^{\infty} \alpha_r^{(m)} C_r^{(n)} = -\frac{4\mathcal{E}^*}{3\pi^2 e^2 \hbar^2 \omega_e} \frac{\mathcal{D}_{m.n}}{\mathcal{D}}, \tag{9.133}$$

where $\mathcal{D}_{m.n}$ and $\mathcal{D}$ were introduced in Section 9.3. (See (9.91) and (9.92)).

The electric conductivity and the thermoelectric power are given by

$$\sigma = \frac{4\mathcal{E}^*}{3\pi^2 \hbar^2 \omega_e}\left[\frac{(\alpha_0^{(3/2)})^2}{d_{00}} + \sum_{n=0}^{\infty} \frac{(\mathcal{D}_\alpha^{(n-1)})^2}{\mathcal{D}^{(n-1)}\mathcal{D}^{(n)}}\right], \quad S = \frac{\zeta}{eT} - \frac{\mathcal{D}_{3/2,5/2}}{eT\,\mathcal{D}_{3/2,3/2}}. \tag{9.134}$$

These expressions are formally the same ones as (9.100) and (9.111).

$\alpha_r^{(n)}$ and d_{rs} are defined by

$$\alpha_r^{(n)} = \int_0^{\infty} E^{n+r} \frac{\partial f_0}{\partial E}\, dE, \quad d_{rs} = (E^r, E^s) = \int_0^{\infty} E^r \mathcal{L}(E^s) \frac{\partial f_0}{\partial E}\, dE. \tag{9.135}$$

Substituting $f_0(E) = \exp\{(\zeta - E)/k_0T\} = e^{\xi} e^{-E/k_0T}$ into (9.135).

we obtain

$$\alpha_r^{(n)} = -\frac{e^{\xi}}{k_0T}\int_0^{\infty} E^{r+n} e^{-E/k_0T}\, dE = -(k_0T)^{r+n}\,\Gamma(r+n+1)\, e^{\xi}. \tag{9.136}$$

$$d_{rs} = -\frac{e^{\xi}}{k_0 T(e^{z}-1)} \int_0^{\infty} E^{r} \Big[\!\Big[(E+\hbar\omega_e)^{s} \Big\{ (2E+\hbar\omega_e)\sinh^{-1}\sqrt{E/\hbar\omega_e} - \sqrt{E(E+\hbar\omega_e)} \Big\}$$

$$-2E^{s+1}\sinh^{-1}\sqrt{E/\hbar\omega_e} + h(E-\hbar\omega_e)e^{z}\Big[(E-\hbar\omega_e)^{s}\Big\{ (2E-\hbar\omega_e)\cosh^{-1}\sqrt{E/\hbar\omega_e}$$

$$-\sqrt{E(E-\hbar\omega_e)}\Big\} - 2E^{s+1}\cosh^{-1}\sqrt{E/\hbar\omega_e}\Big]\Big]\!\Big] e^{-E/k_0T} dE., \qquad (9.137)$$

where $z = \hbar\omega_e / k_0 T$ and h is the step function defined by (9.122). By the replacement of $E \rightarrow E + \hbar\omega_e$ in the term including $h(E - \hbar\omega_e)$ d_{rs} is rewritten as follows :

$$d_{rs} = \frac{(k_0 T)^{r+s+1} e^{\xi}}{e^{z}-1} \int_0^{\infty} \Big[2\big\{ y^{r+s+1} + (y+z)^{r+s+1} \big\} \sinh^{-1}\sqrt{y/z}$$

$$- \big\{ y^{r}(y+z)^{s} + (y+z)^{r} y^{r} \big\} \big\{ (2y+z)\sinh^{-1}\sqrt{y/z} - \sqrt{y(y+z)} \big\} \Big] e^{-y} dy, \qquad (9.138)$$

where $\int_{-\hbar\omega_e}^{\infty} h(E)F(E)dE = \int_0^{\infty} F(E)\,dE$, $\sinh^{-1}\sqrt{x} = \cosh^{-1}\sqrt{x+1}$

are employed. Inserting the relation $\sinh^{-1} t = \ln(t + \sqrt{t^2+1})$ and integrating by parts, we obtain

$$\begin{cases} d_{rs} = (k_0 T)^{r+s+1} e^{\xi} z e^{\frac{1}{2}z} \delta_{rs} / (e^{z}-1), \\ \delta_{rs} = P_{rs}(z) K_0(\tfrac{1}{2}z) + Q_{rs}(z) K_1(\tfrac{1}{2}z). \end{cases} \qquad (9.139)$$

K_0 and K_1 are the modified Bessel functions and defined by

$$\int_0^\infty (y^2+2xy)^{p-1/2} e^{-sy} dy = \pi^{1/2} \Gamma(p+1/2) \left(\frac{2x}{s}\right)^p e^{sx} K_p(sx), \quad p \geqq 0. \tag{9.140}$$

$P_{rs}(z)$ and $Q_{rs}(z)$ are polynomials in Z. δ_{rs} for small r, s are given in the following:

$$\left\{\begin{aligned} &\delta_{00} = K_1\left(\tfrac{1}{2}z\right), \quad \delta_{01} = \delta_{10} = z K_0\left(\tfrac{1}{2}z\right) + 2K_1\left(\tfrac{1}{2}z\right), \\ &\delta_{11} = \frac{7}{2} z K_0\left(\tfrac{1}{2}z\right) + (z^2+6) K_1\left(\tfrac{1}{2}z\right), \\ &\delta_{02} = \delta_{20} = \frac{5}{2} z K_0\left(\tfrac{1}{2}z\right) + (z^2+6) K_1\left(\tfrac{1}{2}z\right), \\ &\delta_{12} = \delta_{21} = (z^2+13z) K_0\left(\tfrac{1}{2}z\right) + (6z^2+24) K_1\left(\tfrac{1}{2}z\right). \end{aligned}\right. \tag{9.141}$$

From (9.134), (9.136) and (9.139) the electrical conductivity is

$$\left\{\begin{aligned} &\sigma = \frac{4\varepsilon^*(k_0 T)^2}{3\pi^2 \hbar^2 w_e} (e^z - 1) G(\xi, z), \\ &G(\xi, z) = \frac{e^{\xi - 1/2 z}}{z} \left[\frac{\{\Gamma(5/2)\}^2}{\delta_{00}} + \sum_{n=2}^{\infty} \frac{(\Delta_r^{(n-1)})^2}{\Delta^{(n-1)} \Delta^{(n)}} \right], \end{aligned}\right. \tag{9.142}$$

where

$$\Delta^{(n)} = \begin{vmatrix} \delta_{00} & \delta_{01} & \cdots & \delta_{0\,n-1} \\ \delta_{10} & \delta_{11} & \cdots & \delta_{1\,n-1} \\ \vdots & \vdots & & \vdots \\ \delta_{n-1\,0} & \delta_{n-1,1} & \cdots & \delta_{n-1\,n-1} \end{vmatrix}, \quad \Delta_r^{(n-1)} = \begin{vmatrix} \delta_{00} & \cdots & \delta_{0\,n-2} & \Gamma(5/2) \\ \delta_{10} & & \delta_{1\,n-2} & \Gamma(7/2) \\ \vdots & & \vdots & \vdots \\ \delta_{n-1\,0} & & \delta_{n-1\,n-2} & \Gamma(n+3/2) \end{vmatrix}. \tag{9.143}$$

The thermoelectric power is given by

$$-\frac{e}{k_0}S = \frac{\begin{vmatrix} 0 & \Gamma(5/2) & \Gamma(7/2) & \Gamma(9/2) & \cdots \\ \Gamma(7/2) & \delta_{00} & \delta_{01} & \delta_{02} & \cdots \\ \Gamma(9/2) & \delta_{10} & \delta_{11} & \delta_{12} & \cdots \\ \Gamma(11/2) & \delta_{20} & \delta_{21} & \delta_{22} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \end{vmatrix}}{\begin{vmatrix} 0 & \Gamma(5/2) & \Gamma(7/2) & \Gamma(9/2) & \cdots \\ \Gamma(5/2) & \delta_{00} & \delta_{01} & \delta_{02} & \cdots \\ \Gamma(7/2) & \delta_{10} & \delta_{11} & \delta_{12} & \cdots \\ \Gamma(9/2) & \delta_{20} & \delta_{21} & \delta_{22} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \end{vmatrix}} - \xi, \qquad (9.144)$$

The value of G obtained by retaining N terms in the series $\sum_{n=2}^{\infty}$ in (9.142) is denoted by $G^{(N)}$, and $S^{(N)}$ is the value of S obtained by retaining $N+2$ rows and columns of the determinants in (9.144). First few approximations for G, S are given by

$$G^{(0)} = 9\pi e^{\xi - \frac{1}{2}z} \Big/ \{16z\, K_1(\tfrac{1}{2}z)\}, \quad -\frac{e}{k_0}S^{(0)} = \frac{5}{2} - \xi, \qquad (9.145)$$

$$\left\{ \begin{aligned} G^{(1)} &= \frac{9\pi}{32}\,\frac{e^{\xi-\frac{1}{2}z}}{z}\,\frac{(4z^2+9)K_1(\frac{1}{2}z) - 6z\,K_0(\frac{1}{2}z)}{2(z^2+2)K_0^2(\frac{1}{2}z) - z\,K_0(\frac{1}{2}z)K_1(\frac{1}{2}z) - 2z^2 K_0^2(\frac{1}{2}z)}, \\ -\frac{e}{k_0}S^{(1)} &= \frac{5}{2}\,\frac{(4z^2+11)K_1(\frac{1}{2}z) - 10z\,K_0(\frac{1}{2}z)}{(4z^2+9)K_1(\frac{1}{2}z) - 6z\,K_0(\frac{1}{2}z)} - \xi. \end{aligned} \right. \qquad (9.146)$$

Now, we consider the two limiting cases: a) high temperatures ($z \ll 1$) and b) low temperatures ($z \gg 1$).

a) *High temperatures* :

For small values of t, $K_0(t)$ and $K_1(t)$ become

$$\begin{cases} K_0(t) = \left(\ln\frac{2}{t} - 0.5722\cdots\right)\left(1+\frac{t^2}{4}+\cdots\right)+\frac{t^2}{4}+\cdots, \\ K_1(t) = \frac{1}{t} - \frac{t}{2}\ln\frac{2}{t}\left(1+\frac{t^2}{8}+\cdots\right). \end{cases} \qquad (9.147)$$

Then, we have

$$G^{(0)} = \frac{9\pi e^{\xi}}{32} = 0.8836\, e^{\xi}, \quad -\frac{e}{k_0}S^{(0)} = \frac{5}{2} - \xi . \qquad (9.148)$$

$$G^{(1)} = \frac{81\pi\, e^{\xi}}{256} = 0.994\, e^{\xi}, \quad -\frac{e}{k_0}S^{(1)} = \frac{55}{18} - \xi = 3.055 - \xi . \qquad (9.149)$$

The exact values of G and S at high temperature limit are readily found from the expression (9.125) for τ. They are

$$G = e^{\xi}, \quad -\frac{e}{k_0}S = 3 - \xi , \qquad (9.150)$$

and (9.149) indicates that $G^{(1)}$ and $S^{(1)}$ provide very good approximations for the exact solutions.

b) *Low temperatures* :

For large values of t, $K_0(t)$ and $K_1(t)$ are given by

$$\begin{cases} K_0(t) = \sqrt{\frac{\pi}{2t}}\, e^{-t}\left(1-\frac{1}{8t}+\cdots\right), \\ K_1(t) = \sqrt{\frac{\pi}{2t}}\, e^{-t}\left(1+\frac{3}{8t}+\cdots\right). \end{cases} \qquad (9.151)$$

Then, we have

$$G^{(0)} = 9\sqrt{\frac{\pi}{z}}\,\frac{e^{\xi}}{16}\,, \quad -\frac{e}{k_0}S^{(0)} = \frac{5}{2} - \xi\,, \tag{9.152}$$

$$G^{(1)} = \frac{3}{8}\sqrt{\pi z}\; e^{\xi}\,, \quad -\frac{e}{k_0}S^{(1)} = \frac{5}{2} - \xi\,. \tag{9.153}$$

It is shown that all the higher correction terms are zero in the limit $z \to \infty$ (the proof is complicated and will not be given here) and the (9.153) are exact in this limit. It should be noted that $G^{(1)} \gg G^{(0)}$ for large values of z. The expressions (9.153) may be obtained formally by assuming that the relaxation time is given by

$$\tau = \frac{\varepsilon^{*}\hbar(\hbar\omega_{l})^{1/2}}{(2m^{*})^{1/2}e^{2}\omega_{l}}\left(e^{\hbar\omega_{l}/k_{0}T} - 1\right). \tag{9.154}$$

Fröhlich and Mott [96)] obtained an expression equal to three times the result (9.154). This is an example illustrating the danger of relying on non-rigorous calculation.

More higher order calculations show that for $z \lesssim 1$ and $z \gg 1$ $G^{(1)}$ gives a good approximation to the exact result within 10%. However, at the intermediate temperatures ($z \sim 5$) the third order approximation $G^{(3)}$ is needed.

Effects of carrier-carrier scattering on the transport coefficients in semiconductors were discussed by using the variation principle.[97, 98) Drastic change of the minority carrier mobility is induced through the scatterings with majority carriers.[98) In some cases, e.g. minority holes in n-type InSb, the drag effects due to the majority electrons is strong enough to give the minority carriers a negative mobility.[98)

9.6 T^2-dependence of the electrical resistivity in the semimetals with elongated Fermi surface

Through the amplitude measurement of the radio frequency size effect (RFSE)[99) in antimony Gantmakher and Dolgopolor[100) obtained the result that temperature-dependent part of the mean free path for electrons and holes is proportional to T^{-2} between 1.17 and 4.2 K. Hartman[101) also observed the T^{-2}-dependence of the Hall coefficient and the magnetoresistance in bismuth in the region of 8 ~ 20 K, and Kukkonen and Sohn[102) reported the T^{-2}-dependence of the low temperature resistivity ($T < 4$ K) in bismuth.

As mentioned briefly in Section 9.1, the T^2-dependence of the resistivity is caused by the highly anisotropic Fermi surface and is not due to the carrier-carrier scattering. Gantmakher et al[100) indicated that the carrier-carrier scattering gives only one order longer mean path than the observed one.

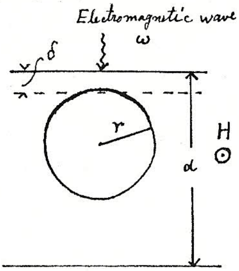


Fig. 9.7 Azbel'-Kaner resonance. $r \ll d$.

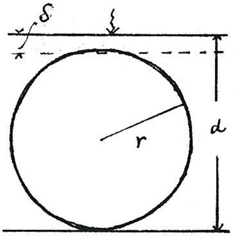


Fig. 9.8 Radio frequency size effect (RFSE) $r \approx d/2$.

Here, we present a brief explanation about RFSE.

Let apply a magnetic field perpendicular to the paper and propagate an electromagnetic wave perpendicular to the sample surface (See Figs. 9.7 and 9.8)).

If the cyclotron orbit r is enough smaller than the sample thickness d, carriers make a resonance absorption of the electromagnetic wave when their orbits enter in the skin depth region δ (Fig. 9.7), and the resonance condition is

$\omega = n\omega_c$ ($n = 1, 2, 3, \cdots$) where ω is the angular frequency of the electromagnetic wave and ω_c the cyclotron frequency. This is the so-called Azbel'-Kaner (AK) resonance, and the detailed discussions will be given in Chapter 13.

With decreasing the field intensity H, the cyclotron orbit becomes larger and RFSE appears in the case of $r \approx d/2$. This effect is not a true "time" resonance such as AK resonance but a geometrical or "space" resonance. Since the order of mismatching is δ, the spectral line width $\Delta H/H$ is $\sim \delta/d$. Resonance peak heights decrease with the carrier mean free path and the line widths remain unchanged. This is the characteristic of the geometrical resonance. Amplitude of the resonance lines A (the resonance lines are obtained by measuring $\partial X/\partial H$, where X is the imaginary part of the surface impedance $Z = R - iX$ (See Chapter 13)) is related to the mean free path l by

$$A \propto \exp(-\Lambda/l), \quad \ln A(T) = \text{const.} - \frac{\Lambda}{l} . \qquad (9.155)$$

As is readily shown from Fig. 9.8, $\pi r \doteqdot \pi d/2 \doteqdot \Lambda$.

Put $l = (l_0^{-1} + T^n/\beta)^{-1}$, where $l_T \equiv \beta/T^n$ is the temperature dependent mean free path. Then, we have

$$\ln\left(\frac{C}{A(T)} + 1\right) = \frac{\pi d}{2 l_0} + \frac{\pi d}{2}\frac{T^n}{\beta}, \quad C : \text{constant}. \qquad (9.156)$$

According to Gantmakher et al [100] l_T for electrons and holes were found to be

$$l_T^{el} = 0.22/T^2 \,(\text{cm}), \quad l_T^{h} = 0.68/T^2 \,(\text{cm}). \qquad (9.157)$$

Spectral lines of RFSE are enough sharp to be separable from many other lines due to the complex Fermi surface. Therefore, RFSE is a powerful tool for studing the Fermi surface.[99]

Since the carrier - carrier scattering also gives the T^2-dependence to the electrical resistivity, we first estimate the probability of the carrier - carrier collision. The differential cross section for the scattering process of an electron from a state k to k' by a screened Coulomb potential $U(r) = (e^2/\kappa r)\exp(-8_s r)$ is given by

$$d\sigma = \left(\frac{2m^* e^2}{\varkappa \hbar^2}\right)^2 \left(|k-k'|^2 + q_s^2\right)^{-2}. \qquad (9.158)$$

The screening constant q_s is comparable to the Fermi momentum k_F and then, we obtain $k_F \approx q_s \approx 1/(100a)$ for Bi and $k_F \approx q_s \approx 1/(10a)$ for Sb, where a denotes the lattice constant. Then the total cross section for $k = k' = k_F$ is expressed in terms of the Fermi energy E_F:

$$\sigma = 16\pi \left(\frac{m^* e^2}{\varkappa \hbar^2}\right)^2 \left[q_D^2 (4k_F^2 + q_D^2)\right]^{-1} \approx \left(\frac{e^2}{\varkappa E_F}\right)^2. \qquad (9.159)$$

Dimensional consideration directly leads to (9.159). In consideration of the Pauli principle the mean free path limited by the electron-electron scattering is given by

$$l_{e-e}^{-1} \approx \sigma \frac{1}{N_e}\left(\frac{\partial N_e}{\partial E}\right)^2_{E=E_F} (k_0 T)^2, \quad l_{e-e} \approx N_e \left(\frac{\varkappa}{e^2}\right)^2 \left(\frac{\partial N_e}{\partial E}\right)^{-2}_{E=E_F} \left(\frac{E_F}{k_0 T}\right)^2, \qquad (9.160)$$

where N_e denotes the carrier density. Substituting $N_e \approx 10^{20}\,\mathrm{cm}^{-3}$, $\partial N_e/\partial E \approx 10^{33}\,\mathrm{erg}^{-1}\mathrm{cm}^{-3}$ and $\varkappa \approx 100$ 103), we obtain $l_{e-e} \approx 10/T^2$, which is one order longer than the observed value (9.157).

In the following we calculate the electrical resistivity due to electron-phonon scattering on a small cylindrical Fermi surface.90) The Fermi surface is approximated by a cylinder with major axis $2k_{F\parallel}$ and minor axis $2k_{F\perp}$ where $k_{F\parallel} \gg k_{F\perp}$. $k_{F\parallel}/k_{F\perp}$ is ~ 5 for electrons and ~ 3 for holes (See (8.54)).

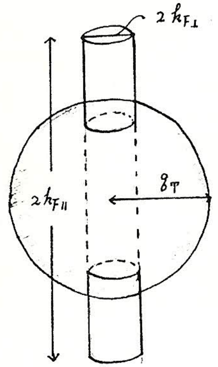


Fig. 9.9 Relation between the cylindrical Fermi surface and the thermal phonons at intermediate temperatures.

average wave vectors q of the phonons excited at a temperature T are

$$q \sim q_T = k_0 T/\hbar v_s . \qquad (9.161)$$

Let introduce the temperatures $T_\parallel$ and $T_\perp$ defined by

$$T_\parallel = 2\hbar k_{F\parallel} v_s / k_0 , \quad T_\perp = 2\hbar k_{F\perp} v_s / k_0 .$$

It can be readily shown that at the temperatures $T \gg T_\parallel$ the resistivity ρ varies as T and for $T \ll T_\perp$ $\rho \propto T^5$. The interesting case arises at intermediate temperatures, $T_\parallel > T > T_\perp$, where the sphere of the excited phonons is larger than the diameter of the cylinder but smaller than the height (see Fig 9.9). In this region we can see $\rho \propto T^2$ as follows. According to (9.50) the resistivity takes the form

$$\rho = \langle |M_{kk'}|^2 n_q (1 - \cos\theta) \rangle . \qquad (9.162)$$

Since $q_T > 2k_{F\perp}$, large angle scattering is allowed and then the factor $(1-\cos\theta) = (1-\cos\theta_\perp)$ does not contribute any temperature dependence, where $\cos\theta_\perp = (k_\perp \cdot k_\perp')/k_\perp k_\perp'$. Apperance of $\theta_\perp$ is due to the fact that only the perpendicular component of q affect the current.

As can been seen from Fig. 9.9, the area of the surface of allowed phonon state is $2\pi k_{F\perp} q_T \propto T$. Combining it with $|M_{kk'}|^2 \propto q$, we obtain $\rho \propto T^2$. More detailed derivation is given in the following. As is shown in Appendix 6, the electrical resistivity arising from electron-phonon scattering has the form

$$\rho = \frac{\sum_{k}\sum_{k'} V(k.k')\left\{\Phi(k)-\Phi(k')\right\}^2}{2k_0 T\left(\sum_{k} e v_k \Phi(k)\frac{\partial f_0}{\partial E_k}\right)^2}, \qquad (9.163)$$

where $V(k.k')$ is given in (9.8). It is rewritten in the form

$$V(k.k') = \frac{\pi D^2}{d\, v_s}\, \delta_{k',k+q}\, q\, f_k^0 (1-f_{k'}^0)\, n_q\, \delta(E_k - E_{k'} + \hbar\omega_q). \qquad (9.164)$$

In the case where $C(E) =$ constant gives a good approximation (see Section 9.1), we can put

$$\Phi(k) = k\cdot u \quad (u \parallel \mathcal{E} \parallel x:\ \text{a constant vector}), \qquad (9.163)$$

and then, u disappears in the numerator and denominator of (9.163). In the present model we assume $m_\parallel/m_\perp \gg 1$ and the electric current does not flow along the major axis direction. Consequently, we should take u being perpendicular to the major axis.

The factor $(\sum_k \cdots)^2$ in the denominater of (9.163), which is independent on T, is calaculated as follows.

$$\sum_k e\, v_x\, \Phi(k) \frac{\partial f_0}{\partial E_k} = - \frac{2 e u \hbar}{(2\pi)^3 m^*} \int d\mathbf{k}\, k_x^2\, \delta(E_k - \zeta) . \qquad (9.166)$$

In consideration of $E_k = (\hbar^2/2m_\perp)\, k_\perp^2 \; (m^* = m_\perp)$, (9.166) becomes

$$- \frac{e u}{2\pi^2 \hbar} \Omega_F , \; (\Omega_F = \pi k_{F\perp}^2 k_{F\parallel}) . \qquad (9.167)$$

Accordingly, we have

$$\text{the denominator of } (9.163) = 2 k_0 T\, u^2 \left(\frac{e \Omega_F}{2\pi^2 \hbar} \right)^2 . \qquad (9.168)$$

On the other hand, the numerator of (9.163) is given by

$$\frac{\pi D^2}{d\, v_s} \frac{2 u^2}{(2\pi)^6} \int d\mathbf{q}\, q\, q_x^2\, n_q \int d\mathbf{k}\, f_0(E_k) \left\{ 1 - f_0(E_k + \hbar\omega_q) \right\} \delta(E_k - E_{k'} + \hbar\omega_q)\, \delta_{k';k+q} . \qquad (9.169)$$

Integration of the δ-function over $\mathbf{q}$ becomes

$$\int d\mathbf{q}\, \delta(E_k - E_{k'} + \hbar\omega_q)\, \delta_{k';k+q} = \int dq_\perp\, q_\perp\, dq_\parallel\, d\varphi_q\, \delta\left[\frac{\hbar^2}{2m^*} (2 k_\perp \cdot q_\perp + q_\perp^2) - \hbar v_s q \right]$$

$$= m^*/(\hbar^2 k_\perp) \int dq_\perp\, dq_\parallel . \qquad (9.170)$$

Neglecting the phonon energy in the δ-function, we get $q_\perp < 2k_\perp$. By changing the variables $(q_\perp, q_\parallel)$ into $(q_\perp, q)$, we obtain

$$\int dq_\parallel \rightarrow 2 \int_0^{q_{max}} \frac{q\, dq}{\sqrt{q^2 - q_\perp^2}} . \qquad (9.171)$$

Using the relation

$$\int f_0(E) \left\{ 1 - f_0(E + \hbar\omega_q) \right\} dE = k_0 T \frac{e^z z}{e^z - 1} , \qquad z \equiv \hbar v_s q / k_0 T . \qquad (9.172)$$

one gets the expression for the numerator of (9.163) as

$$\frac{2u^2 D^2}{(2\pi)^4 d v_s}\left(\frac{m^*}{\hbar^2}\right)^2\left(\frac{k_{F\parallel}}{k_{F\perp}}\right)k_0 T\left(\frac{k_0 T}{\hbar v_s}\right)^2\int_0^{2k_{F\perp}} dq_\perp\, q_\perp^2 \int_{Z_\perp}^{Z_{max}} \frac{dZ\, Z^3 e^Z}{\sqrt{1-\left(\frac{Z_\perp}{Z}\right)^2}\,(e^Z-1)^2}\,, \qquad (9.173)$$

where $Z_\perp = 2\hbar v_s q_\perp / k_0 T$, $Z_{max} = \hbar v_s q_{max} / k_0 T$.

The resistivity (9.163) becomes

$$\rho = \frac{\hbar^2 D^2}{4 e^2 d v_s \Omega_F^2}\left(\frac{m^*}{\hbar^2}\right)^2\left(\frac{k_{F\parallel}}{k_{F\perp}}\right)\left(\frac{k_0 T}{\hbar v_s}\right)^2\int_0^{2k_{F\perp}} dq_\perp\, q_\perp^2 \int_{Z_\perp}^{Z_{max}} \frac{dZ\, Z^3 e^Z}{\sqrt{1-\left(\frac{Z_\perp}{Z}\right)^2}\,(e^Z-1)^2}\,. \qquad (9.174)$$

In the case of $Z_\perp \ll 1$, $Z_{max} \gg 1$, we can put $Z_\perp \to 0$ and $Z_{max} \to \infty$. Accordingly, we obtain $\rho \propto T^2$. Comparison between (9.174) and the observed resistivity in bismuth is shown in Fig. 9.10, where $k_{F\parallel}/k_{F\perp}$ is assumed.90)
The Bloch formula gives a reasonable fit to the data up to only below 1.5 K. Rapid increase of the observed resistivity at 4 ~ 5 K is attributed to intervalley electron-phonon scattering.

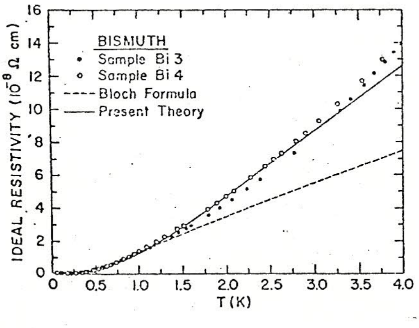


Fig. 9.10 Temperature-dependent resistivity of Bi: Comparison of theory with experiment.

9.7 Validity of the Boltzmann-Bloch Equation

The conventional theory of the electrical resistivity of metals is based on the Boltzmann-Bloch equation. The usual derivation of the equation includes two important assumptions.$^{104)}$

(1). For simplicity, we consider the case in which the origin of the scattering is an irregular static potential. The scattering potential is assumed to be the combined effect of a large number of similar centers:

$$W(r) = \sum_n w(r - R_n). \tag{9.175}$$

If an exact eigenfunction of the system is expanded in terms of the eigenstates of the unperturbed Hamiltonian as

$$\psi(r.t) = \sum_{k.l} a_{kl}(t)\, \psi_{kl}(r)\, e^{-iE_l(k)t/\hbar}, \tag{9.176}$$

(9.176) leads to the equation

$$i\hbar\, \dot{a}_{kl} = \sum_{k'l'} \langle k.l \,|\, W \,|\, k'.l' \rangle e^{i\{E_l(k) - E_{l'}(k')\}t/\hbar} a_{k'l'}. \tag{9.177}$$

where

$$\langle k.l \,|\, W \,|\, k'l' \rangle = \int \psi^*_{kl}(r)\, W(r)\, \psi_{k'l'}(r)\, dr. \tag{9.178}$$

In first order approximation we may regard the a on the right-hand side of (9.177) as constant: hence

$$a_{k\ell}(t) = -\sum_{k'\ell'} \langle k.\ell \,|\, W \,|\, k'.\ell' \rangle\, a_{k'\ell'}(0)\, \frac{e^{i(E-E')t/\hbar} - 1}{E - E'}, \tag{9.179}$$

where $E = E_\ell(k)$ and $E' = E_{\ell'}(k')$.

If the electron is in a state $(k.\ell)$ at $t=0$; then probability of finding it in the state $(k'.\ell')$ at time t is

$$|\langle k'\ell' \,|\, W \,|\, k.\ell \rangle|^2\, 2\, \frac{1-\cos(E'-E)t/\hbar}{(E'-E)^2} . \tag{9.180}$$

This is the transition probability from state $(k.\ell)$ to $(k'.\ell')$. If we take more than one of the $a(0)$ into account in (9.179), cross terms appear in the square (9.180).

The first assumption states that the expansion coefficients $a_{k\ell}$ in (9.176) have randomly distributed phases and the cross terms do not appear in the transition probability. This is called "repeated random phase" assumption.104)

The repeated random phase assumption has been discussed in connection with the Boltzmann equation by Kohn-Luttinger105) and Greenwood.106) They derived the usual Boltzmann equation from the equation of motion of the density matrix and showed that in the case of elastic scattering by rigid impurity centers, the random phase approximation can be replaced by the assumption of spatially random distribution of the scattering centers.

(2). From (9.180) the change in the distribution function due to collisions is given by

$$f(k,l.t) - f(k,l.0) = \sum_{k'l'} |\langle k'l'|W|k.l\rangle|^2 \{f(k'l') - f(k.l)\} D(t), \tag{9.181}$$

where

$$D(t) = 2\,\frac{1-\cos(E'-E)t/\hbar}{(E'-E)^2}. \tag{9.182}$$

The function D, considered as a function of E', has a steep maximum at $E'=E$, and its peak height is given by $(t/\hbar)^2$. The width of this maximum is of the order of $\hbar/t$. Therefore, the area formed by D is proportional to $t/\hbar$. Actually, we have

$$\int D\,dE = \frac{2\pi t}{\hbar}. \tag{9.183}$$

Then, if the variation of the other factors in (9.18) with E' is weak, we may insert their values for $E'=E$ and carry out the integration on D. Using the relation (9.183), we obtain

$$\dot{f}(k.l) = \frac{2\pi}{\hbar}\sum_{k'l'} |\langle k'l'|W|k.l\rangle|^2 \{f(k'l') - f(kl)\}\,\delta(E'-E). \tag{9.184}$$

$f(k'l')$ changes by a large amount over an interval k_0T around E_F, which is the most important region in the conduction phenomena.

Accordingly, (9.184) is valid only if the following is satisfied:

$$k_0T > \frac{\hbar}{t}. \tag{9.185}$$

Since we have used the first order perturbation, the collision time τ should be longer than t. Therefore, we have

$$k_0 T > \frac{\hbar}{\tau} . \qquad (9.186)$$

With decreasing temperatures τ tends to a constant limit. Then, at low temperatures the assumption (9.186) is no more valid Therefore, one might consider that the Boltzmann-Bloch equation is founded on a unsound basis. However, Landau has argued in an abstract way that as long as we are dealing with elastic scatterings, we can derive the results of the theory by a slightly different approach without using (9.186).[104, 107] More detailed arguments have been given in a more direct way.[106,108] It is concluded from these arguments that (9.186) should be replaced by a much weaker inequality

$$E_F > \frac{\hbar}{\tau} . \qquad (9.187)$$

This condition is pratically always satisfied in metals.

Chapter 10 Interaction with Localized Spins

10.1 Magnetic Semiconductors

Since the magnetic semiconductors contain the atoms with magnetic moment, these materials behave in different way from the usual semiconductors without magnetic moment.

In the presence of a magnetic field spins tend to align along the field direction. This alignment modifies the interaction between carriers and magnetic moments and the transport properties are affected by the magnetic field. EuS and $CdCr_2Se_4$, which are ferromagnetic semiconductors, exhibit large magnetoresistance and around the Curie temperature T_c marked maximum of the magnetoresistance appears. Mobility of EuS is strongly enhanced near T_c by applying a magnetic field and n-type $CdCr_2Se_4$ shows a large negative magnetoresistance in the vicinity of T_c. These behaviors indicate that carriers are strongly scattered by the interactions with localized spins.

Ferrimagnetic semiconductor $FeCr_2Se_4$ and antiferromagnetic semiconductor MnTe exhibit the magnon drag effect in the thermoelectric phenomena, and in MnTe the thermoelectric power and the electrical resistivity show anomaly at the Néel temperature T_N (See Fig 10.3).

Band structures of the magnetic semiconductors have been extensively studied. However, the information obtained still remains in the stage of a qualitative interpretation in comparison with the ypical semiconductors Ge. Si, GaAs, InSb and so on. Techniques f synthesizing crystals and controlling impurity content are more difficult than the cases in the typical semiconductors abovementioned.

In many magnetic semiconductors the electric current is carried by the electrons and/or holes belonging narrow d-bands, and the conduction mechanism is different from that of usual semiconductors in which carriers are moving in the broad bands.

In Sections 10.1 — 10.4 we consider the case in which the carriers moving in the broad band interact with the localized spins through the s-d interaction.

10.2 s-d interaction

We write the s-d exchange interaction between the conduction electron and the localized spin in the form

$$H' = -2 \sum_n J(r - R_n)(\mathbf{s} \cdot \mathbf{S}_n) , \qquad (10.1)$$

where $\mathbf{s}$ denotes the electron spin, $\mathbf{S}_n$ the localized spin at R_n and J the exchange integral. (10.1) is called "s-d interaction". If the localized moment is specified by $\mathbb{J}$ instead of $\mathbf{S}$, $\mathbf{S}_n$ in (10.1) should be replaced by

$$(g-1)\,\mathbb{J} = \mathbf{S} , \qquad (10.2)$$

where g is the g-factor. Proof of (10.2) is as follows:

As is well known, there are the following relations between $\mathbf{J}$, $\mathbf{S}$ and $\mathbf{L}$

$$g\mathbb{J} = \mathbb{L} + 2\mathbb{S}, \quad \mathbb{J} = \mathbb{L} + \mathbb{S}. \tag{10.3}$$

From (10.3) we arrive at the result of $(g-1)\mathbb{J} = \mathbb{S}$.

Total Hamiltonian is given by

$$H = H_e + H' + H_s, \tag{10.4}$$

where H_e is the unperturbed Hamiltonian of the electron system and H_s the corresponding Hamiltonian of the localized spin system. Throught Sections 10.2 - 10.4 we assume that H' is small enough so that the perturbation theory is applicable. However, this assumption is not always satisfied in actual magnetic semiconductors.

Nevertheless, the following treatments are useful since the results obtained from the perturbational calculation reveal qualitatively many interesting characteristics of the magnetic semiconductors.

The follwing calculations are mainly due to Haas.[109]

We consider the case in which the influence on the spin system exerted by the electron system may be neglected since electron number is enough small.

Eigenstates of the electron system are expressed by the Bloch functions φ_{bK} (b: band index) and those of the localized spins by α.

α forms a quasi-continuous spectrum because α takes $(2S+1)^N$ different values, where N is the concentration of the localized spins.

In the case where the localized spins are strongly coupled each other, $(2S+1)^N$ levels form the spin wave (magnon) state.

As the electronic motion is much faster than the spin motion, it is permitted to treat the spin states adiabatically when we consider the electronic states. Accordingly, the first order energy shift of the electron energy is given by

$$\Delta E_{bk}^{(1)} = \sum_{\alpha} w_\alpha \langle \varphi_{bk}(r).t,\alpha | H' | \varphi_{bk}(r)\, t,\alpha \rangle$$

$$= -2 \sum_{n} \int |u_{bk}(r)|^2 J(r-R_n)\,dr \, \langle t|s|t\rangle \sum_{\alpha} w_\alpha \langle \alpha | S_n | \alpha \rangle , \qquad (10.5)$$

where the Bloch function is expressed by $\varphi_{bk}(r) = e^{ikr} u_{bk}(r)$, w_α is the probability for α-state and t denotes the electron spin state + or −.

average value of S_n is assumed to be parallel to the z-axis.

If all magnetic atoms are equivalent, we can put

$$\int |u_{bk}(r)|^2 J(r-R_n)\,dr = J_{bk}/N, \qquad (10.6)$$

where $\varphi_{bk}(r)$ is normalized in a unit volume.

Hence,

$$\Delta E_{bk\pm}^{(1)} = \mp S J_{bk} \left(\frac{M(T)}{M(0)} \right), \qquad (10.7)$$

where $M(0)$ is the saturation magnetization $-Ng\mu_B S$ (μ_B : Bohr magneton) and $M(T)$ is given by

$$M(T) = \sum_n \langle S_n \rangle = \sum_n \sum_\alpha w_\alpha \langle \alpha | S_n | \alpha \rangle . \tag{10.8}$$

(10.7) indicates that at the temperature $T < T_c$ an energy gap appears between + spin state and − state of the conduction electron (spin splitting of the band). at $T > T_c$ where $M(T) = 0$, magnetic field induces the magnetization $M = \chi H$ (χ : susceptibility), then

$$\Delta E^{(1)}_{bk\pm} = \mp S J_{bk} \left(\frac{\chi H}{M(0)} \right) . \tag{10.9}$$

From (10.7) change of the band gap becomes

$$\Delta E_G = - S (|J_c| + |J_v|) \frac{M(T)}{M(0)} , \tag{10.10}$$

where J_c and J_v represent the exchange integrals for the conduction and valence bands. Temperature dependence of the band gap E_G is schematically represented by Fig. 10.1. $E_G(T)$ has a term $-\beta T$ which is usually seen in the non-magnetic semiconductors. Behavior represented by Fig. 10.1 is, for example, observed in $CdCr_2Se_4$.110)

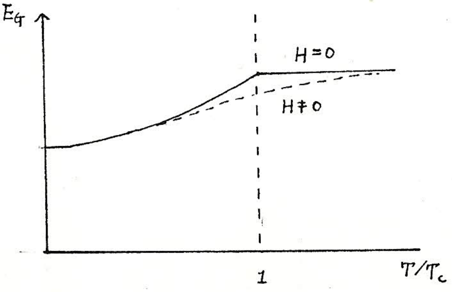


Fig. 10.1 Temperature dependence of E_G in the ferromagnetic semiconductors.

On the other hand in the antiferromagnetic semiconductors the band splitting appears only in the presence of a magnetic field.

Consider the shallow donor level just below the conduction band. Eigenstate of an electron trapped in the shallow level is formed by the superposition of the states near the conduction band edge. Therefore, the level splitting of the shallow level is given by (10.7) for $k = 0$.

Accordingly, the energy gap between the conduction band edge and the impurity level with identical spin remain unchanged. The situation is the same in the shallow acceptor level. On the other hand the spin splitting in the deep level may be negligibly small since the exchange integral is small due to small spatial extension of the impurity wave function.

10.3 Spin Disorder Scattering due to Localized Spins

In the previous section we mentioned that s-d interaction lifts the spin degeneracy of the band. Non-diagonal part of the same interaction becomes an origin of the scattering of electrons.

At finite temperatures spin continually fluctuates. This fluctuation causes the scattering of electrons. This is called "spin disorder scattering" and usually this scattering process is more important than the collisions with phonons and impurity centers.

Semiconducting carriers with long wave length are strongly scattered by long wave length component of the spin fluctuation.

In ferromagnetics the long wave spin fluctuation is enhanced around Tc. This phenomena is due to the critical fluctuation related to the second order phase transition at Tc. Therefore, it is expected that the spin disorder scattering in the ferromagnetic semiconductors exhibits a maximum at Tc. This behavior is clearly observed in Gd-doped EuS.[111]

In the following the mobility controlled by the spin disorder scattering is calculated in the approximation of the perturbational calculation.

Transition probabilities for spin conserving and spin flip processes are given by

$$P(k\pm,\alpha,\ k'\pm,\alpha') = \frac{2\pi}{\hbar}\left|\langle k\pm\alpha|\mathcal{H}'|k'\pm\alpha'\rangle\right|^2 \delta(E_{k\pm}+\varepsilon_\alpha-E_{k'\pm}-\varepsilon_{\alpha'}), \quad (10.11)$$

$$P(k\pm\alpha,\ k'\mp\alpha') = \frac{2\pi}{\hbar}\left|\langle k\pm\alpha|\mathcal{H}'|k'\mp\alpha'\rangle\right|^2 \delta(E_{k\pm}+\varepsilon_\alpha-E_{k'\mp}-\varepsilon_{\alpha'}), \quad (10.12)$$

where ε_α and $\varepsilon_{\alpha'}$ correspond to the energy of the spin system. Matrix elements corresponding to (10.11) and (10.12) are given by

$$\langle k\pm\alpha|\mathcal{H}'|k'\pm\alpha'\rangle = \mp\sum_n e^{i(k'-k)\cdot R_n}\langle\alpha|S_{nz}|\alpha'\rangle\int|u(r)|^2 e^{i(k'-k)(r-R_n)}$$

$$\times J(r-R_n)\,d\mathbf{r}, \quad (10.13)$$

where the Bloch function is written as $\varphi_k = e^{ikr}u(r)$ and the band index is omitted.

Defining

$$J(k) \equiv N\int|u(r)|^2 e^{ik(r-R_n)} J(r-R_n)\,d\mathbf{r}, \quad (10.14)$$

we obtain

$$\langle k\pm\alpha \,|\, H' \,|\, k'\pm\alpha' \rangle = \mp \frac{1}{N} J(k'-k) \sum_n \langle \alpha \,|\, S_{nz} \,|\, \alpha' \rangle e^{i(k'-k)\cdot R_n} . \qquad (10.15)$$

Similarly, by using the relations

$$\begin{cases} \mathbf{s}\cdot \mathbf{S}_n = s_z S_{nz} + \frac{1}{2}(s^+ S_n^- + s^- S_n^+), \\ s^\pm \equiv s_x \pm i s_y , \; S_n^\pm \equiv S_{nx} \pm i S_{ny} , \end{cases} \qquad (10.16)$$

the matrix element of the spin flip process is

$$\langle k\pm\alpha \,|\, H' \,|\, k'\mp\alpha' \rangle = -\frac{1}{N} J(k'-k) \sum_n \langle \alpha \,|\, S_{n\pm} \,|\, \alpha' \rangle e^{i(k'-k)\cdot R_n} . \qquad (10.17)$$

Change of the distribution function due to the collision process is expressed by

$$\left(\frac{\partial f_{k+}}{\partial t}\right)_{coll.} = \sum_\alpha \sum_{\alpha'} w_{\alpha'} \left[f_{k'+}(1-f_{k+}) P(k'+\alpha', k+\alpha) + f_{k'-}(1-f_{k+}) P(k'-\alpha, k+\alpha) \right]$$

$$- \sum_\alpha \sum_{\alpha'} w_\alpha \left[f_{k+}(1-f_{k'+}) P(k+\alpha, k'+\alpha') + f_{k+}(1-f_{k'-}) P(k+\alpha, k'-\alpha) \right] . \qquad (10.18)$$

On making use of $E_{k\pm} = E_{0\pm} + (\hbar^2/2m^*)k^2$, the drift term becomes

$$\left(\frac{\partial f_{k+}}{\partial t}\right)_{drift} = e\mathcal{E} \frac{\hbar k_x}{m^*} \frac{\partial f_{k\pm}}{\partial E_{k\pm}} , \quad (\mathcal{E} \,/\!/\, x) . \qquad (10.19)$$

Similarly, we can obtain the equation for f_{k-}. Thus, the Boltzmann equation is

$$\left(\frac{\partial f_{k\pm}}{\partial t}\right)_{coll.} + \left(\frac{\partial f_{k\pm}}{\partial t}\right)_{drift} = 0 . \qquad (10.20)$$

Assume $f_{k\pm}$, as usual, as

$$f_{k\pm} = f_{k\pm}^{0} - \Phi_{k\pm}\frac{\partial f_{k\pm}^{0}}{\partial E_{k\pm}} . \tag{10.21}$$

Throughout this Chapter we assume that the spin system is in thermal equilibrium. This corresponds to neglect of the magnon drag effect.

Retaining the linear terms in $\Phi_{k\pm}$, we obtain

$$\left(\frac{\partial f_{k+}}{\partial t}\right)_{coll.} = \sum_{\alpha}\sum_{\alpha'} w_\alpha \frac{\partial f_{k+}^{0}}{\partial E_{k+}}\left[P(k+\alpha, k'+\alpha')\left(\frac{1-f_{k'+}^{0}}{1-f_{k+}^{0}}\right)(\Phi_{k+}-\Phi_{k'+})\right.$$

$$\left. + P(k+\alpha, k'-\alpha')\left(\frac{1-f_{k'-}^{0}}{1-f_{k+}^{0}}\right)(\Phi_{k+}-\Phi_{k'-})\right] . \tag{10.22}$$

Energy change of the spin system in the δ-functions included in (10.11) and (10.12) may be neglected as compared with that of the carrier system (elastic scattering approximation).

On making use of the relation, which is satisfied for any operators A and B:

$$\sum_{\alpha} w_\alpha \sum_{\alpha'} \langle\alpha|A|\alpha'\rangle\langle\alpha'|B|\alpha\rangle = \sum_{\alpha} w_\alpha \langle\alpha|AB|\alpha\rangle = \langle AB\rangle , \tag{10.23}$$

we obtain from (10.15) and (10.17)

$$\sum_{\alpha}\sum_{\alpha'} w_\alpha P(k+\alpha, k'+\alpha') = \frac{2\pi}{\hbar}\left|\frac{J(k-k')}{N}\right|^2 \delta(E_{k+}-E_{k'+})\sum_{n}\sum_{m}\langle S_{nz}S_{mz}\rangle$$

$$\times e^{i(k-k')(R_n-R_m)} , \tag{10.24}$$

$$\sum_{\alpha}\sum_{\alpha'} w_\alpha P(k+\alpha, k'-\alpha') = \frac{2\pi}{\hbar}\left|\frac{J(k-k')}{N}\right|^2 \delta(E_{k+}-E_{k'-})\sum_{n}\sum_{m}\langle S_n^{+}S_m^{-}\rangle$$

$$\times e^{i(k-k')(R_n-R_m)} . \tag{10.25}$$

$\sum_{n,m} \langle S_{nz} S_{mz} \rangle e^{i(k-k')(R_n-R_m)}$ and $\sum_{n\cdot m} \langle S_n^+ S_m^- \rangle e^{i(k-k')(R_n-R_m)}$ are the Fourier components of the spin correlation function which specifies a spatial extension of the spin fluctuation.

By introducing the generalized susceptibility

$$\chi_{ij}(k) = \left(\frac{g^2 \mu_B{}^2}{k_0 T}\right) \sum_n \sum_m \left\{ \langle S_{ni} S_{mj} \rangle - \langle S_{ni} \rangle \langle S_{mj} \rangle \right\} e^{ik(R_n-R_m)}, \qquad (10.26)$$

we can rewrite (10.24) and (10.25) and obtain the relaxation time by inserting $\Phi_{k\pm} = -e\,\mathcal{E}(\hbar k_x/m^*)\,\tau_{k\pm}$ into (10.22).

$$\frac{1}{\tau_{k\pm}} = \frac{2\pi}{\hbar}\frac{k_0 T}{(N g \mu_B)^2} \left\{ \sum_{k'} |J(k-k')|^2 \chi_z(k-k')\,\delta(E_{k\pm} - E_{k'\pm}) \right.$$

$$+ \sum_{k'} |J(k-k')|^2 \chi_x(k-k')\,\delta(E_{k\pm} - E_{k'\mp})$$

$$\left. + \sum_{k'} |J(k-k')|^2 \chi_y(k-k')\,\delta(E_{k\pm} - E_{k'\mp}) \right\}, \qquad (10.27)$$

where $\chi_{ij} = \chi_i \delta_{ij}$ and we employ that the terms including $\langle S_{ni} \rangle \langle S_{mj} \rangle$ vanish after integrating over k' since $\langle S_{ni} \rangle$ and $\langle S_{mj} \rangle$ do not depend on spational position.

How about $m = n$.

Mobility of electron is given by

$$\mu_\pm = -\frac{e\hbar^2}{m^{*2}} \frac{\sum_k (1/3)\, k^2 \left(\partial f^0_{k\pm}/\partial E_{k\pm}\right) \tau_{k\pm}}{\sum_k f^0_{k\pm}}. \qquad (10.28)$$

Since k is small in the semiconductors, $1/\chi_{ij}(k)$ may be expanded as

$$1/\chi_{ij}(k) = 1/\chi_{ij} + A_{ij} k^2, \qquad (10.29)$$

χ_{ij} is the susceptibility in the uniform magnetic field. A_{ij} was calculated by de Gennes - Villain.[112] If the magnetic atoms constitute a simple cubic lattice with lattice constant a and the exchange interaction is assumed to be finite only between the nearest neighbor atoms, A_{ij} is given by

$$A_{ij} = \delta_{ij}\, k_0 T_c\, a^2 / 2N(g\mu_B)^2 S(S+1). \qquad (10.30)$$

In the semiconductors with small carrier concentration $A_{ij}k^2$ term can be disregarded in comparison with $1/\chi_{ij}$. This is a good approximation in the region except $T \sim T_c$. In the same reason k-dependence of $J(k-k')$ may be neglected and we can put $J(k-k') \simeq J =$ constant.

Thus, (10.28) leads to

$$\mu_\pm = \frac{2(2\pi)^{1/2}(Ng\mu_B)^2 e \hbar^4}{3(m^*)^{5/2} J^2 (k_0 T)^{3/2}} \int_0^\infty \frac{t\, e^{-t}\, dt}{\chi_z + 2\lambda_\pm \chi_x [1 \mp (\delta/t)]^{1/2}}, \qquad (10.31)$$

where

$$\delta = (E_{0-} - E_{0+})/k_0 T = 2SJ\, M(T)/(M(0) k_0 T),$$

$$\lambda_\pm = \begin{cases} 1 : \text{ if } [1 \mp (\delta/t)]^{1/2} \text{ is real}, \\ 0 : \text{ if } [1 \mp (\delta/t)]^{1/2} \text{ is imaginary}. \end{cases} \qquad (10.32)$$

(10.31) indicates that mobility depends on the spin orientation. With the notation $n_\pm$ for carrier density the resistivity is given by $1/\rho = n_+ e\mu_+ + n_- e\mu_-$. Using $n_+/n_- = e^{\delta}$ and $n = n_+ + n_-$, one obtains

$$\frac{1}{\rho} = ne\left[\frac{\mu_+ e^{\delta/2} + \mu_- e^{-\delta/2}}{e^{\delta/2} + e^{-\delta/2}}\right]. \tag{10.33}$$

Let consider the qualitative feature of the mobility in the ferromagnetic semiconductors derived from (10.31).

At $T < T_c$ most of the electrons are populated in the + spin sub-band and then we observe the mobility μ_+. Since $\delta \gg 1$. we have $\mu_+ \propto (T^{3/2}\chi_z)^{-1}$. As T approaches T_c, the susceptibility χ becomes very large due to the critical fluctuation and $\mu_\pm \to 0$. Above the Curie temperature $\delta = 0$ and, therefore, $\mu = \mu_+ = \mu_-$. In this region χ obeys the Curie-Weiss law : $\chi = C/(T - \Theta)$, then $\mu \propto \{T^{3/2}(T-\Theta)\}^{-1}$. Qualitative characteristic of the mobility is shown in Fig. 10.2. More detailed considerations are needed in the vicinity of T_c.

Mobility of the photoexcited electron in EuS exhibits a similar behavior to Fig. 10.2 113) (See Section 10.6).

Mobility of the antiferromagnetic semiconductors is also given by

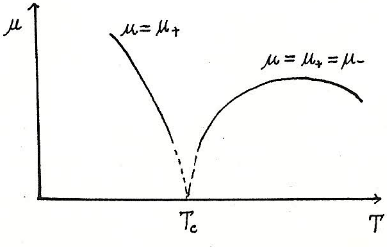


Fig. 10.2 Mobility in the ferromagnetic semiconductors

(10.31) with $\delta = 0$. Accordingly, we have

$$\mu = \frac{2(2\pi)^{1/2}(Ng\mu_B)^2 e\hbar^4}{3(m^*)^{5/2} J^2 (k_0 T)^{3/2}} (\chi_\parallel + 2\chi_\perp)^{-1}, \tag{10.34}$$

where $\chi_\parallel = \chi_z$, $\chi_\perp = \chi_x = \chi_y$. Hence, the mobility is inversely proportional to the average susceptibility $(\chi_\parallel + 2\chi_\perp)/3$.

Provided $E = \sum_i (\hbar^2/2m_i) k_i^2$, the factor $(m^*)^{5/2}$ included in the mobility μ_i along i-th direction should be replaced by

$$m_i^* (m_1^* m_2^* m_3^*)^{1/2}. \tag{10.35}$$

In antiferromagnetic crystals there is no long wave critical fluctuation around the Néel temperature T_N and the anomaly corresponding to Fig. 10.2 does not appear. However, a bend is observed at T_N, which is expected from (10.34). An example observed in MnTe is shown in Fig. 10.3.$^{114, 27)}$

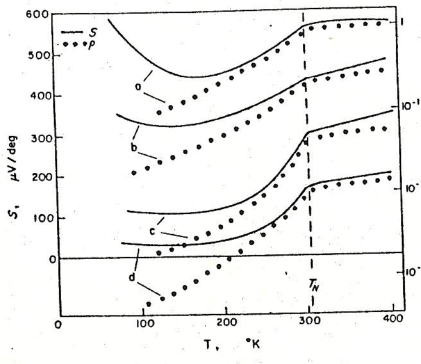


Fig. 10.3 Temperature dependences of the resistivity and the thermoelectric power of MnTe.$^{114, 27)}$

a, b, c : non-degenerate samples,

d : degenerate sample. $n \simeq 10^{20}\,\mathrm{cm}^{-3}$

$T_N = 307\,K$.

Behaviors of the thermoelectric power S at $T < T_N$ in Fig. 10.3 are explained in consideration of the magnon drag effect.

In the degenerate antiferromagnetic semiconductors the expression of the mobility is obtained by a replacement $(k_0 T)^{3/2} \rightarrow k_0 T \, E_F^{1/2}$. Namely, we obtain

$$\mu = \frac{\pi (N g \mu_B)^2 e \hbar^4}{\sqrt{2}\,(m^*)^{5/2} J^2 k_0 T \, E_F^{1/2}} \left(\chi_{\parallel} + 2 \chi_{\perp} \right)^{-1}, \qquad (10.36)$$

where E_F is measured from the band edge.

In the degenerate ferromagnetic semiconductors the mobility takes the form:

$$\mu_{\pm} = \frac{\pi (N g \mu_B)^2 e \hbar^4}{\sqrt{2}\,(m^*)^{5/2} J^2 k_0 T} \left[\chi_{\parallel} (E_F^{\pm})^{1/2} + 2 \chi_{\perp} (E_F^{\mp})^{1/2} \right]^{-1}, \qquad (10.37)$$

where $E_F^{\pm}$ are measured from the each subband edge.

10.4 Magnetoresistance of the Ferromagnetic Semiconductors

Magnetic field affects the mobility and the carrier concentration; both effects lead to a magnetoresistance.

At first we consider the change of the carrier concentration caused by an applied magnetic field. For definiteness we assume that the charge carriers are supplied by excitation from the donor centers, and the exchange coupling between the donor electron and the neighboring magnetic atom is given by γJ $(\gamma < 1)$, where J denotes the magnitude of the s-d interaction.

As has been mentioned in Section 10.2, γ is nearly equal to unity in the case of the shallow donor level, while $\gamma \ll 1$ for the deep level.

Since the energy change of conduction electrons with spin + or − is given by $E_\pm = \mp SJM(T)/M(0)$, the carrier densities in the ± subbands are given by

$$\left\{ \begin{aligned} n_\pm &= \frac{1}{2} N_c \exp\left[\{\zeta \mp SJM(T)/M(0)\}/k_0T\right], \\ N_c &= (m^* k_0 T/2\pi\hbar^2)^{3/2}. \end{aligned} \right. \tag{10.38}$$

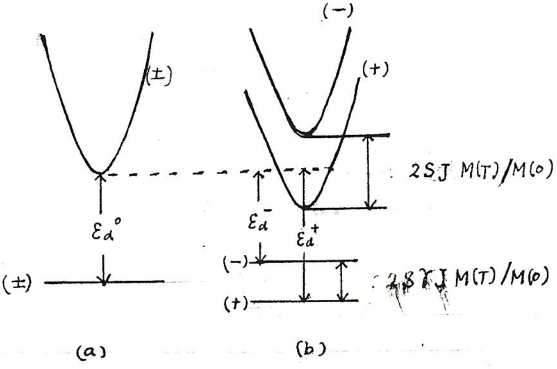


Fig. 10.4 Energy levels of the conduction band and the donor level without and with spin splitting.

Let denote the concentration of donor atoms occupied by electrons with + or - spin by $n_d^{\pm}$. $n_d^{\pm}$ is given by

$$n_d^{+} = (N_d - n_d^{-})\, f(\epsilon_d^{+}), \quad n_d^{-} = (N_d - n_d^{+})\, f(\epsilon_d^{-}), \qquad (10.39)$$

where N_d is the concentration of donor atom. $f(\epsilon_d^{\pm})$ is given by

$$f(\epsilon_d^{\pm}) = \exp[(\zeta - \epsilon_d^{\pm})/k_0T],$$

and $\mathcal{E}_d^{\pm}$ is shown in Fig. 10.4. Since the ionized donor concentration is given by $N_i = N_d - (n_d^{+} + n_d^{-})$, $n_d^{\pm}$ is rewritten as

$$n_d^{\pm} = N_i \exp\left[\{\zeta - \epsilon_d^{0} \pm \gamma S J M(T)/M(0)\}/k_0T\right], \qquad (10.40)$$

where $\mathcal{E}_d^{0} = \frac{1}{2}(\mathcal{E}_d^{+} + \mathcal{E}_d^{-})$ (See Fig. 10.4), The number of ionized donors is equal to the total concentration of the conduction electrons (at least if the crystal is uncompensated; i.e. if there are no acceptors present); then $N_i = n^{+} + n^{-}$. In the case where only a small fraction of the donors is ionized (i.e. $n_d^{+} + n_d^{-} \simeq N_d$), the total carrier concentration $n = n^{+} + n^{-}$ is given by

$$n = \left(\frac{1}{2} N_c N_d\right)^{1/2} \exp(\epsilon_d^{0}/2k_0T) \left\{\frac{\cosh(SJM/M(0)k_0T)}{\cosh(S\gamma JM/M(0)k_0T)}\right\}^{1/2}. \qquad (10.41)$$

By applying a magnetic field $M(H)$ and accordingly n increases.

The magnetoresistance $\Delta\rho/\rho_0 = (\rho(H) - \rho_0)/\rho_0$ is given by

$$\frac{\Delta\rho}{\rho_0} = \left\{ \frac{\cosh\left(SJM(H=0)/M(0)k_0T\right)\cosh\left(\gamma JM(H)/M(0)k_0T\right)}{\cosh\left(\gamma SJM(H=0)/M(0)k_0T\right)\cosh\left(SJM(H)/M(0)k_0T\right)} \right\}^{1/2} - 1 \;, \qquad (10.42)$$

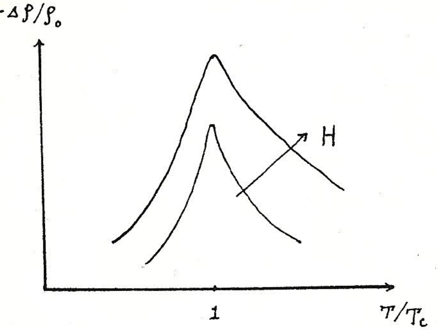


Fig. 10.5 Negative magnetoresistance of the ferromagnetic semiconductors, assuming a field independent mobility.

where $M(H)$ is the magnetization in a field intensity H and $M(0)$ is the spontaneous magnetization at $T = 0$ °K. Qualitative feature of (10.42) is shown in Fig. 10.5. The magnetoresistance exhibits a pronounced maximum at T_c. At the temperatures below T_c most of the carriers are populated in the (+) subband. By applying a magnetic field ordering of the spin system is enhanced and then, the probability of the spin disorder scattering decreases. Namely, the effect of a magnetic field on the mobility at $T < T_c$ also leads to the negative magnetoresistance. In this case $\Delta\rho/\rho_0$ becomes

$$\frac{\Delta\rho}{\rho_0} = \frac{\chi_z(H)}{\chi_z(0)} - 1 < 0 \,. \qquad (10.43)$$

In deriving (10.43) we assume a field independent charge carrier concentration.

(10.43) has a maximum at T_c. Detailed discussions are given in reference 109).

10.5 Critical Scattering around the Curie Temperature 115)

As was discussed in Section 10.3, for the purpose of calculating the resistivity of the magnetic semiconductors it is essentially important to know the behavior of the spin correlation function. In this Section we briefly introduce the theory of the critical scattering of the resistivity based on the theory of the second order phase transition due to Landau.

For simplicity the present discussion is limited to the case of a degenerate semiconductor and the band splitting and the anisotropy of susceptibility will be neglected. Then the resistivity takes the form:

$$\rho(T) = \frac{\rho(\infty)}{2} \int_0^{\pi} d\theta \sin\theta \, (1-\cos\theta) \sum_r g(r)\, e^{i q \cdot r}, \quad q = 2k_F \sin\left(\frac{\theta}{2}\right), \quad (10.44)$$

where $\rho(\infty)$ is the resistivity for $T \gg T_c$ and $g(r)$ is the spin correlation function defined by

$$g(r) \propto \langle [S(r) - \langle S(r)\rangle][S(0) - \langle S(0)\rangle]\rangle. \quad (10.45)$$

In his theory of the second order phase transition 116) Landau assumed that the thermodynamic potential Φ (Gibbs free energ) may be expanded in power series of the order parameter (in this case the

~~order~~ parameter is the magnetization $M(r)$) as :

$$\Phi = \int dr\, \phi(r),$$

$$\phi(r) = \phi_0 - B(r)\, M(r) + a(T)\, M(r)^2 + b(T)\, M(r)^4 + C(T)\, (\nabla M(r) . \nabla M(r)). \tag{10.46}$$

the second term denotes the effect of an applied magnetic field, the third and the fourth terms the energy and entropy terms and the last one corresponds to the spatial fluctuation of the magnetization.

At $T \sim T_c$ Landau proposed the following form for a.

$$a(T) = a'(T - T_c). \tag{10.47}$$

and assumed b and C to be independent on T. Then, the correlation function $g(r-r')$ is given by

$$g(r-r') = \frac{\exp(-|r-r'|\xi)}{|r-r'|} \left(\frac{k_0 T}{8\pi C}\right), \tag{10.48}$$

$$\xi^{-1} = \begin{cases} (C/a')^{1/2} (T - T_c)^{-1/2} & : T > T_c \\ (C/2a')^{1/2} (T_c - T)^{-1/2} & ; T < T_c, \end{cases} \tag{10.49}$$

(See appendix 7).

The critical scattering arises from the divergence of the correlation length ξ^{-1} as $T \to T_c$, which is a consequence of a large fluctuation of the magnetization. Integration over $(r.\theta)$ in (10.44) introduces the following factor :

$$1 - \left(\frac{\xi}{2k_F}\right)^2 \ln\left[1 + \left(\frac{2k_F}{\xi}\right)^2\right]. \qquad (10.50)$$

Defining a temperature $T_0 = 4k_F^2 c/a'$, one obtains

$$\begin{cases} \rho = \dfrac{2T\rho(\infty)}{T_0}\left[1 - \dfrac{T-T_c}{T_0}\ln\left(1 + \dfrac{T_0}{T-T_c}\right)\right] & : T > T_c \\ \rho = \dfrac{2T\rho(\infty)}{T_0}\left[1 - \dfrac{2(T_c-T)}{T_0}\ln\left(1 + \dfrac{T_0}{2(T_c-T)}\right)\right] & : T < T_c . \end{cases} \qquad (10.51)$$

Accordingly, ρ exhibits a maximum at T_c which becomes larger and sharper as k_F is decreased.

Fisher and Langer117) criticized the above theory on the following basis:

(1) To consider the correlation function $g(r)$ as a continuous function of r is not valid. The continuous model of $g(r)$ should be modified for the nearest neighbor pair, which play a most important role.

(2) It is meaningless to extend the correlation length ξ^{-1} infinity because the correlation over the mean free path is negligible.

10.6 Examples of the Magnetic Semiconductors

In the preceding Sections 10.3~10.5 the effects of the s-d interaction on the conduction processes are discussed in connection with the carriers moving in the broad band. However, in actual case the magnetic semiconductors belonging to such a category are few in number, and on the contrary most of the carriers moves in the d-bands which have a strong correlation.

Materials called "magnetic semiconductor" include various kinds of substances. In this Section we give only few examples of the magnetic semiconductors and make mention of the interesting properties of these materials.

i) EuS, $Eu_{1-x}Gd_xS$:

Density of states of the rare earth chalcogenides EuS, GdP and GdS is illustrated in Fig 10.6.$^{113)}$ $3p^6$ corresponds to the band of S^{2-} and $4f^7$, 5d and 6s levels stem from

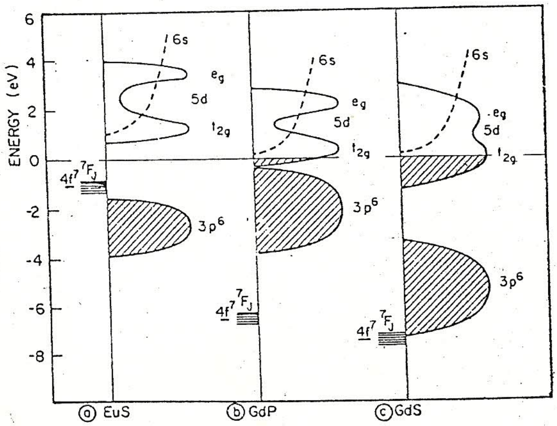


Fig. 10.6 Density of states scheme of (a) EuS, (b) GdP. and (c) GdS. EuS is ferromagnetic. GdP and GdS are antiferromagnetic.

Eu^{2+} and Gd^{3+}. GdS has one more extra electron than EuS and this electron enters into the t_{2g} subband which comes from the crystal-field splitting of the 5d-bands (See Fig. 10.6). Consequently, GdS is expected to be an ionic or polar metal. Among the three presented in Fig. 10.6 only EuS is insulating. GdP has an intermediate character between that of EuS and GdS.

Energy gap between the t_{2g}- and $3p^6$-band is very small and the Fermi energy is small. EuS is ferromagnetic and its ordering temperature is $T_c = 16.5$ K. For a theoretical derivation of the exchange integrals we can exclude 4f overlap. Goodenough[118)] proposed that the exchange interaction related to the 12 nearest neighbors of Eu^{2+} ions is the ferromagnetic superexchange with virtual transfer of a 4f electron to the 5d t_{2g} excited state of a neighboring cation.

In Europium chalcogenides addition of a few atomic percents a trivalent rare earth impurity such as Gd strongly increases the Curie temperature and may even modify the magnetic order (EuSe changes from an antiferromagnetic insulator to a ferromagnetic metal).

In $Eu_{0.99}G_{0.01}S$ the Curie temperature becomes 50K. Such a strong enhancement of Tc was explained by Kasuya and Yanase[119)] as follows.

The range of the 5d-wave function of the Gd^{3+} ion is extended to the nearest neighbor Eu^{2+} ions (See Fig. 10.7). Then the exchange

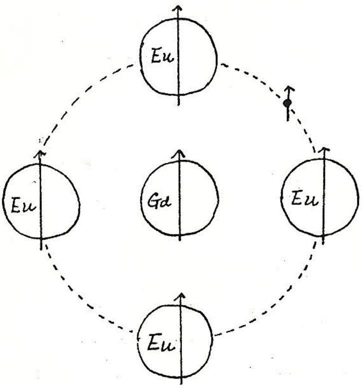


Fig. 10.7 Giant spin molecule in Gd-doped Eu chalcogenide.[119]

interaction is able to align the spin of the Gd ion at which the electron is localized and the spins of the neighboring Eu ions. This effect is neither important for $T < T_c$ where the spins are aligned nor for $T > T_c$ where the spins are thermally disordered, but it is important around T_c and the exchange coupled system Gd + electron + neighboring Eu ions is called the giant spin molecule.[119]

By writing the additional exchange interaction between a dopant electron and the 4f spins of the neighboring Eu ions as

$$-2\sum_{n} J_{i,n}\, \mathbf{S}_n \cdot s_i \, . \tag{10.52}$$

where n is summed over the number of 4f spins, the enhancement of the Curie temperature is given by

$$k_0 \Delta T_c = 2\sum_{i,n} J_{i,n} \langle \mathbf{S}_n \cdot s_i \rangle = (N_{el}/N_{Eu})\Big(2\sum_{n} J_n(|r-R_n|)\langle s \cdot \mathbf{S}_n\rangle\Big)$$

$$= (N_{el}/N_{Eu})(2\Delta E) . \tag{10.53}$$

Here, N_{el}/N_{Eu} is the relative concentration of dopant electrons and ΔE is a quantity corresponding to the red shift of the absorption edge.[120]

Magnetic impurity state is stabilized in the temperature range except for high ($T > T_c$) and low temperatures ($T < T_c$). This situation also affect the conductivity. Because the energy gap between the bottom of the conduction band and the occupied Gd level is expected to be large, only a very few carriers are excited in the conduction band and the conduction will be due to the hopping of an electron from an occupied Gd site to an empty one. The spin polarization will be transferred by the hopping process frome one site to another and the activation energy will be strongly dependent on the temperature and the magnetic field near T_c.[119]

In EuS : Gd with a Gd concentration $\lesssim 10^{20}$ cm^{-3} a donor state with an electron configuration $4f^7 5d^1$ is formed with an activation energy between 10 and 30 meV. For Gd concentrations above 10^{20} cm^{-3} an impurity band will merge with the 5d-conduction band of EuS. Then the conduction becomes metallic with $d\rho/dT$ being positive for $T \gg T_c$.

In Fig. 10.8 the resistivity of $Eu_{0.99}Gd_{0.01}S$ single crystals is shown.[111] Hall effect measurements on these samples provide a temperature-independent carrier concentration of 2.2×10^{20} cm^{-3}. Then Fig. 10.8 represents the inverse of the carrier mobility. At room temperature one obtains $\mu = 14.2$ cm^2/Volt sec. which increases only by a factor 2 when magnetic saturation is realized at 4.2 K.

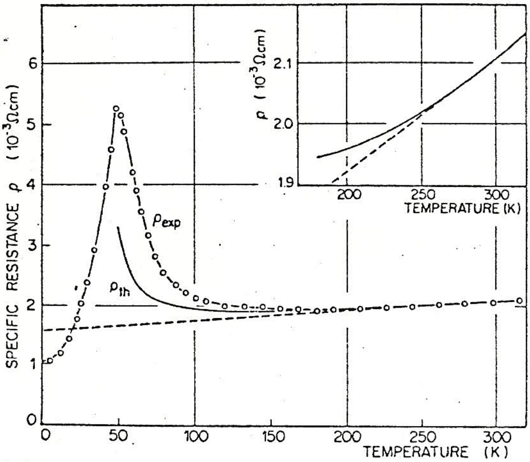


Fig. 10.8 Temperature dependence of the resistivity of $Eu_{0.99}Gd_{0.01}S$.[111)]

Samples with Gd concentrations $\lesssim 10^{20}\,cm^{-3}$ usually are semiconducting with an activated mobility and an activated free-carrier concentration.

The resistivity of undoped EuS at 300K exceeds $10^9\,\Omega\,cm$ with a negative $d\rho/dT$.

Photosensitivity data of EuS single crystals are shown in Fig. 10.9.[113)]

The photosensitivity strongly decreases with lowering temperature below 100K and exhibits a pronounced minimum at the ordering temperature $T_c = 16.5\,K$.

The photosensitivity P_s is expressed by

$$P_s = Q\mu\tau, \qquad (10.54)$$

where Q is the quantum efficiency, μ the mobility of the photoelectron and τ its life time in the conduction band. Since Q and τ are temperature-independent below 100K, so P_s is proportional to the mobility $\mu(T)$. The curve for $H=0$ is considered to be

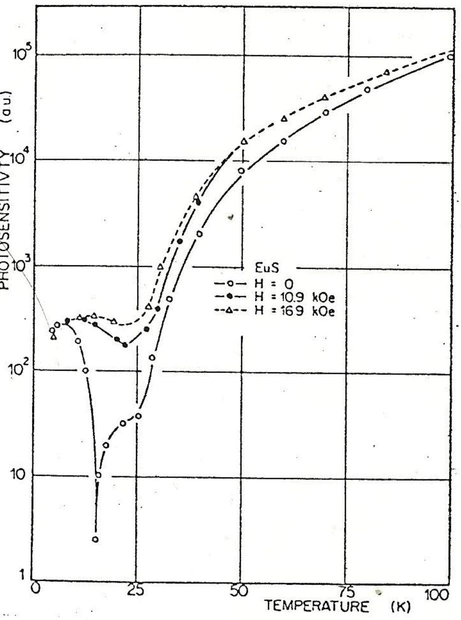


Fig 10.9 Temperature and field dependence of EuS single crystals.[113]

corresponding to Fig. 10.2 obtained by Haas.[109]

Decrease of the minimum by applying a magnetic field may be explained due to a decrease of the susceptibility.

It should be noted that there is a marked difference between Fig. 10.8 and 10.9. In Fig. 10.8 the temperature dependence of the mobility is small, whereas it is very large in Fig. 10.9.

ii) $CdCr_2Se_4$:

$CdCr_2Se_4$ crystallizes in the spinel structure and it becomes ferromagnetic below 130 K. Undoped $CdCr_2Se_4$ is usually observed to be a p-type semiconductor with an average carrier density of 10^{16} cm^{-3} at room temperature. It can be readily "doped" with Ag and In by substitution for Cd. The Ag-doped material shows p-type conduction while the In-doped materials show n-type conduction.

The conductivity of the n-type sample shows a minimum at

150 K and increases sharply with further decreasing temperature (See Fig. 10.10.[121)]). It has a maximum at 50 K and drops to $5\times10^{-2}\ (\Omega\,cm)^{-1}$ at 4.2 K. The change of the conductivity with temperature is greatest around the Curie temperature.

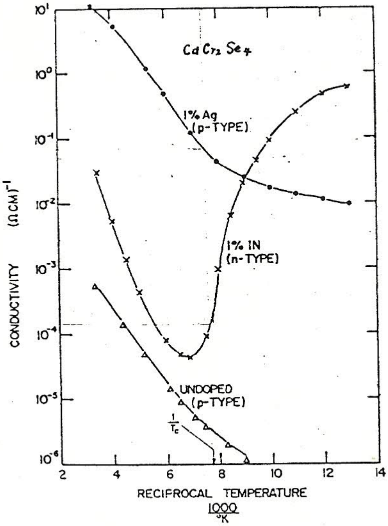


Fig. 10.10 Electrical Conductivity of 3 different samples of $CdCr_2Se_4$.[121)]

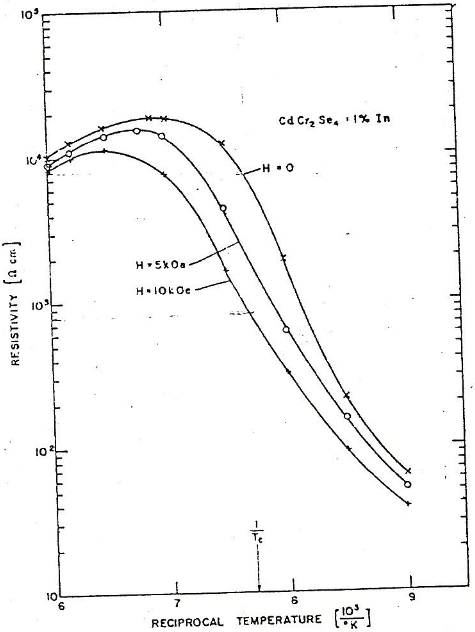


Fig. 10.11 Transverse magnetoresistance $\Delta\rho/\rho_0$ of $CdCr_2Se_4$ with 1% In.[121)]

Fig. 10.10 shows that the temperature dependences of n- and p-type $CdCr_2Se_4$ are strikingly different. The conductivity of the p-type sample shows a gradual change of the slope in the neighbor-hood of T_c. Fig. 10.11 shows the transverse magnetoresistance of n-type $CdCr_2Se_4$ as a function of magnetic field and reciprocal temperature, respectively.$^{121)}$ $\Delta\rho/\rho_0$ is always negative and exhibits a maximum at T_c (130K). On the other hand at high temperature $\Delta\rho/\rho_0$ is positive and proportional to H^2, as one would expect from ordinary transport theory. As the temperature is lowered ($T < 120K$) $\Delta\rho/\rho_0$ becomes negative and shows a saturation effect at low temperature (77K).$^{121)}$

These results indicates that the interactions with the localized magnetic moments seem to be much more prounced in the case of electrons than of the holes.

These different behaviors in the conductivity and the magnetoresistance of the n-type and p-type $CdCr_2Se_4$ suggest that in the p-type (Ag-doped) sample the conduction is due to the wide valence band (formed mainly from the 4 p-orbita of the anions), with a small localized spin interaction,$^{109)}$ while in the n-type sample the conduction electrons would belong to a narrow d-band derived from the Cr^{2+} levels.$^{122)}$

In Fig. 10.12 the temperature dependence of the band edge of $CdCr_2Se_4$ is shown.$^{110)}$ This indicates that the ordinary shift which is proportional to T coexists with the magnetic shift represented by Fig. 10.1.

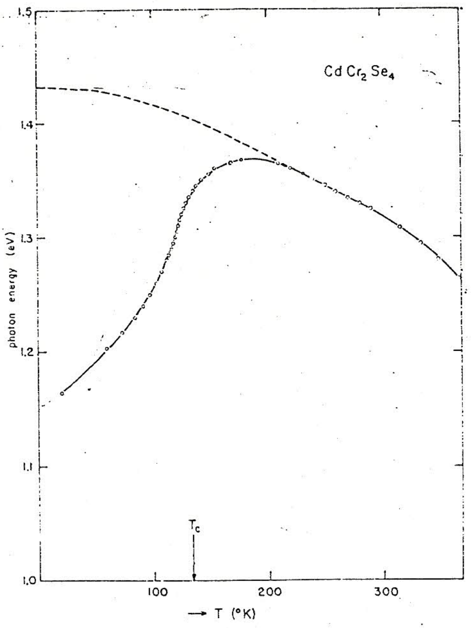


Fig. 10.12 Temperature dependence of the band edge of $CdCr_2Se_4$.110)

iii) MnTe :

In Fig. 10.3 the temperature dependences of the resistivity ρ and the thermoelectric power S of MnTe are shown.114, 27) MnTe cryptallizes in the NiAs structure and is the antiferromagnetic semiconductor with $T_N = 307\,K$. Its mobility is large and attains to $\sim 100\ cm^2/volt\ sec$ at 77K.114) Conduction carriers belong to the wide 5p-band holes. The resistivity is given by

$$\rho \propto T^{3/2} (\chi_{\parallel} + 2\chi_{\perp})/n , \qquad (10.55)$$

(See (10.34)) and the bend of ρ at T_N is due to the susceptibility. The temperature dependence of S can not be explained by the diffusion term but it needs to consider the magnon drag effect.

Recently, the materials called "semimagnetic semiconductors" have attracted a good deal of attentions of many investigators.[123) Typical examples of them are $Hg_{1-x}Mn_xTe$ and $Cd_{1-x}Mn_xTe$.

$Hg_{1-x}Cd_xTe$ is a material which belongs to the narrow gap semiconductors and its properties have been extensively studied. Mn is in the state of $(3d)^5$, $S = 5/2$. Therefore, the investigation on the semimagnetic semiconductors will provide useful and interesting information about the interaction between the localized spins and the high mobility carriers.

10.7 Kondo Theory of the Resistance Minimum

When small amounts of transition metal elements are dis
in a non-magnetic metal, the resulting alloy may or may no
diplay a localized moment (Table 10.1).[124]

Impurity	Host Au	Cu	Ag	Al
Ti	×	—	—	×
V	?	—	—	×
Cr	O	O	O	×
Mn	O	O	O	?
Fe	O	O	—	×
Co	?	?	—	×
Ni	×	×	—	×

Table 10.1 Presence or absence of localized magnetic moments when transition metal elements are dissolved in non magnetic metals.[124] O : presence, × : absence.

The alloys with localized magnetic moments are called mag
dilute alloys. The existence of localized moments in dilute alloy
which couple to the conduction electrons through the s-d int
has important consequences for the electrical conductivity. As
been discussed in Sections 10.3 and 10.4 the magnetic impurit

act as scattering centers, and if they are the predominant type of impurity scattering, then at low temperatures the scattering due to localized moments will be a most important mechanism of electrical resistance.

In Section 10.4 we mentioned that s-d interaction causes the negative magnetoresistance. In the magnetic dilute alloys magnetic field align the localized spins and, then the probability of the spin disorder scattering decreases. This is the origin of the negative magnetoresistance. Yoshida presented a detailed theory on this problem.[125)]

In nonmagnetic metals the resistivity monotonically decreases with lowering temperature and reaches a temperature independent value (the so-called residual resistivity). In magnetic alloys, however, it has been known since 1930[126)] that the resistivity has a shallow minimum at 10K ~ 30K that depends weakly on the concentration of magnetic impurities (Fig. 10.13). This problem has survived for more than thirty years as an unsolved and difficult problem in Solid State Physics until Kondo removed a veil of mystery.[127)] Prior to Kondo theory, the spin disorder scattering was treated only to the first order Born approximation and the result obtained was not to differ qualitatively from the nonmagnetic scattering. Kondo pointed out, however, that in all higher orders of perturbation theory the s-d scattering cross section is divergent, yielding an infinite resistivity. At finite temperatures the resistivity has a log T-term, which becomes infinite with decreasing temperature. This term is the origin of the resistance minimum.

Apperance of the log T term stems from a sharp cutoff in the electron distribution function at $k = k_F$ and noncommuting property of the spin operators.

Kondo theory has brought forward the so-called Kondo problem in which the stability of the coupled system (electrons plus localized spin) comes into question without relying on a simple perturbation theory. This problem exceeds over the level of this text book and, then we do not touch it.[127)

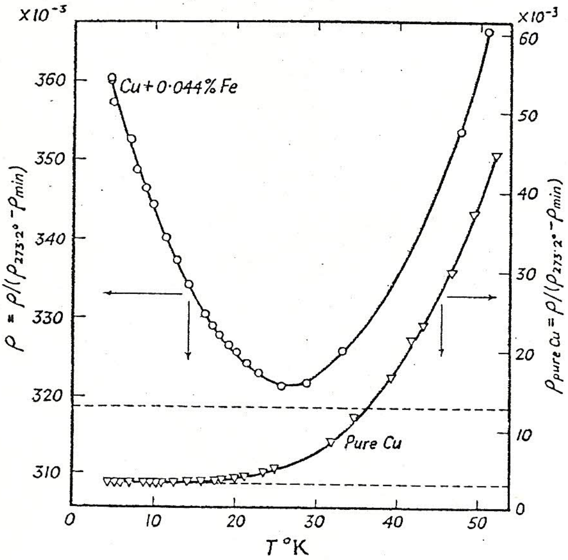


Fig. 10.13 The resistance minimum of Cu-Fe dilute alloy. (after W.B. Pearson 126))

Now, let proceed to consider the Kondo theory.

The s-d interaction (10.1) is rewritten in terms of the second quantization operators as follows:

$$H' = -\left(\frac{J}{N}\right)\sum_{n}\sum_{k,k'} e^{i(k-k')\cdot R_n}\Big\{(a^{+}_{k'+}a_{k+} - a^{+}_{k'-}a_{k-})S_{nz}$$

$$+\ a^{+}_{k'+}a_{k-}S_{n-} + a^{+}_{k'-}a_{k+}S_{n+}\Big\}, \qquad (10.56)$$

$a^{+}_{k\pm}$ and $a_{k\pm}$ represent the creation and annihilation operators of $k\pm$-electron, respectively. Though in general J is a function of $k-k'$ as shown in (10.14), for simplicity it is assumed to be a constant. Unperturbed Hamiltonian of the election system is

$$H_0 = \sum_{k,s} E_k\, a^{+}_{ks}\, a_{ks}\,. \quad (s=\pm). \qquad (10.57)$$

When the localized spins are isolated and the correlation between them may be neglected, the first Born approximation gives rise to the resistivity being temperature-independent:

$$\rho = \frac{2\pi\,\eta(E_F)\,m^{*}c}{Ne^{2}\hbar}\,J^{2}S(S+1), \qquad (10.58)$$

where S is the magnitude of the localized spin, $\eta(E_F)$ the density of states at E_F, and c denotes the ratio of the spin concentration to the lattice point density. ρ given by (10.58) is equal to $\rho(\infty)$ in (10.51).

Kondo has clarified that if the scatter has an internal degree of freedom such as the spin operator, the second order Born approximation adds an extra term proportional to $\log T$ to the resistivity and this term is the origin of the resistance minimum.[127]

Then, it needs to carry out further calculation beyond the first order Born approximation.

T-matrix associated with (10.56) and (10.58) is given by

$$T = H' + H'(E_a - H_0 + i\varepsilon)^{-1}H' + H'(E_a - H_0 + i\varepsilon)^{-1}H'(E_a - H_0 + i\varepsilon)^{-1}H'$$
$$+ \cdots, \quad (\varepsilon \to 0) \tag{10.59}$$

Transition probability for $a \to b$ process is

$$W(a\to b) = \frac{2\pi}{\hbar}\,\delta(E_a - E_b)\,|T_{ab}|^2, \tag{10.60}$$

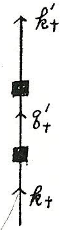
(See appendix 8). By retaining up to the second Born approximation, (10.60) becomes

$$W(a\to b) = \frac{2\pi}{\hbar}\,\delta(E_a - E_b)\left\{ H'_{ab}H'_{ba} + \left[\sum_{c\neq a}\frac{H'_{ac}H'_{cb}H'_{ba}}{E_a - E_c} + \sum_{c\neq b}\frac{H'_{bc}H'_{ca}H'_{ab}}{E_b - E_c}\right]\right\}, \tag{10.61}$$

where E_a, E_b and E_c denotes the energies of the electron and spin system. The two terms in the square bracket of (10.61) are complex conjugate each other, since $E_a = E_b$. These terms are usually a factor J/E_F smaller than the first term (the first Born approximation). However, the logarithmic term $\log|E - E_F|$ is included in them and they become essentially important in discussing the resistance minimum.

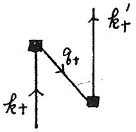
At first we consider the transitions without spin flip : $|k+\rangle \to |k'+\rangle$. These transitions are classified into four types according to the intermediate states. 1) and 2) correspond to the intermediate states without spin flip process, while 3) and 4) to the intermediate states with spin flip process.

)



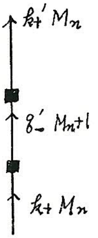
An electron k_+ is scattered into an unoccupied state q'_+ and finally makes transitions to k'_+. Direction from downward to upward coincides with the one of the time axis. ■ indicates the s-d interaction. This type of scattering is induced by the term $\overset{+}{a}_{k'+} a_{k+} S_{nz}$ in (10.56).

)



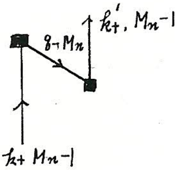
This is the inverse process of 1). At first an electron q_+ is scattered into k'_+ and finally the electron in the initial state k_+ makes transition into q_+ state.

)



This process is induced by the term $\overset{+}{a}_{k'\pm} a_{k\mp} S_{n\mp}$ in (10.56). M_n denotes the z-component of the localized spin.

)



This is the inverse process of 3).

In consideration of 1) – 4) the square bracket in (10.61) is given by

$$\sum_{q'} H'_{k+,q'+} H'_{q'+,k'+} H'_{k'+,k+} (1-f^\circ_{q'})/(E_k - E_{q'})$$

$$-\sum_{q} H'_{q+,k'+} H'_{k+,q+} H'_{k'+,k+} f^\circ_q/(E_q - E_{k'})$$

$$+\sum_{n,q} H'_{k+M_n,\, q'-,\, M_n+1} H'_{q'-,\, M_n+1,\, k+M_n} H'_{k'+,k+} (1-f^\circ_{q'})/(E_k - E_{q'})$$

$$-\sum_{n,q} H'_{q-M_n,\, k'+,\, M_n-1} H'_{k+M_n-1,\, q-M_n} H'_{k'+,k+} f^\circ_q/(E_q - E_{k'}) \qquad (10.62)$$

+ complex conjugate,

where f° denotes the equilibrium Fermi function. Since the spin correlation is disregarded in the present problem, (10.62), in consideration of (10.56), is reduced to

$$2\left(-\frac{J}{N}\right)^3 \sum_n M_n^3 \sum_{q'} (1-f^\circ_{q'})/(E_k - E_{q'})$$

$$-2\left(-\frac{J}{N}\right)^3 \sum_n M_n^3 \sum_q f^\circ_q/(E_q - E_{k'})$$

$$+2\left(-\frac{J}{N}\right)^3 \sum_n M_n (S-M_n)(S+M_n+1) \sum_{q'} (1-f^\circ_{q'})/(E_k - E_{q'})$$

$$-2\left(-\frac{J}{N}\right)^3 \sum_n M_n (S+M_n)(S-M_n+1) \sum_q f^\circ_q/(E_q - E_{k'}) . \qquad (10.63)$$

Sum of the first and second terms of (10.63) becomes

$$2\left(-\frac{J}{N}\right)^3 \sum_n M_n^3 \sum_q 1/(E_k - E_q), \qquad (10.64)$$

where the energy conservation $E_k = E_{k'}$ is employed.

10.64) is just what is obtained when we take no account of the Pauli principle. We usually encounter such situations when the perturbing system has no internal degrees of freedom. The scattering processes without spin flip may be regarded of the same nature as the potential scattering.

As a result of this fact, the expression (10.64) has little dependence on the initial energy E_k and can be neglected. For the same reason we shall disregard the terms which do not involve f_q° in the third and fourth term of (10.62). Finally, the important term we concern is given by

$$4\left(\frac{J}{N}\right)^3 \sum_n M_n^2 \sum_q f_q^\circ/(E_q - E_k). \qquad (10.65)$$

As is clearly seen in the processes 3) and 4), the spin quantum number changes in order of $M_n \to M_{n+1} \to M_n$ in the process 3), while in 4) the corresponding order is $M_n \to M_n - 1 \to M_n$. Combining them, we get (10.65). Namely, (10.65) is the result of the non-commuting property of the spin operator : $S_+ S_- - S_- S_+ = 4 S_z \neq 0$.

From the assumption that the localized spins are randomly oriented we have

$$\sum_n M_n^2 = \{S(S+1)/3\} cN. \qquad (10.66)$$

Introducing the notation

$$g(E) = (1/N) \sum_q f_q^\circ/(E_q - E). \qquad (10.67)$$

and using (10.66), we obtain the following expression of the transition probability including the first order and second order Born approximation :

$$W(k+ \to k'+) = \{2\pi J^2 S(S+1) c/3\hbar N\}\{1+4J g(E_k)\}\delta(E_k - E_{k'}) . \qquad (10.68)$$

Similar result is obtained for $W(k- \to k'-)$.

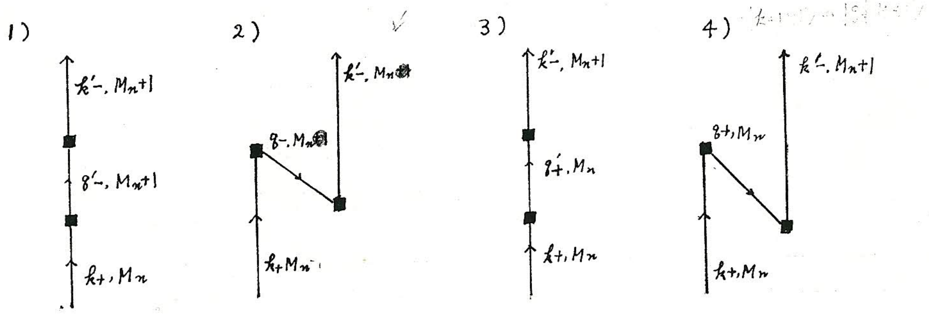
In the next place we shall consider the process in which the electron $k+$ is scattered into the state $k'-$ and simultaneously the n-th spin increases its z-component by unity ($M_n \to M_n+1$).

This process is classified into four types according its intermediate state.

$|q-, M\rangle \to |k'- M\rangle$, $|k+ M$, $|q- M+1\rangle$, $|k'- M+1\rangle \to$ [illegible]

$|q+ M\rangle \to |k' M+1\rangle$

[illegible]



The transition probability is easily obtained as in the case of $k\pm \to k'\pm$ and is given by

$$W(k+, M_n \to k'-, M_n+1) = (2\pi J^2/\hbar N^2)(S-M_n)(S+M_n+1)$$

$$\times \{1+4J g(E_k)\}\delta(E_k - E_{k'}) . \qquad (10.69)$$

Similarly, we obtain

$$W(k-, M_n \rightarrow k'+, M_n-1) = (2\pi J^2/\hbar N^2)(S+M_n)(S-M_n+1)$$

$$\times \left\{1 + 4J\, g(E_k)\right\} \delta(E_k - E_{k'}). \tag{10.70}$$

Then, the total transition probability of the spin-flip processes is given by

$$W(k\pm \rightarrow k'\mp) = \sum_n W(k\pm M_n \rightarrow k'\mp, M_n \pm 1)$$

$$= \left\{4\pi J^2 S(S+1)\, c/3\hbar N\right\}\left\{1 + 4J\, g(E_k)\right\} \delta(E_k - E_{k'}), \tag{10.71}$$

which is just twice of (10.68).

At the absolute zero temperature the Fermi function f_q° can be replaced by a step function : $f_q^\circ = 1$ for $q < k_F$ and $f_q^\circ = 0$ for $q > k_F$.

Assuming $E_k = \hbar^2 k^2/2m^*$, we have

$$g(E_k) = \frac{3}{2E_F}\left\{1 + (k/2k_F)\log\left|(k-k_F)/(k+k_F)\right|\right\}. \tag{10.72}$$

g becomes $-\infty$ with $k \rightarrow k_F$ and this singularity is a reflection of the sharpness of the Fermi function at $T = 0\,°K$. From (10.72), (10.71) and (10.68), we can see that the transition probability increases with $k \rightarrow k_F$, if J is negative. At finite temperatures the mean value of $|k - k_F|$ is proportional to T, then it is concluded that the resistivity has a term proportional to $\log T$.

Let proceed to calculate the resistivity at finite temperatures.

The rate of change of $f_k^\pm$ due to the collision with the localized spins is given by

$$\left(\frac{\partial f_k^{\pm}}{\partial t}\right)_{coll} = \sum_{k'} W(k\pm \to k'\pm)(f_{k'}^{\pm} - f_k^{\pm})$$

$$+ \sum_{k'} W(k\pm \to k'\mp)(f_{k'}^{\mp} - f_k^{\pm}). \qquad (10.73)$$

When the electric field is applied along the x-direction, we may put

$$f_k^{\pm} = f_k^{\circ} - \mathcal{E} k_x \chi(E_k). \qquad (10.74)$$

Then, (10.73) becomes

$$\left(\frac{\partial f_k^{\pm}}{\partial t}\right)_{coll} = -(f_k^{\pm} - f_k^{\circ})\sum_{k'}\{W(k\pm \to k'\pm) + W(k\pm \to k'\mp)\}$$

$$= -(f_k^{\pm} - f_k^{\circ})/\tau_k. \qquad (10.75)$$

where

$$1/\tau_k = (2\pi\eta(E_F)c/\hbar)J^2 S(S+1)\{1+4Jg(E_k)\}. \qquad (10.76)$$

Inserting the relaxation time τ_k into the expression of the conductivity

$$\sigma = -\frac{e^2}{12\pi^3}\int dk\, \tau_k v_k^2 \frac{\partial f_k^{\circ}}{\partial E_k}, \qquad (10.77)$$

we obtain the resistivity due to the s-d interaction

$$\rho_{spin} = c\rho_M\left\{1 - (\hbar^2 J/\pi m^* k_F)\int dk\, g(E_k)\frac{\partial f_k^{\circ}}{\partial E_k}\right\}, \qquad (10.78)$$

where

$$\rho_M = (2\pi\eta m^*/Ne^2\hbar)J^2 S(S+1). \qquad (10.79)$$

In getting the explicit expression of ρ_{spin} all the terms in the order of $(k_0T/E_F)^2$ are neglected. The integral in (10.78) is carried out as follows:

$$\int dk\, g(E_k)\frac{df_k^0}{dE_k} = \frac{\Omega}{8\pi^3 N}\iint f_{k'}^0 \frac{df_k^0}{dE_k}\frac{dk\,dk'}{E_{k'}-E_k}$$

$$= -\frac{4m^{*3}\Omega}{\pi\hbar^6 N}\iint (EE')^{1/2} f^0(E)\frac{df^0}{dE'}\frac{dE\,dE'}{E'-E} = -\frac{8m^{*3}\Omega E_F}{\pi\hbar^6 N}$$

$$-\frac{4m^{*3}\Omega E_F}{\pi\hbar^6 N}\iint \log\left|(\sqrt{E}-\sqrt{E'})/(\sqrt{E}+\sqrt{E'})\right|\frac{df^0}{dE}\frac{df^0}{dE'}\,dE\,dE'. \qquad (10.80)$$

The first term in the last expression of (10.80) gives a constant $(2\pi/3)(J/E_F)$ in the curly bracket of (10.78). Then, it may be neglected as compared with unity. The integral in the second term becomes

$$\cong \iint \log\left|(E-E')/4E_F\right|\frac{df^0}{dE}\frac{df^0}{dE'}\,dE\,dE' = \text{const.} + \log T. \qquad (10.81)$$

Inserting this expression into (10.78), we have

$$\rho_{spin} = c\,\rho_M\left\{1+\left(\frac{3J}{E_F}\right)\log T\right\}, \qquad (10.82)$$

where the relation of $E_F = (\pi^2\hbar^2/2m^*)\{(3/\pi)(N/\Omega)\}^{2/3}$ is employed. Then, we arrive at an important conclusion that the term involving $\log T$ increases with decreasing temperature, if J is negative.

Combining with the lattice scattering resistivity and the potential scattering contribution, we obtain the resultant resistivity

$$\rho = aT^5 + c\rho_0 - c\rho_1\log T, \qquad (10.83)$$

where $c\rho_0$ includes $c\rho_M$ and the ordinary potential scattering due to the magnetic impurities and aT^5 denotes the lattice scattering term (cf. Section 9.1). From (10.83) the temperature at which the resistivity minimum appears is given by

$$T_{min} = (\rho_1/5a)^{1/5}c^{1/5}. \qquad (10.84)$$

Such a weak dependence on the impurity concentration is in good agreement with the observed results.

Direct exchange interaction between the localized and conduction electrons gives a positive sign of J, while a negative J may be derived from the Anderson Hamiltonian[128] which involves the s-d mixing interaction. Assuming a single d-level related to the magnetic impurity, we obtain an effective s-d exchange integral as follows:

$$J = -N|V_{sd}|^2\left\{\frac{1}{U+E_d} + \frac{1}{-E_d}\right\}, \qquad (10.85)$$

where V_{sd} represents the s-d mixing interaction, E_d the d-level and U the Coulomb energy between the electrons with + and − spins in the d-level. Energy level is measured from the Fermi level.

Let us imagine that E_d is placed sufficiently below the Fermi level, while E_d+U is located above the Fermi level. In this the localized moment is formed and J is negative.[128,129]

The whole sign of J is determined by the balance of the two contributions.

In Fig. 10.14[129] the three curves drawn represent the three functions $0.20 - 0.0078 \log T$, $0.077 - 0.04 \log T$ and $0.034 - 0.0016 \log T$,

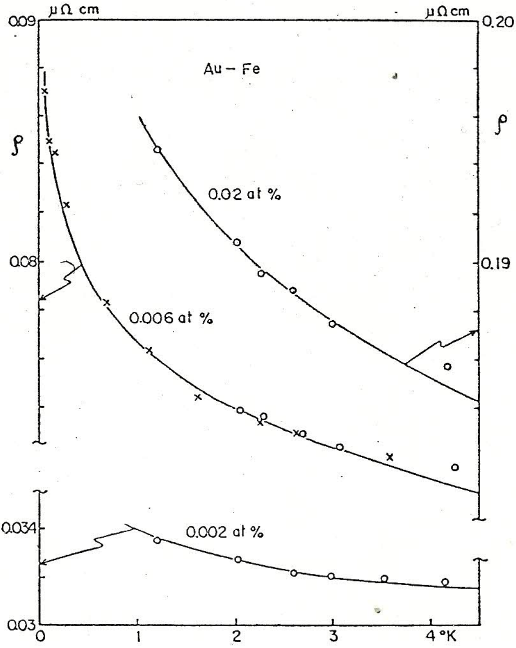


Fig. 10.14 Resitivities of Au-Fe alloys. The theoretical curves are based on (10.83).127) The experimental points are due to reference 129).

respectively from the above, in units of $\mu\Omega$ cm.126) From (10.83) both the constant term and the coefficient of the logarithmic term should be proportional to concentration.

In the three curves the three constant terms are in the ratio of 2.5 : 1 : 0.44, while the logarithmic terms are in the ratio of 2.0 : 1 : 0.40. This agrees with (10.83).

Let define the Kondo temperature at which the logarithmic term in curly bracket of (10.82) becomes comparable to unity:

$$T_K \sim e^{-E_F/3|J|}. \tag{10.86}$$

Below T_K the present calculation loses its validity, since the second Born approximation exceeds the first order contribution. In this temperature region it is needed to treat the coupled system composed of the conduction electrons and the localized spins without relying on the perturbation calculation. This is the so-called Kondo problem which is beyond the scope of this book.126)

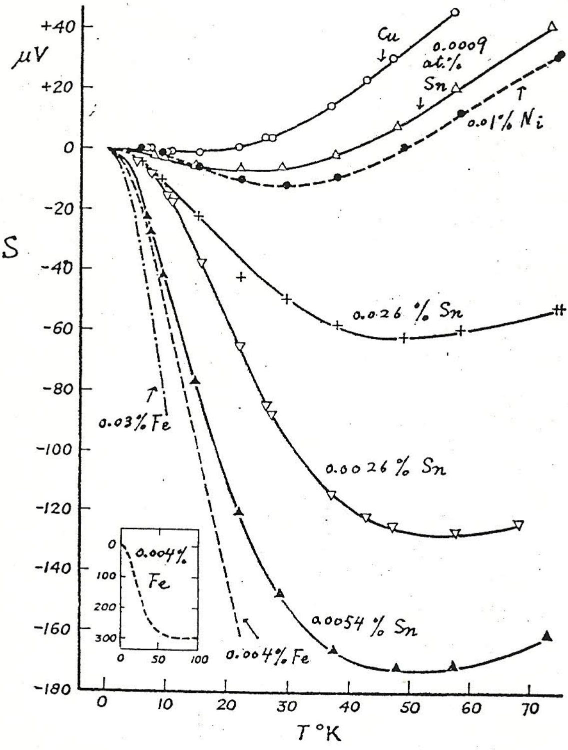


Fig. 10.15 Thermoelectric power of Cu-alloys.130)

Dilute magnetic alloys exhibit a large thermoelectric power, whose magnitude is often nearly independent of T and c in a fairly large region of these parameters. One of these results is shown in Fig. 10.15.130) Kondo has shown that the interference effect between the s-d interaction and the ordinary potential scattering provides a reasonable explanation to the anomalous thermoelectric power.126)

$$\mathcal{H} = \frac{1}{2m}\left(p + \frac{e}{c}A\right)$$

Chapter 11 Conduction in Strong Magnetic Field (I)

11.1 Wave Function in Magnetic Field, Landau level

In Section 5.2 we have verified that the energy levels in the presence of a magnetic field are approximately given by

$$E\left(-i\nabla + \frac{e}{\hbar c}A\right)\psi = \mathcal{E}\psi \quad (e>0), \tag{11.1}$$

where $E(k)$ is the energy for the unperturbed periodic potential and A denotes the vector potential of the magnetic field.

In the first place we shall consider a simplest case in which $E(k)$ is given by $\hbar^2k^2/2m$. For the convenience of latter use we assume that an electric field is applied along the x-direction. Then, the Hamiltonian becomes

$$\mathcal{H} = \frac{1}{2m}\left\{p_x^2 + \left(p_y + \frac{eH}{c}x\right)^2 + p_z^2\right\} + e\mathcal{E}x, \tag{11.2}$$

Landau gauge

where the gauge of the vector potential is taken to be $A = (0, Hx, 0)$. Since $[\mathcal{H}, p_z] = [\mathcal{H}, p_y] = 0$, p_y and p_z may be treated as the c-number. Rewriting (11.2), we get

$$\mathcal{H} = \frac{p_x^2}{2m} + \frac{m\omega_0^2}{2}(x - X)^2 + \frac{p_z^2}{2m} + e\mathcal{E}X + \frac{1}{2}\frac{e^2\mathcal{E}^2}{m\omega_0^2}, \tag{11.3}$$

where

$$\left\{\begin{aligned} X &= -\frac{\hbar k_y}{m\omega_0} - \frac{e\mathcal{E}}{m\omega_0^2} = -\frac{k_y}{s} - \frac{e\mathcal{E}}{m\omega_0^2}, \quad (p_y = \hbar k_y) \\ \omega_0 &= \frac{eH}{mc}, \quad s = \frac{eH}{\hbar c} = 1.52\times 10^7 H. \end{aligned}\right. \tag{11.4}$$

$\mathcal{H}$ is composed of the two contributions : one is the energy of a linear harmonic oscillator around X and the other is the kinetic energy of the free motion along the z-direction. Then, the wave function is expressed by

$$\begin{cases} \Psi_{N,k} = (L_y L_z)^{-1/2}\,\phi_N(x-X)\,e^{i(k_y y + k_z z)}, \quad k \equiv (k_y, k_z), \\ \phi_N(x) = \left[\sqrt{\frac{s}{\pi}}\,\frac{1}{2^N N!}\right]^{1/2} e^{-\frac{s}{2}x^2}\,H_N(\sqrt{s}\,x). \end{cases} \tag{11.5}$$

L_y and L_z denote the length of the crystal along the y- and z-axes and H_N is the N-th order Hermite function. H_N is obtained by a generating function $G(x,t)$ as follows :

$$G(x,t) \equiv e^{-t^2+2t(s^{1/2}x)} = \sum_{N=0}^{\infty} t^N \frac{H_N(\sqrt{s}\,x)}{N!}. \tag{11.6}$$

Energy level corresponding to (11.5) is given by

$$E_{N,k} = \hbar\omega_0(N+1/2) + \frac{\hbar^2 k_z^2}{2m} + e\mathcal{E}X, \quad (P_z = \hbar k_z) \tag{11.7}$$

The Schrödinger equation for a free electron in magnetic field was first solved by Landau 131) in connection with the diamagnetism of the conduction electrons, and (11.5) is called the Landau state and (11.7) the Landau level.

An electric field $\mathcal{E}$ displaces the center coordinate of the harmonic oscillator and gives an energy shift $e\mathcal{E}X$. In the absence of an electric field the energy level is independent of the center coordinate

X. Each level is highly degenerate. The number of levels with energy 11.7) ($\mathcal{E} = 0$) for a given N and k_z lying in $(k_z, k_z + \Delta k_z)$ is

$$\frac{L_z}{2\pi}\,\Delta k_z\,\frac{L_y}{2\pi}\int dk_y = \frac{L_z L_y \Delta k_z}{(2\pi)^2}\, s\int dX = \frac{L_x L_y L_z}{(2\pi)^2}\, s\,\Delta k_z \, . \qquad (11.8)$$

To obtain an explicit expression of H_N it is more convenient to employ the formula :

$$\left\{\begin{array}{l} H_N(\xi) = (-1)^N e^{\xi^2}\dfrac{d^N e^{-\xi^2}}{d\xi^N}, \\ H_0 = 1, \quad H_1 = 2\xi, \quad H_2 = 4\xi^2 - 2, \quad H_3 = 8\xi^3 - 12\xi, \\ H_4 = 16\xi^4 - 48\xi^2 + 12, \quad H_5 = 32\xi^5 - 160\xi^3 + 120\xi, \\ H_6 = 64\xi^6 - 480\xi^4 + 720\xi^2 - 120, \\ H_7 = 128\xi^7 - 1344\xi^5 + 3360\xi^3 - 1680\xi . \end{array}\right. \qquad (11.9)$$

Putting $X = 0$ and operating x and $\partial/\partial x$ on $\phi_N(x)$, we obtain

$$\left\{\begin{array}{l} x\,\phi_N = \sqrt{\dfrac{1}{2s}}\left\{\sqrt{N}\,\phi_{N-1} + \sqrt{N+1}\,\phi_{N+1}\right\}, \\ \dfrac{\partial}{\partial x}\phi_N = \sqrt{\dfrac{s}{2}}\left\{\sqrt{N}\,\phi_{N-1} - \sqrt{N+1}\,\phi_{N+1}\right\}. \end{array}\right. \qquad (11.10)$$

and then,

$$\left(s x \pm \frac{\partial}{\partial x}\right)\phi_N = \sqrt{2s}\left\{\begin{array}{l} \sqrt{N}\,\phi_{N-1} , \\ \sqrt{N+1}\,\phi_{N+1} . \end{array}\right. \qquad (11.11)$$

From (11.11) we can introduce the creation and annihilation operators b^+ and b as follows (in the general case for $X \neq 0$) :

$$\begin{cases} b^+ = \sqrt{\frac{1}{2s}}\left\{s(x-X) - \frac{\partial}{\partial x}\right\}, \quad b = \sqrt{\frac{1}{2s}}\left\{s(x-X) + \frac{\partial}{\partial x}\right\}. \\ b^+\phi_N = \sqrt{N+1}\,\phi_{N+1}, \quad b\phi_N = \sqrt{N}\,\phi_{N-1}, \quad b^+ b\,\phi_N = N\phi_N. \\ [b, b^+] = 1. \end{cases} \tag{11.12}$$

By using $k = -i\nabla + \frac{e}{\hbar c}A$, b^+ and b are rewritten as

$$b^+ = -i\sqrt{\frac{1}{2s}}\,k_+, \quad b^- = i\sqrt{\frac{1}{2s}}\,k_-, \quad k_\pm = k_x \pm ik_y. \tag{11.13}$$

The Landau state for $A = (0, Hx, 0)$ is represented by the product of the plane wave $e^{ik_z z}$ and the linear oscillator wave function along the x-axis and the quantum number is given by a set $\mu \equiv (N, X, k_z)$. It should be noted that the wave function in magnetic field depends on the gauge of the vector potential. For example, let choose the gauge $A = \frac{1}{2}H \times r$, $(H \parallel z)$. In the cylindrical coordinate (ρ, φ, z) $A_\varphi = \frac{1}{2}H\rho$, $A_z = A_\rho = 0$ and the Schrödinger equation becomes

$$-\frac{\hbar^2}{2m}\left[\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial\psi}{\partial\rho}\right) + \frac{\partial^2\psi}{\partial z^2} + \frac{1}{\rho^2}\frac{\partial^2\psi}{\partial\varphi^2}\right] - \frac{ie\hbar H}{2mc}\frac{\partial\psi}{\partial\varphi} + \frac{e^2H^2}{8mc^2}\rho^2\psi = E\psi. \tag{11.14}$$

Assuming

$$\psi = \frac{1}{\sqrt{2\pi}}R(\rho)e^{iM\varphi}e^{ik_z z}. \tag{11.15}$$

we obtain

$$\left\{\begin{aligned} R &= e^{-\xi/2}\,\xi^{|M|/2}\,w(\xi)\ , \quad \left(\xi \equiv \tfrac{1}{2}s\rho^2\right) \\ w(\xi) &= F\left\{-\left(\beta - \frac{|M|+1}{2}\right), |M|+1, \xi\right\}, \left(\beta \equiv \frac{(2mE - \hbar^2 k_z^2)c}{2\hbar eH} + \frac{M}{2}\right), \end{aligned}\right. \tag{11.16}$$

where F is the confluent hypergeometric function defined by

$$F(a, b, z) = \sum_{s=0}^{\infty} \frac{\Gamma(a+s)\,\Gamma(b)\,z^s}{\Gamma(a)\,\Gamma(b+s)\,\Gamma(1+s)} \ . \tag{11.17}$$

In order to keep the wave function finite everywhere, $\beta - (|M|+1)/2$ must be equal to a non-negative integer n_ρ. Therefore, the energy level is given by

$$E = \hbar\omega_0\left(n_\rho + \frac{|M| - M + 1}{2}\right) + \frac{\hbar^2 k_z^2}{2m} \ . \tag{11.18}$$

We often encounter the case in which several bands couple together. In this case the Landau state can not be expressed by single harmonic oscillator. In general it needs infinite number of the harmonic oscillator wave function.

As an example, let consider the Landau level of graphite. As was shown in Section 8.4, π-band in graphite is composed of the four bands E_1, E_2, E_3 and E_3' and they are coupled through the $\mathbf{k}\cdot\mathbf{p}$-perturbation (See (8.57)).

If the matrix element H_{33}, which connects E_3- and E_3'-states, is non-zero, it needs infinite number of the harmonic oscillator wave function to describe the Landau state. For simplicity, we assume $H_{33} = 0$. In consideration of (11.13) the Hamiltonian matrix (8.57) becomes

$$\mathcal{H} = \begin{vmatrix} E_1 & 0 & -i\sqrt{2s}\,P_1 b^+ & i\sqrt{2s}\,P_1 b \\ 0 & E_2 & i\sqrt{2s}\,P_2 b & i\sqrt{2s}\,P_2 b \\ i\sqrt{2s}\,P_1 b & -i\sqrt{2s}\,P_2 b & E_3 & 0 \\ -i\sqrt{2s}\,P_1 b^+ & -i\sqrt{2s}\,P_2 b^+ & 0 & E_3 \end{vmatrix} , \qquad (11.19)$$

where $P_1 = \eta_0(1-\nu)/\sqrt{2}$, $P_2 = \eta_0(1+\nu)/\sqrt{2}$.

We now proceed to the exact calculation of the energy spectrum, using the method of Luttinger and Kohn.$^{132)}$ According to L K the wave function in magnetic field is given by the product of the Bloch function for $k_x = k_y = 0$ and the slowly varying envelope function. In this case the wave function is written as

$$\Psi_\lambda = \begin{bmatrix} c(\lambda_1)\,\phi_N \\ c(\lambda_2)\,\phi_N \\ c(\lambda_3)\,\phi_{N-1} \\ c(\lambda_4)\,\phi_{N+1} \end{bmatrix} = N^{-1/2} \sum_{t=1}^{4} c(\lambda_t)\,\phi_{N_t}(x-X)\,e^{ik_y y}\,\psi_{k_z}^{(t)} , \qquad (11.20)$$

where $\psi_{k_z}^{(t)}$ represents the Bloch function for $k_x = k_y = 0$ and ϕ_N is the harmonic oscillator state. b and b^+ operate on ϕ_N. Operating $\mathcal{H}$ on Ψ_λ, we obtain the following secular equation :

$$\begin{vmatrix} E_1 - E & 0 & -i\sqrt{2SN}\,P_1 & i\sqrt{2S(N+1)}\,P_1 \\ 0 & E_2 - E & i\sqrt{2SN}\,P_2 & i\sqrt{2S(N+1)}\,P_2 \\ i\sqrt{2SN}\,P_1 & -i\sqrt{2SN}\,P_2 & E_3 - E & 0 \\ -i\sqrt{2S(N+1)}\,P_1 & -i\sqrt{2S(N+1)}\,P_2 & 0 & E_3 - E \end{vmatrix} = 0 \quad . \tag{11.21}$$

For small N, retaining the terms up to $O(\mathcal{E}^2)$, where $\mathcal{E} = E - E_3$ we obtain 84)

$$\left\{ \begin{aligned} E &= E_3 + 2\eta_0^2 S \left[-\frac{1}{2}\left(N+\frac{1}{2}\right)(\omega_1+\omega_2) \pm \left\{ \left(\frac{N+1/2}{2}\right)^2 (\omega_1-\omega_2)^2 + \frac{\omega_1\omega_2}{4} \right\}^{1/2} \right], \\ E &= E_{1,2} + 2\eta_0^2 S\,(N+1/2)\,\omega_{1,2} \, , \end{aligned} \right. \tag{11.22}$$

where

$$\omega_1 = \frac{(1-\nu)^2}{E_1 - E_3} \, , \quad \omega_2 = \frac{(1+\nu)^2}{E_2 - E_3} \, . \tag{11.23}$$

It should be noted that in the first formula of (11.22) the root corresponding to $+\{\cdots\}^{1/2}$ is equal to E_3 for $N=0$. This means that this level does not include the zero point energy $\hbar\omega_0/2$. This situation is more clearly seen in the case of two-dimensional graphite. The two-dimensional unit cell contains two atoms, A and B (See Fig 8.15). Putting all the band parameters except γ_0 to zero, we obtain the Hamiltonian matrix as follows: 133)

$$\mathcal{H} = \begin{vmatrix} E_f & \eta_0 k_\xi e^{i\alpha}/\sqrt{2} \\ \eta_0 k_\xi e^{-i\alpha}/\sqrt{2} & E_f \end{vmatrix} \, , \quad \eta_0 = \sqrt{3}\,\gamma_0 a/\sqrt{2} \, , \tag{11.24}$$

and then we have

$$E - E_f = \pm \frac{\sqrt{3}\,\gamma_0 a}{2} k_f \qquad (11.25)$$

near the corners of the Brillouin zone. The corresponding Hamiltonian in magnetic field is given by

$$\mathcal{H} = \begin{vmatrix} E_f & i\sqrt{2s}\,p_0 b \\ -i\sqrt{2s}\,p_0 b^+ & E_f \end{vmatrix} , \quad p_0 = \gamma_0/\sqrt{2} , \qquad (11.26)$$

and the Landau levels are [134]

$$\begin{cases} E_0 - E_f = 0 , \\ E_N^{\pm} - E_f = \pm\sqrt{2sN}\,p_0 , \quad N = 1, 2, 3 \cdots \end{cases} \qquad (11.27)$$

The level for $N = 0$ is independent of the magnetic field. Appearance of the $N = 0$ state is one of the main reason for the large diamagnetism in graphite. [134]

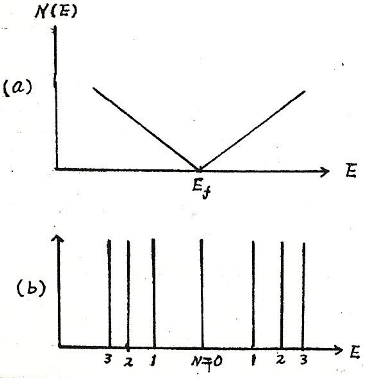


Fig. 11.1 (a) Density of states of two-dimensional graphite for $H = 0$.

(b) Landau levels of two-dimensional graphite.

11.2 Theory of Transverse Conductivity (Adams-Holstein Theory)

Classical motion of the electrons in magnetic field is a spiral motion around the axis parallel to the magnetic field, and the diagonal element of the velocity perpendicular to the magnetic field is zero. In the quantum theory the matrix elements of v_x and v_y are obtained as follows:

$$\begin{cases} v_x = \dot{x} = \dfrac{1}{i\hbar}[x, \mathcal{H}] = \dfrac{\hbar}{im}\dfrac{\partial}{\partial x}, \\ v_y = \dot{y} = \dfrac{1}{i\hbar}[y, \mathcal{H}] = \dfrac{\hbar}{im}\dfrac{\partial}{\partial y} + \omega_0 x, \end{cases} \qquad (11.28)$$

$$\begin{cases} \langle N', k_y', k_z' | v_x | N, k_y, k_z \rangle = \dfrac{1}{i}\sqrt{\dfrac{\hbar\omega_0}{2m}}\left\{-\sqrt{N+1}\,\delta_{N+1,N'} + \sqrt{N}\,\delta_{N-1,N'}\right\}\delta_{k.k'}, \\ \langle N', k_y', k_z' | v_y | N, k_y, k_z \rangle = \sqrt{\dfrac{\hbar\omega_0}{2m}}\left\{\sqrt{N+1}\,\delta_{N+1,N'} + \sqrt{N}\,\delta_{N-1,N'}\right\}\delta_{k.k'} \\ \qquad\qquad - \dfrac{e\mathcal{E}}{m\omega_0}\delta_{N.N'}\delta_{k.k'}, \end{cases} \qquad (11.29)$$

where we employ (11.10).

If the orbital quantization is disregarded, the current density can be calculated by the usual formula : $j_x = -(e/\Omega)\sum_k v_x(k) f_k$, where f_k is determined by solving the Boltzmann equation. However, in the "strong magnetic field" regime for which the cyclotron angular frequency ω_0 is greater than the reciprocal time between collisions, namely & $\hbar\omega_c \gg k_0T$ $\omega_0\tau \gg 1$ the crystal momentum k loses its meaning specifying the quantum state. Instead of the Bloch function we must use the Landau state. In this case f_k is replaced by the density matrix (Appendix 9).

In this Section we shall present a brief review about the theory due to Adams and Holstein.[135)]

In terms of the density matrix ρ the current density is given by

$$\mathbf{j} = -\frac{e}{\Omega}\sum_{\mu,\mu'} \rho_{\mu\mu'}(\boldsymbol{v})_{\mu'\mu} \, , \tag{11.30}$$

where μ and μ' denote the Landau state. Inserting (11.29) into (11.30), we have

$$\begin{aligned} j_x &= -\frac{e}{\Omega}\sum_{N,k}\left\{ \rho_{N,N-1}(v_x)_{N-1,N} + \rho_{N,N+1}(v_x)_{N+1,N} \right\} \\ &= \frac{ie\hbar}{2m\Omega}\sum_{N,k}\sqrt{2S(N+1)}\left\{ \rho_{N+1,N}(k) - \rho_{N,N+1}(k)\right\} . \end{aligned} \tag{11.31}$$

$$j_y = -\frac{e\hbar}{2m\Omega}\sum_{N,k}\sqrt{2S(N+1)}\left\{\rho_{N+1,N}(k) + \rho_{N,N+1}(k)\right\} + eV_d n, \tag{11.32}$$

where $V_d = c\mathcal{E}/H$ and $n = \Omega^{-1}\sum_{N,k}\rho_{NN}(k)$. V_d is the drift velocity along $-y$-direction induced by the Lorentz force.

Combining equations (11.31) and (11.32), we find :

$$j_y + i j_x = \frac{eV_d}{\Omega}\sum_{N,k}\rho_{NN}(k) - \frac{e\hbar}{m\Omega}\sum_{N,k}\sqrt{2S(N+1)}\;\rho_{N+1,N}(k) . \tag{11.33}$$

(11.33) expresses the current in terms of the matrix elements ρ_{NN} and $\rho_{N+1,N}$ of the density matrix, which connects states of the same wave number.

Our next step will be to develop an expansion of ρ as a perturbation series in the scattering interaction V. We will treat V as static, and V is expressed in terms of its Fourier components

V_g according to the formula :

$$V(r) = \sum_g V_g \, e^{igr}. \qquad (11.34)$$

The density matrix obeys the equation (Appendix 9)

$$-i\hbar \frac{\partial \rho}{\partial t} = [\rho . \mathcal{H}], \quad \mathcal{H} = \mathcal{H}_0 + V. \qquad (11.35)$$

We will use the Laplace transform method of solving the differential equation of motion of the density matrix :

$$P(\varepsilon) = \varepsilon \int_0^\infty e^{-\varepsilon t} \rho(t) dt. \qquad (11.36)$$

We can obtain the value of the density matrix ρ after such a long time that all transients have disappeared by $\lim_{\varepsilon \to 0} P(\varepsilon)$.

By applying an operation $\varepsilon \int_0^\infty dt\, e^{-\varepsilon t} \dots$ on the both sides of equation (11.35), we obtain

$$-i\hbar\varepsilon P(\varepsilon) = [P(\varepsilon), \mathcal{H}] - i\hbar \varepsilon \rho(0). \qquad (11.37)$$

We will choose as the initial density matrix

$$\rho_{\mu\nu}(0) = \delta_{\mu\nu} f(\mathcal{E}_\mu), \quad \mu \equiv (N, k) \qquad (11.38)$$

where f is the Fermi function and $\mathcal{E}_\mu$ represents the part of the energy that does not depend on electric field. To solve (11.37) we express $P(\varepsilon)$ as the sum of three parts :

$$P_{\mu\nu}(\varepsilon) = f_\mu \delta_{\mu\nu} + D_{\mu\nu}(\varepsilon) + G_{\mu\nu}(\varepsilon), \qquad (11.39)$$

here $f_\mu \delta_{\mu\nu}$ represents the Laplace transform of the initial density matrix, while $D_{\mu\nu}$ and $G_{\mu\nu}$ represent the Laplace transform of the change in the distribution function resulting from the combined action of the scattering and the electric field. $D_{\mu\nu}$ does not vanish only for $k_\mu = k_\nu$ and $G_{\mu\nu}$ is defined so as to vanish unless k_μ and k_ν are different.

From (11.37) D and G satisfy

$$\begin{cases} (\varepsilon_{\mu\nu} + e\mathcal{E}X_{\mu\nu} - i\hbar\varepsilon)\,G_{\mu\nu} = f_{\mu\nu}V_{\mu\nu} + [D, V]_{\mu\nu} + [G, V]_{\mu\nu}, \\ (\varepsilon_{NN'} - i\hbar\varepsilon)\,D_{NN'} = [G, V]_{NN'}, \end{cases} \tag{11.40}$$

where

$$\varepsilon_{\mu\nu} = \varepsilon_\mu - \varepsilon_\nu, \quad f_{\mu\nu} = f_\mu - f_\nu \quad (k_\mu \neq k_\nu), \quad \varepsilon_{NN'} = \varepsilon_N - \varepsilon_{N'}. \tag{11.41}$$

The lowest non-vanishing approximations to the solutions of (11.40) are

$$\begin{cases} G_{\mu\nu} = f_{\mu\nu}V_{\mu\nu}/(\varepsilon_{\mu\nu} + e\mathcal{E}X_{\mu\nu} - i\hbar\varepsilon), \\ D_{NN'} = \dfrac{1}{\varepsilon_{NN'} - i\hbar\varepsilon}\sum_\nu V_{N\nu}V_{\nu N'}\left[\dfrac{f_{N\nu}}{\varepsilon_{N\nu} + e\mathcal{E}X_{N\nu} - i\hbar\varepsilon} - \dfrac{f_{N'\nu}}{\varepsilon_{N'\nu} + e\mathcal{E}X_{N'\nu} + i\hbar\varepsilon}\right], \end{cases} \tag{11.42}$$

where $k_N = k_{N'} \neq k_\nu$.

(11.31) and (11.32) indicate that in calculating the current density we need only $D_{NN'}$ with $N = N' \pm 1$. Using the relation

$$\lim_{\varepsilon \to 0^+} \frac{1}{z - i\varepsilon} = P\left(\frac{1}{z}\right) + i\pi\delta(z), \tag{11.43}$$

we obtain

$$D_{NN'} = \frac{i\pi}{\varepsilon_{NN'}} \sum_{\nu} V_{N\nu} V_{\nu N'} \Big[\{ f(\varepsilon_N) - f(\varepsilon_\nu) \} \delta(\varepsilon_{N\nu} + e\mathcal{E} X_{N\nu})$$

$$- \{ f(\varepsilon_{N'}) - f(\varepsilon_\nu) \} \delta(\varepsilon_{N'\nu} + e\mathcal{E} X_{N'\nu}) \Big] . \qquad (11.44)$$

By developing the δ-function to the first power of $\mathcal{E}$, (11.44) becomes

$$D_{N+1,N} = \frac{i\pi e\mathcal{E}}{\hbar\omega_0} \sum_{\nu} V_{N+1,\nu} V_{\nu N} X_{\nu N} \frac{\partial f(\varepsilon_\nu)}{\partial \varepsilon_\nu} \left[\delta(\varepsilon_{N+1.\nu}) + \delta(\varepsilon_{N.\nu}) \right] . \qquad (11.45)$$

If we insert the approximation (11.45) for the density matrix elements $\rho_{N+1.N}$ into the expression (11.33) for the current, we obtain a formula for the current density

$$j_y + i j_x = e V_d n - \frac{i\pi e^2 \mathcal{E}}{\Omega m \omega_0} \sum_{\mu,\nu} \delta(\varepsilon_{N\nu}) \frac{\partial f}{\partial \varepsilon_\nu} X_{\mu\nu} \Big[\sqrt{2s(N+1)}\, V_{N+1,\nu} V_{\nu,N}$$

$$+ \sqrt{2sN}\, V_{N,\nu} V_{\nu N-1} \Big] , \quad \mu \equiv (N.k), \quad \nu \equiv (N'.k') . \qquad (11.46)$$

In consideration of (11.10) and (11.11), the term in square bracket of (11.46) is transformed as follows:

$$\sqrt{2s(N+1)}\, V_{N+1,\nu} V_{\nu,N} + \sqrt{2sN}\, V_{N.\nu} V_{\nu,N-1} = \{ s(x - X_\mu) V \}_{\mu\nu} V_{\nu\mu}$$

$$+ \left(\frac{\partial}{\partial x} V \right)_{\mu\nu} V_{\nu\mu} + V_{\mu\nu} \{ V s(x - X_\mu) \}_{\nu\mu} + V_{\nu\mu} \left(V \frac{\partial}{\partial x} \right)_{\nu\mu} , \qquad (11.47)$$

where

$$\left(\frac{\partial}{\partial x} V \right)_{\mu\nu} \equiv \int \psi_\mu^* \frac{\partial}{\partial x} (V \psi_\nu)\, d\tau , \qquad (11.48)$$

and $\sum_{\mu,\nu} \cdots$ in (11.46) becomes

$$\sum_{\mu\nu} \delta(\varepsilon_{\mu\nu}) \frac{\partial f_\nu}{\partial \varepsilon_\nu} X_{\nu\mu}\left[s(xV - Vx)_{\mu\nu} V_{\nu\mu} + X_{\nu\mu}\, s\, V_{\mu\nu} V_{\nu\mu} + \left(\frac{\partial V}{\partial x}\right)_{\mu\nu} V_{\nu\mu}\right]$$

$$= \sum_{\mu\nu} \delta(\varepsilon_{\mu\nu}) \frac{\partial f_\nu}{\partial \varepsilon_\nu} \frac{q_y}{s} (q_y + i q_x) |V_q|^2 |(e^{iqr})_{\mu\nu}|^2, \tag{11.49}$$

where $k_\mu - k_\nu = q$.

Then, we have

$$j_x = -\frac{\pi e^2 \mathcal{E}}{\Omega m \omega_0 s} \sum_{\mu\nu} \delta(\varepsilon_{\mu\nu}) \frac{\partial f_\nu}{\partial \varepsilon_\nu} q_y^2 |V_q|^2 |(e^{iqr})_{\mu\nu}|^2. \tag{11.50}$$

Hence,

$$\sigma_{xx} = -\frac{e^2}{\Omega} \sum_{\mu,\nu} \frac{2\pi}{\hbar} \delta(\varepsilon_{\mu\nu}) \frac{\partial f_\nu}{\partial \varepsilon_\nu} \frac{1}{2} X_{\mu\nu}^2 |V_{\mu\nu}|^2$$

$$= \frac{1}{\Omega} \sum_{N,k} e^2 \frac{\partial f}{\partial \zeta} \sum_{E_N = E_\nu} \frac{1}{2} X_{\mu\nu}^2 \omega_{N\nu}, \tag{11.51}$$

where $\omega_{N\nu}$ denotes the relaxation rate for $N \to \nu$ transition.

By introducing a relaxation time τ, (11.51) is rewritten in the form

$$\sigma_{xx} = e^2 \left\langle \frac{dn}{d\zeta} \left\langle \frac{1}{2} \frac{d^2}{\tau} \right\rangle \right\rangle, \tag{11.52}$$

where

$$\frac{1}{\Omega} \frac{d}{d\zeta} \sum_{N,k} f(E_{Nk}) = \frac{dn}{d\zeta}, \quad \left\langle \frac{d^2}{\tau} \right\rangle = \sum_{E_N = E_\nu} X_{\mu\nu}^2 \omega_{N\nu}. \tag{11.53}$$

The outer angular bracket in (11.52) denotes a thermal average, the inner an average over jumps,

From (11.46), we have

$$\sigma_{xy} = -\frac{ec}{H} n. \tag{11.54}$$

In the case of non-degenerate system, (11.52) becomes

$$\sigma_{xx} = n e \mu , \ \mu = \frac{e}{k_0 T n} \langle n \langle \frac{1}{2} \frac{d^2}{\tau} \rangle \rangle \ . \qquad (11.55)$$

The expression (11.55) is closely related to the Einstein-relation for the electrical conductivity in terms of the diffusivity.

It will be shown in the latter Sections that the present theory is essentially identical with that of Titeica, which will be discussed in the next Section.

11. 3 Titeica Theory on the Transverse Conductivity in Strong Magnetic Field.

The first calculation on the transverse conduction in strong magnetic field was done by Titeica.[136)] He calculated the transverse current by tacitly assuming that it is produced only by the drift of centers of the cyclotron orbits of the electrons in the magnetic field due to the electric field and the scattering processes. This semiclassical method of calculation of Titeica was justified by the procedure based on the density matrix. His pioneer work has not attracted notice for long time since at that time the research works in strong magnetic field were very scarce.

Titeica calculated the electrical conductivity related to the acoustic phonon scattering. We will present a brief sketch of the theory.

Apply an electric field $\mathcal{E}$ along the x-direction and consider the yz-plane passing through $x=0$, where H is parallel to the z-axis. According to Titeica, the electric current is proportional to the difference in the jumping transition rate between the processes $X(<0) \rightarrow X'(>0)$ and its reverse processes, where X and X' denote the centers of the Landau orbit. The perturbing potential is taken to be as (See (7.4)),

$$V(r) = \frac{1}{\sqrt{\Omega}} \sum_q{}' \left\{ C(q)\, b_q e^{iqr} + C^*(q)\, b_q^+ e^{-iqr} \right\}, \quad C(q) = iD\sqrt{\frac{\hbar}{2d\omega_q}}\, q, \tag{11.56}$$

where $\sum_q{}'$ denotes a summation over half the phase parallelpiped.

The current density is given by

$$j_x = -\frac{e}{\Omega} \sum_{X_\mu<0} \sum_{X_\nu>0} \sum_q{}' \frac{2\pi}{\hbar} \frac{|C(q)|^2}{\Omega} \left|(e^{iqr})_{\mu\nu}\right|^2 \Big[\left\{ f_\nu(1-f_\mu)N_q - f_\mu(1-f_\nu)(N_q+1) \right\} \delta(E_\mu - E_\nu - \hbar\omega_q) + \left\{ f_\nu(1-f_\mu)(N_q+1) - f_\mu(1-f_\nu)N_q \right\} \delta(E_\mu - E_\nu + \hbar\omega_q) \Big], \tag{11.57}$$

where

$$\begin{cases} E_\mu = \hbar\omega_0(N+1/2) + \dfrac{\hbar^2 k_z^2}{2m} + e\mathcal{E}X_\mu, \\ E_\nu = \hbar\omega_0(N'+1/2) + \dfrac{\hbar^2 k_z'^2}{2m} + e\mathcal{E}X_\nu, \end{cases} \tag{11.58}$$

and f_μ and f_ν are the Fermi function specified by E_μ and E_ν.

Rewriting (11.57), we obtain

$$j_x = -\frac{\pi\hbar}{2}\,\frac{eD^2}{d\Omega\,\hbar v_s}\left(\frac{L}{2\pi}\right)^5\left(\frac{m\omega_0}{\hbar}\right)^2\sum_{N,N'}\int_{X<0,\,X'>0} du\,dv\,dX\,dX'\,dq_x\,|J_{NN'}|^2\times[\cdots], \tag{11.59}$$

where $[\cdots]$ denotes the square bracket in (11.57), and

$$\begin{cases} u = k_z + k_z', \quad v = k_z - k_z', \quad X = X_\mu, \quad X' = X_\nu, \\ J_{NN'} = \displaystyle\int_{-\infty}^{\infty} dx\, e^{iq_x x}\,\phi_N(x-X)\,\phi_{N'}(x-X'), \quad L: \text{length of the edge of the sample.} \end{cases} \tag{11.60}$$

Developing the δ-function to the first power of $\mathcal{E}$ and integrating over u, one obtains

$$j_x = -\frac{\pi}{2}\,\frac{m}{\hbar}\,\frac{e\mathcal{E}}{k_0T}\,\frac{eD^2}{d\Omega\,\hbar v_s}\left(\frac{L}{2\pi}\right)^2\left(\frac{m\omega_0}{\hbar}\right)^2\sum_{NN'}\int dv\,dr\,ds\,dq_x\, r\,(A-B), \tag{11.61}$$

where

$$\begin{cases} r = X' - X, \quad s = X' + X, \\ A = \dfrac{q}{|v|}\,|J_{NN'}|^2 N_q(N_q+1)\,[f(\varepsilon') - f(\varepsilon)] \;:\; \varepsilon' - \varepsilon - \hbar\omega_q = 0, \\ B = \dfrac{q}{|v|}\,|J_{NN'}|^2 N_q(N_q+1)\,[f(\varepsilon') - f(\varepsilon)] \;:\; \varepsilon' - \varepsilon + \hbar\omega_q = 0. \end{cases} \tag{11.62}$$

Integration over s is performed in the range $(-r, r)$ and the one over r is done in the range $(0, \infty)$. Since the integrand does not depend on s, (11.61) becomes

$$j_x = -\frac{\pi m}{\hbar}\,\frac{e\mathcal{E}}{k_0T}\,\frac{eD^2}{d\Omega\,\hbar v_s}\left(\frac{L}{2\pi}\right)^5\left(\frac{m\omega_0}{\hbar}\right)^2\sum_{NN'}\int dr\,dv\,dq_x\, r^2(A-B), \tag{11.63}$$

where $r = (k_y - k_y')/s = q_y/s$. Writing $q_x = q_\rho \cos\theta$, $q_y = q_\rho \sin\theta$ and integrating over θ, we obtain

$$j_x = -\frac{\pi^2}{2}\frac{m}{\hbar}\frac{e\mathcal{E}}{k_0 T}\frac{eD^2}{d\Omega\hbar v_s}\left(\frac{L}{2\pi}\right)^5\frac{\hbar}{m\omega_0}\sum_{N,N'}\int dq_\rho\, q_\rho^3\, dv\,(A-B). \qquad (11.64)$$

To calculate (11.64) for arbitrary values of N and N' is not easy. The reader should be referred to Titeica's paper. The result for $N = N' = 0$ (quantum limit) will be shown in Section 11.8.

11.4 Kubo Formula

The linear response of a statiscal ensemble to an external time-dependent perturbations is investigated in this Section. We consider mechanical perturbations as the external perturbations. By mechanical perturbations, we mean only those perturbations which represent the action of external fields and which can be described completely by adding the corresponding energy of interaction of the system with the field to the Hamiltonian.

Kubo gave the most general proof of the linear response theory, and applied them widely to the theory of linear dissipative processes.[137)]

Let denote the external perturbation as

$$H_1 = -A F(t), \qquad (11.65)$$

where F is the external force and A is the dynamic variable.

The density matrix satisfies

$$\frac{d}{dt}\rho(t) = \frac{1}{i\hbar}[H + H_1(t), \rho(t)], \qquad (11.66)$$

and the initial condition $\rho(-\infty) = \rho_0$, which means that, at $t=-\infty$, the system was in a state of statistical equilibrium, where $[\mathcal{H}, \rho_0]=0$. Retaining the first order terms in $\mathcal{H}_1$, we obtain

$$\frac{d}{dt}\rho_1(t)=\frac{1}{i\hbar}\left\{[\mathcal{H}, \rho_1(t)]-F(t)[A, \rho_0]\right\}, \qquad (11.67)$$

and

$$\rho_1(t)=-\frac{1}{i\hbar}\int_{-\infty}^{t} e^{-i(t-t')\mathcal{H}/\hbar}[A, \rho_0]\, e^{i(t-t')\mathcal{H}/\hbar} F(t')\,dt'. \qquad (11.68)$$

Accordingly, the linear response of an operator B is given by

$$\Delta B(t)=\mathrm{Tr}\,\rho_1(t)B=-\frac{1}{i\hbar}\mathrm{Tr}\int_{-\infty}^{t} e^{-i(t-t')\mathcal{H}/\hbar}[A, \rho_0]\, e^{i(t-t')\mathcal{H}/\hbar} B F(t')\,dt'$$

$$=-\frac{1}{i\hbar}\mathrm{Tr}\int_{-\infty}^{t}[A, \rho_0]\, B(t-t')\, F(t')\,dt', \qquad (11.69)$$

where

$$B(t)=e^{it\mathcal{H}/\hbar} B\, e^{-it\mathcal{H}/\hbar}. \qquad (11.70)$$

Then,

$$\dot{B}(t)=\frac{1}{i\hbar}[B(t), \mathcal{H}]. \qquad (11.71)$$

It is worthy of note that the order of the commutator in (11.71) is different from that in (11.66). $\Delta B(t)$ is rewritten in terms of the response function

$$\Delta B(t)=\int_{-\infty}^{t}\phi_{BA}(t-t')F(t')\,dt', \qquad (11.72)$$

where

$$\phi_{BA}(t)=-\frac{1}{i\hbar}\mathrm{Tr}[A, \rho_0]\, B(t). \qquad (11.73)$$

If the external perturbation contains only one harmonic of frequency ω, i.e.: $F(t) = F_0 \cos\omega t$, $\Delta B(t)$ is expressed by introducing the admittance χ_{BA} as

$$\Delta B(t) = \mathrm{Re}\, \chi_{BA}(\omega) F_0 e^{i\omega t}, \tag{11.74}$$

where

$$\chi_{BA}(\omega) = \int_0^\infty \phi_{BA}(t) e^{-i\omega t} dt = \lim_{\varepsilon \to +0} \int_0^\infty \phi_{BA}(t) e^{-i\omega t - \varepsilon t} dt$$

$$= \lim_{\varepsilon \to +0} \frac{1}{i\omega + \varepsilon} \left\{ \phi_{BA}(0) + \int_0^\infty \dot{\phi}_{BA}(t) e^{-i\omega t - \varepsilon t} dt \right\}. \tag{11.75}$$

In the next place we shall prove the identity[137]:

$$[\rho_0, A] = \int_0^\beta \rho_0 e^{\lambda H} [A, H] e^{-\lambda H} d\lambda = i\hbar \int_0^\beta \rho_0 \dot{A}(-i\hbar\lambda) d\lambda, \tag{11.76}$$

where $\rho_0 = \exp(-\beta H)/\mathrm{Tr}\exp(-\beta H)$. In consideration of (11.70) and (11.71) the last relation is derived from the second term. We shall now derive the Kubo identity (11.76). We put

$$\left[e^{-\beta H}, A \right] = e^{-\beta H} S(\beta), \tag{11.77}$$

where $S(\beta)$ is an operator to be determined. Differentiating (11.77) with respect β, we obtain a differential equation for $S(\beta)$:

$$\frac{\partial S}{\partial \beta} = e^{\beta H} [A, H] e^{-\beta H}, \tag{11.78}$$

with the intial condition $S|_{\beta=0} = 0$. Integrating this, taking the initial condition into account, we obtain Kubo identity (11.76).

Substituting (11.76) into (11.73) and using the invariance of trace with respect to a cyclic permutations of the operators, we obtain

$$\Phi_{BA}(t) = \int_0^\beta \mathrm{Tr}\, \rho_0\, \dot{A}(-i\hbar\lambda)\, B(t)\, d\lambda = -\int_0^\beta \mathrm{Tr}\, \rho_0\, A(-i\hbar\lambda)\, \dot{B}(t)\, d\lambda. \qquad (11.79)$$

We shall apply the above expressions to the calculation of the electrical conductivity. In this case the external force is

$$H_1(t) = -\sum_i e_i\, \mathbf{r}_i \cdot \mathcal{E}(t). \qquad (11.80)$$

Let consider that $\mathcal{E}$ is applied along the ν-direction. The response function $\Phi_{\mu\nu}$ is given by

$$\begin{aligned}\Phi_{\mu\nu}(t) &= \frac{1}{i\hbar}\, \mathrm{Tr}\left[\rho_0, \sum_i e_i x_{i\nu}\right] \sum_j e_j \dot{x}_{j\mu} \\ &= \int_0^\beta \langle j_\nu(-i\hbar\lambda)\, j_\mu(t)\rangle\, d\lambda, \quad j_\mu = \sum_i e_i \dot{x}_{i\mu}.\end{aligned} \qquad (11.81)$$

Accordingly, the conductivity tensor $\sigma_{\mu\nu}$ takes the form

$$\sigma_{\mu\nu}(\omega) = \frac{1}{\Omega} \int_0^\infty dt\, e^{-i\omega t} \int_0^\beta \langle j_\nu(-i\hbar\lambda)\, j_\mu(t)\rangle\, d\lambda, \qquad (11.82)$$

and the static conductivity becomes

$$\sigma_{\mu\nu} = \frac{1}{\Omega} \int_0^\infty dt \int_0^\beta \langle j_\nu(-i\hbar\lambda)\, j_\mu(t)\rangle\, d\lambda. \qquad (11.83)$$

Completely analogous formula is obtained in the presence of a spatially uniform oscillating magnetic field. The operator corresponding

(11.80) is

$$H_1(t) = -(M \cdot H)\cos\omega t, \tag{11.84}$$

where M is the total magnetic moment of the system. The magnetic susceptibility tensor $\chi_{\alpha\beta}(\omega)$ can also be written in the form

$$\chi_{\alpha\beta}(\omega) = \frac{1}{\Omega}\int_0^\infty dt\, e^{i\omega t}\int_0^\beta \langle \dot{M}_\beta M_\alpha(t+i\hbar\lambda)\rangle\, d\lambda, \tag{11.85}$$

which is analogous to (11.83). This formula was derived by Kubo and Tomita and applied to the problem of magnetic resonance.138)

A remarkable feature of the Kubo relations is that they express non equilibrium dissipative properties in terms of a state of statistical equilibrium and have an extremely general character. These relations are called "fluctuation-dissipation therem."

Here, we notice that an equivalent expression to (11.83) was independently derived by Nakano.139)

The Onsager's relation is naturally verified by use of the Kubo formula,

11.5 Quantum Theory of the Electrical Conduction in Strong Magnetic Field

Kubo formula exhibits its effectiveness in the application to the galvanomagnetic effect in strong magnetic field. The discussions developed in the following several Sections are mainly due to the works done by Kubo and his collaborators.140), 141)

We consider crystal electrons which are described by the Bloch states $E_0(P)$ where p is crystal momentum $\hbar k$. In the presence of a perturbation potential $V(r)$, the crystal electrons may be described by the effective Hamiltonian,

$$\mathcal{H} = H_e + V(r), \quad H_e = E_0(\pi). \quad \pi = P + \frac{e}{c} A . \tag{11.86}$$

Since curl $A = H$, π satisfies the commutation relation,

$$\pi \times \pi = \frac{\hbar e}{i c} H . \tag{11.87}$$

If the direction of H is chosen as the z-axis, non-zero commutation relations are

$$[\pi_x, \pi_y] = \frac{\hbar e}{i c} H, \quad [\pi_x, x] = [\pi_y, y] = [p_z, z] = \frac{\hbar}{i} . \tag{11.88}$$

Now let us introduce a new set of variables instead of the cartesian coordinates and their conjugate momenta:

$$\xi = \frac{c}{eH} \pi_y , \quad \eta = -\frac{c}{eH} \pi_x , \tag{11.89}$$

and

$$X = x - \xi , \quad Y = y - \eta . \tag{11.90}$$

It is shown that the coordinates (X, Y) specify the center coordinates of the cyclotron motion perpendicular to the magnetic field.

Since (X, Y) commute with π, then they commute with the unperturbed Hamiltonian $E_0(\pi)$. This means that the coordinates (X, Y) remain unchanged in the cyclotron motion. Therefore, we can consider (X, Y) as the center coordinates. From (11.89) and (11.90) we obtain the following commutation relations:

$$\begin{cases} [\xi, \eta] = -i\ell^2, \quad [X, Y] = i\ell^2, \\ [\xi, X] = [\eta, X] = [\xi, Y] = [\eta, Y] = 0, \\ \ell^2 = s^{-1} = \hbar c/eH. \end{cases} \tag{11.91}$$

Then, we can see that the variables (ξ, η), (X, Y) and (P_z, z) make a complete set of canonical variables. From (11.91) we obtain the uncertainty relation

$$\Delta X \Delta Y \cong 2\pi\ell^2 = 2\pi\hbar c/eH, \tag{11.92}$$

from which results that each eigenstate $E_0(\pi_x, \pi_y, P_z)$ has the degeneracy of $1/2\pi\ell^2$ per unit area of the x-y plane. This leads to the degree of the degeneracy for the Landau state $(N, (P_z, P_z+\Delta P_z))$

$$\frac{L_x L_y L_z}{2\pi\ell^2}\left(\frac{\Delta P_z}{\hbar}\right), \tag{11.93}$$

which is already obtained in (11.8). ℓ corresponds to the extension of the Landau wave function with $N=0$ (see (11.5)).

In the presence of the perturbing potential $V(r)$ the equation of motion of the center coordinates (X, Y) is given by

$$\begin{cases} \dot{X} = \frac{i}{\hbar}[\mathcal{H}, X] = \frac{i}{\hbar}[V, X] = \frac{c}{eH}\frac{\partial V}{\partial y}, \\ \dot{Y} = \frac{i}{\hbar}[\mathcal{H}, Y] = \frac{i}{\hbar}[V, Y] = -\frac{c}{eH}\frac{\partial V}{\partial x}, \end{cases} \tag{11.94}$$

and the motion along the z-axis is given by

$$\dot{z} = \frac{\partial E_0}{\partial p_z}, \quad \dot{p}_z = -\frac{\partial V}{\partial z}. \tag{11.95}$$

The wave function ψ_{N,X,p_z} given by (11.5) corresponds to the set of the conjugate variables (x, π_x), (X, y), and (p_z, z).

Let us rewrite (11.83) by introducing the quantized wave functions. The current density operator $\mathbf{j}_\mu$ is expressed by

$$\mathbf{j}_\mu = \int \Psi(r)^* j_\mu \Psi(r)\, d\mathbf{r}, \tag{11.96}$$

where j_μ is the current operator for one electron, $j_\mu = -e v_\mu$. Quantized wave functions normalized in unit volume are written in terms of the second quantization operators as

$$\Psi(r) = \sum_i a_i \psi_i(r), \quad \Psi(r)^* = \sum_i a_i^+ \psi_i(r)^*, \tag{11.97}$$

where ψ_i and ψ_i^* denote the Landau state wave functions.

From (11.90), the electric current can be written as

$$j_x \pm i j_y = -e\left\{(\dot{\xi} \pm i\dot{\eta}) + (\dot{X} \pm i\dot{Y})\right\}, \tag{11.98}$$

We may conveniently use the complex representation : $j_\pm = j_x \pm i j_y$, $\xi_\pm = \xi \pm i\eta$, $X_\pm = X \pm iY$. The current components are

$$\left\{\begin{aligned} \mathbf{j}_\pm &= -e(\dot{\mathbf{X}}_\pm + \dot{\boldsymbol{\xi}}_\pm), \\ \mathbf{X}_\pm &= \int \Psi(r)^* X_\pm \Psi(r)\, d\mathbf{r}, \quad \boldsymbol{\xi}_\pm = \int \Psi(r)^* \xi_\pm \Psi(r)\, d\mathbf{r}. \end{aligned}\right. \tag{11.99}$$

In the following it will be shown that we obtain a simple expression of the conductivity tensor if the Fermi surface is closed. Namely, the cross terms between $\mathbf{X}_\pm$ and $\xi_\pm$ vanish and we have

$$\begin{cases} \sigma_{xx} = \dfrac{e^2}{\Omega} \displaystyle\int_0^\infty dt\, e^{-\varepsilon t} \int_0^\beta d\lambda \langle \dot{\mathbf{X}}(-i\hbar\lambda)\dot{\mathbf{X}}(t)\rangle, \quad (\varepsilon \to +0) \\ \sigma_{xy} = -\dfrac{nec}{H} + \dfrac{e^2}{\Omega} \displaystyle\int_0^\infty dt\, e^{-\varepsilon t} \int_0^\beta d\lambda \langle \dot{\mathbf{Y}}(-i\hbar\lambda)\dot{\mathbf{X}}(t)\rangle. \end{cases} \tag{11.100}$$

Proof :

In the first place, let take notice of

$$\langle \dot{\xi}_\pm \rangle = 0, \quad \langle \dot{\mathbf{X}}_\pm \rangle = 0, \tag{11.101}$$

if the cyclotron orbit is closed. The first relation directly follows from the situation that the cyclotron orbit is closed and so the variables (ξ, η) are bounded. The second relation comes from the first one and $\langle \mathbf{j}_\pm \rangle = 0$.

$$\int_0^\infty dt\, e^{-\varepsilon t} \int_0^\beta d\lambda \langle \dot{\xi}_\mp(-i\hbar\lambda)\dot{\xi}_\pm(t)\rangle = \lim_{t\to\infty} \int_0^\beta d\lambda \langle \dot{\xi}_\mp(-i\hbar\lambda)\xi_\pm(t)\rangle$$

$$-\int_0^\beta d\lambda \langle \dot{\xi}_\mp(-i\hbar\lambda)\xi_\pm \rangle = \int_0^\infty d\lambda \langle \dot{\xi}_\mp(-i\hbar\lambda)\rangle\langle \xi_\pm\rangle - \frac{1}{i\hbar} \mathrm{Tr}\left([\rho, \xi_\mp]\, \xi_\pm\right)$$

$$= -\frac{1}{i\hbar} \mathrm{Tr}\left(\rho [\xi_\mp, \xi_\pm]\right) = \pm 2i \frac{nc}{eH} \Omega . \tag{11.102}$$

In deriving (11.102), (11.101) and the Kubo identity (11.76) are employed, and the last expression is obtained by the commutation relation

$$Tr\left(\rho[\xi_\mp, \xi_\pm]\right) = Tr\,\rho\left(\int \Psi(r)^* [\xi_\mp, \xi_\pm]\, \Psi(r)\, d\mathbf{r}\right)$$

$$= \pm\, 2\, l^2\, Tr\,\rho\left(\int \Psi^*(r)\, \Psi(r)\, d\mathbf{r}\right) = \pm 2 n \frac{c\hbar}{eH} . \tag{11.103}$$

Similary, we obtain

$$\int_0^\infty dt\, e^{-\varepsilon t} \int_0^\beta d\lambda \langle \dot{\mathbb{X}}_\pm(-i\hbar\lambda)\, \dot{\xi}_\mp(t)\rangle = -\int_0^\infty d\lambda \langle \dot{\mathbb{X}}_\pm(-i\hbar\lambda)\, \xi_\mp(0)\rangle$$

$$= -\frac{1}{i\hbar}\, Tr\left(\rho[\mathbb{X}_\pm, \xi_\mp]\right) = 0. \tag{11.104}$$

By using the relations (11.101) – (11.104) and the similar ones, (11.100) can be proved.

In the next place we shall rewrite (11.100) into more convenient form.

$$\int_0^\beta d\lambda \langle \dot{\mathbb{X}}(-i\hbar\lambda)\, \dot{\mathbb{X}}(-t)\rangle = \int_0^\beta d\lambda\, Tr\left\{e^{-(\beta-\lambda)\mathcal{H}+\beta\zeta N}\, \dot{\mathbb{X}}\, e^{-\lambda\mathcal{H}}\, e^{-it\mathcal{H}/\hbar}\, \dot{\mathbb{X}}\, e^{it\mathcal{H}/\hbar}\right\}$$

$$\times \left\{Tr\, e^{-\beta(\mathcal{H}-\zeta N)}\right\}^{-1}, \tag{11.105}$$

where $\langle \cdots \rangle$ represents the average over the grand partition function as follows :

$$\langle A \rangle = Tr(\rho A), \quad \rho = e^{-\beta(\mathcal{H}-\zeta N)} \Big/ Tr\, e^{-\beta(\mathcal{H}-\zeta N)}, \tag{11.106}$$

and N is the carrier density operator. Replacing $\beta - \lambda$ by μ and in consideration of the relation $[N, \dot{\mathbb{X}}] = 0$, we have

$$(11.105) = \int_0^\beta d\mu \, \mathrm{Tr}\left\{ e^{-\mu H} \dot{\mathbb{X}} e^{-itH/\hbar} \, e^{(\mu-\beta)H + \beta\zeta N} \dot{\mathbb{X}} e^{itH/\hbar} \right\} / \mathrm{Tr}\, e^{-\beta(H-\zeta N)}$$

$$= \int_0^\beta d\mu \, \langle \dot{\mathbb{X}}(-i\hbar\mu) \dot{\mathbb{X}}(t) \rangle . \qquad (11.107)$$

The last expression is obtained by a cyclic permutation of the operators in $\mathrm{Tr}\{\cdots\}$. Combining with (11.100), we obtain

$$\sigma_{xx} = \frac{e^2}{2\Omega} \int_{-\infty}^{+\infty} dt \int_0^\beta d\lambda \, \langle \dot{\mathbb{X}}(-i\hbar\lambda) \dot{\mathbb{X}}(t) \rangle . \qquad (11.108)$$

It is readily shown that the double integral in (11.108) can be transformed into a single integral.

$$\int_{-\infty}^{+\infty} dt \int_0^\beta d\lambda \, \langle \dot{\mathbb{X}}(-i\hbar\lambda) \dot{\mathbb{X}}(t) \rangle = \int_{-\infty}^{+\infty} dt \int_0^\beta d\lambda \, \langle \dot{\mathbb{X}}(0) \dot{\mathbb{X}}(t + i\hbar\lambda) \rangle$$

$$= \int_0^\beta d\lambda \int_{-\infty + i\hbar\lambda}^{+\infty + i\hbar\lambda} ds \, \langle \dot{\mathbb{X}}(0) \dot{\mathbb{X}}(s) \rangle = \int_0^\beta d\lambda \int_{-\infty}^{+\infty} ds \, \langle \dot{\mathbb{X}}(0) \dot{\mathbb{X}}(s) \rangle$$

$$= \beta \int_{-\infty}^{+\infty} dt \, \langle \dot{\mathbb{X}}(0) \dot{\mathbb{X}}(t) \rangle . \qquad (11.109)$$

Here, the path of integration is shifted. Since the integrand does not seem to have any singularity between the new and the old integration paths, this procedure will be justified, and the change of the order of integration is also permissible.

Finally, we obtain a simple formula

$$\sigma_{xx} = \frac{e^2}{2k_0T\Omega}\int_{-\infty}^{+\infty} dt \langle \dot{X}(0)\dot{X}(t)\rangle . \qquad (11.110)$$

Above expression indicates that the conductivity at high magnetic field is described by the migration of the center of cyclotron motion. This put the Titeica's intuitive treatment on the sound basis.

In a similar way, the longitudinal conductivity becomes

$$\sigma_{zz} = \frac{e^2}{2k_0T\Omega}\int_{-\infty}^{+\infty} dt \langle v_z(0)v_z(t)\rangle , \qquad (11.111)$$

11.6 Impurity Scattering in Strong magnetic Field.

It will be shown in this Section that (11.110) leads to the Adamo-Holstein theory.

From (11.99), we have

$$\langle \dot{X}(0)\dot{X}(t)\rangle = \langle Tr\{f(H)\dot{X}(0)[1-f(H)]\dot{X}(t)\}\rangle , \qquad (11.112)$$

where $\dot{X}(t) = e^{itH/\hbar}\dot{X}e^{-itH/\hbar}$, and Tr is taken over the one-electron coordinate. $\langle\cdots\rangle$ means the average over the scatters. Then,

$$\int_{-\infty}^{+\infty} dt \langle \dot{X}(0)\dot{X}(t)\rangle = \int_{-\infty}^{+\infty} dt \langle Tr\{f(H)\dot{X}[1-f(H)]e^{itH/\hbar}\dot{X}e^{-itH/\hbar}\}\rangle$$

$$= \int_{-\infty}^{+\infty} dt \int dE\, f(E)\langle Tr\{\delta(E-H)\dot{X}[1-f(H)]e^{itH/\hbar}\dot{X}e^{-itH/\hbar}\}\rangle$$

$$= \int_{-\infty}^{+\infty} dE\, f(E) \langle \mathrm{Tr} \{ \delta(E-\mathcal{H}) \dot{X} [1-f(\mathcal{H})] \int_{-\infty}^{+\infty} dt\, e^{it(\mathcal{H}-E)/\hbar}\, \dot{X} \rangle$$

$$= 2\pi\hbar \int_{-\infty}^{+\infty} dE\, f(E) \{ 1-f(E) \} \langle \mathrm{Tr}\, \delta(E-\mathcal{H}) \dot{X}\, \delta(E-\mathcal{H}) \dot{X} \rangle, \qquad (11.113)$$

where $f(E)$ is the Fermi function and in deriving the last expression we assumed that the scattering processes are elastic. Substituting (11.113) into (11.110), we obtain

$$\sigma_{xx} = \frac{\pi\hbar e^2}{\Omega} \int_{-\infty}^{+\infty} dE \left(-\frac{\partial f}{\partial E} \right) \langle \mathrm{Tr}\, \delta(E-\mathcal{H}) \dot{X}\, \delta(E-\mathcal{H}) \dot{X} \rangle . \qquad (11.114)$$

Similary, σ_{zz} becomes as follows:

$$\sigma_{zz} = \frac{\pi\hbar e^2}{\Omega} \int_{-\infty}^{+\infty} dE \left(-\frac{\partial f}{\partial E} \right) \langle \mathrm{Tr}\, \delta(E-\mathcal{H})\, v_z\, \delta(E-\mathcal{H})\, v_z \rangle . \qquad (11.115)$$

Appearance of the two delta functions is due to the density of states for the initial and final states in the scattering process. In consideration of (11.94), (11.114) can be calculated in the Born approximation as follows:

$$\sigma_{xx} = \frac{2\pi e^2}{\Omega\hbar} \int_{-\infty}^{+\infty} dE \left(-\frac{\partial f}{\partial E} \right) \sum_{NXp_z} \sum_{N'X'p_z'} \delta(E-E_N(p_z)) \left| \langle NXp_z | V | N'X'p_z' \rangle \right|^2$$

$$\times\, \delta(E-E_{N'}(p_z'))\, (X-X')^2, \qquad (11.116)$$

where the factor two in front of the integral comes from spin degeneracy.

After carring out integration over E, we obtain the following expression which is just the Adams - Holstein formula (11.51):

$$\sigma_{xx} = \frac{2e^2}{\Omega} \sum_{NXP_z} \sum_{N'X'P_z'} \left\{ -\frac{\partial f(E_N(P_z))}{\partial E_N(P_z)} \right\} \frac{1}{2} (X-X')^2 \frac{2\pi}{\hbar} \left| \langle NXP_z | V | N'X'P_z' \rangle \right|^2 \delta\left(E_N(P_z) - E_{N'}(P_z')\right). \tag{11.117}$$

To apply the Kubo formula to the coupled bands such as (11.20) can be straightforwardly carried out.

With increasing the field intensity, the electrons are finally populated only in the lowest Landau level $N=0$. This regime is called the quantum limit. In the quantum limit orbital quantization has a large effect on the galvanomagnetic coefficients. In the semiconductors or the semimetals with small carrier density and small effective mass the quantum limit is easily realized. By way of example consider n-type InSb. We shall estimate the quantum limit condition.

In Fig. 11.2 we obtain the relations:

$$\left\{ \begin{aligned} &\hbar\omega_0 = \zeta_c - \frac{\hbar\omega_0}{2}, \quad \omega_0 = \frac{eH}{m^*c}, \\ &n_c = \frac{2}{(2\pi)^2 \ell^2} \sum_n \int dk_z \\ &\quad = \frac{S}{\pi^2} (k_z)_m, \\ &\frac{\hbar^2}{2m^*} (k_z)_m^2 \doteq \hbar\omega_0, \end{aligned} \right. \tag{11.118}$$

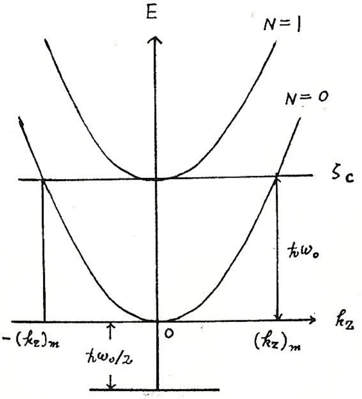


Fig. 11.2 The condition of the quantum limit is $\zeta_c > \zeta$. (Degenerate system)

where n_c is the carrier density in the case where the Fermi level ζ coincides with ζ_c.

Inserting $m^* = 0.014\, m_0$ and $H = 2$ KOe into (11.118), we have

$$\begin{cases} \hbar\omega_0 = 2.65 \times 10^{-15} \text{erg} \ (= 19.2\text{K}), \\ n_c = 7.20 \times 10^{14}\ \text{cm}^{-3}. \end{cases} \tag{11.119}$$

Then, at helium temperature ($\ll \hbar\omega_0/k_0$) n-type InSb with electron density $n \sim 10^{14}$ cm^{-3} ($< n_c$) is in the quantum limit in several kOe.

With further increase of a field intensity, the carrier system becomes non-degenerate since the maximum energy $E_{N=0} - \frac{1}{2}\hbar\omega_0 = P_z^2/2m^*$ which is proportional to H^{-2} is smaller than $k_0 T$ in intense magnetic field.

We shall calculate the quantum limit conductivity limited by the impurity scattering, where the scattering potential is assumed to be

$$V(r) = \frac{1}{\Omega} \sum_i \sum_q v(q)\, e^{iq(r - R_i)}. \tag{11.120}$$

R_i denotes the position of i-th impurity center.

In consideration of (11.5), (11.117) becomes

$$\sigma_{xx} = 2e^2 n_I \sum_{NXP_z} \sum_{N'X'P_z'} \sum_q \left(- \frac{\partial f(E_N(P_z))}{\partial E_N(P_z)} \right) \frac{1}{2} (X - X')^2 \frac{|v(q)|^2}{\Omega^2} |J_{NN'}(q_\perp)|^2$$

$$\times\, \delta(E_N(P_z) - E_{N'}(P_z'))\, \delta_{k_z, q_z + k_z'}\, \delta_{k_y, q_y + k_y'}$$

$$= 2e^2 n_I \sum_{N,N'} \frac{s\Omega}{(2\pi)^2} \frac{\Omega}{(2\pi)^3} \int dk_z \int d\mathbf{q}\, \frac{1}{2} \frac{q_y^2}{s^2} \frac{|v(q)|^2}{\Omega^2} |J_{NN'}(q_\perp)|^2 \left(- \frac{\partial f(E_N(P_z))}{\partial E_N(P_z)} \right)$$

$$\times\, \delta(E_N(P_z) - E_{N'}(P_z - \hbar q_z)), \tag{11.121}$$

where

$$\left\{ \begin{array}{l} n_I : \text{impurity concentration}, \quad q_\perp^2 = q_x^2 + q_y^2, \quad X - X' = -\dfrac{q_y}{s}, \\[2ex] J_{NN'}(q_\perp) = \displaystyle\int \phi_N(x - X)\, e^{i q_x x}\, \phi_{N'}(x - X')\, dx \, . \end{array} \right. \qquad (11.122)$$

Explicit expression of $|J_{NN'}(q_\perp)|^2$ is given by

$$|J_{NN'}(q_\perp)|^2 = \frac{\min(N.N')!}{\max(N.N')!}\, \xi^{|N-N'|} \left\{ L_{\min(N.N')}^{|N-N'|}(\xi) \right\}^2 e^{-\xi}, \quad \xi = \frac{q_\perp^2}{2s},$$

$$(11.123)$$

$$L_p^{(q)}(x) = \sum_{r=0}^{p} \binom{p+q}{p-r} \frac{(-x)^r}{r!} \quad (\text{associated Laguerre function}).$$

By putting $N = N' = 0$ in (11.121), the electrical conductivity in the quantum limit takes the form

$$\sigma_{xx} = \frac{e^2 n_I}{s(2\pi)^5} \frac{1}{2} \int dk_z \int d\mathbf{q}\, q_\perp^2\, |v(\mathbf{q})|^2 e^{-q_\perp^2/2s} \left(-\frac{\partial f(E_0(P_z))}{\partial E_0(P_z)} \right) \delta\big(E_0(P_z) - E_0(P_z - \hbar q_z)\big).$$

$$(11.124)$$

In deriving (11.124), q_y^2 is replaced by $\frac{1}{2} q_\perp^2$. (11.124) is rewritten as

$$\sigma_{xx} = \frac{e^2 n_I}{s(2\pi)^5} \frac{m^*}{2\hbar^2} \int \frac{dk_z}{|k_z|} \left(-\frac{\partial f(E_0(P_z))}{\partial E_0(P_z)} \right) \int d\mathbf{q}_\perp \left\{ |v(q_\perp, 0)|^2 + |v(q_\perp, 2k_z)|^2 \right\} e^{-q_\perp^2/2s},$$

$$(11.125)$$

where $v(\mathbf{q}) \equiv v(q_\perp, q_z)$.

In the following we shall treat (11.125) in the two limiting cases:

(A). Force range a of the scattering potential is short range $(a \ll l)$;

(B). a is much larger l (long range force).

The extension of the Landau orbit for $N=0$ is given by

$$l = (\hbar c/eH)^{1/2} = 8.11 \times 10^{-6}/\sqrt{H(KOe)}\ \text{cm}, \qquad (11.126)$$

which is considerably longer than the lattice spacing in ordinary field strength.

(A). We are interested in the semimetals and the degenerate semiconductors with small Fermi momentum and the non-degenerate semiconductors at low temperatures. Then, it is plausible to assume $2k_z \ll a^{-1}$.

Since $a \ll l$, we have

$$v(q_\perp, 0) \cong v(q_\perp, 2k_z) \cong v(0,0) \equiv v(0). \qquad (11.127)$$

Accordingly, (11.125) becomes

$$\sigma_{xx} = \frac{e^2 n_I}{(2\pi)^4} \frac{s m^*}{\hbar^2} |v(0)|^2 \int \frac{dE_z}{E_z}\left(-\frac{\partial f}{\partial E_z}\right). \qquad (11.128)$$

In general $v(0)$ is a function of magnetic field. The factor $1/E_z$ comes from the product of the density of states before and after the collision.

In considering the problem of removing the divergence around $E_z \sim 0$ the following two cases are treated: (1) Concentration of the scatterers is large enough. In this case collision broadening of the nergy caused by the scattering with the impurity centers is important;

2) If the impurity concentration is small enough, multiple scattering f the electron by a single scatterer should be taken into account.

The problem (1) was first treated by Davydov and Pomeranchuk.142) in connection with an oscillatory large magnetoresistance of bismuth at low temperatures.

An electron with small P_z ($E_z \sim 0$) is described by the wave packet elongated along the z-direction with an extension $\hbar/|P_z|$. Then, the electron is simultaneously scattered by several scatterers and this induces the collision broadening of the electron energy. In consideration of this effect the δ-function is replaced by the Lorentz distribution:

$$\delta\left(\frac{P_z^2}{2m^*} - E\right) \rightarrow \frac{\Gamma/\pi}{\left(\frac{P_z^2}{2m^*} - E\right)^2 + \Gamma^2} . \qquad (11.129)$$

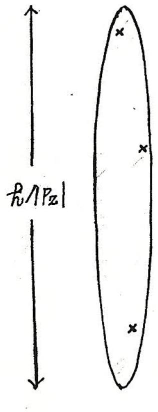


Fig. 11.3 wave packet elongated along the z-direction. × denotes scatterer.

As stated already, the divergence factor $1/E_z$ stems from the product of the density of states $1/\sqrt{E_z}$ before and after the collision, and $1/\sqrt{E_z}$ arises from the integration

$$\int d\left(\frac{P_z}{\sqrt{2m^*}}\right) \delta\left(\frac{P_z^2}{2m^*} - E_z\right) = \frac{1}{2\sqrt{E_z}} . \qquad (11.130)$$

Then, we have

$$\frac{1}{\sqrt{E_z}} \rightarrow \int_{-\infty}^{+\infty} d\left(\frac{P_z}{\sqrt{2m^*}}\right) \frac{\Gamma/\pi}{\left(\frac{P_z^2}{2m^*} - E_z\right)^2 + \Gamma^2} = \left\{ \frac{E_z + (E_z^2 + \Gamma^2)^{1/2}}{2(E_z^2 + \Gamma^2)} \right\}^{1/2}. \qquad (11.131)$$

Accordingly, (11.128) is replaced by

$$\sigma_{xx} = \frac{e^2 n_I}{(2\pi)^4} \frac{s m^*}{\hbar^2} |v(0)|^2 \int_{-\infty}^{+\infty} dE_z \frac{E_z + (E_z^2 + \Gamma^2)^{1/2}}{2(E_z^2 + \Gamma^2)} \left(-\frac{\partial f}{\partial E_z}\right). \qquad (11.132)$$

We shall estimate Γ according to Davydov-Pomeranchuk and Kubo. Let assume the scattering potential in the form

$$\frac{2\pi\hbar^2}{m^*} f\,\delta(r-R), \qquad (11.133)$$

where f corresponds to the scattering amplitude of an electron associated with (11.133) (See Appendix 1). Since the extension of the wave packet along the z-axis is $\sim \hbar/|P_z|$, the duration time τ_d of single collision is $\sim \hbar/|P_z v_z| \sim \hbar/E_z$. Electron circulates $\omega_0/2\pi$ times in unit time and encounters with single scatterer $\tau_d\,\omega_0/2\pi$ times during τ_d. As shown in Appendix 1, the scattering cross section due to the impurity potential (11.133) is given by $4\pi f^2$. Hence, the scattering rate becomes

$$1/\tau \sim n_I\, 4\pi f^2 (\hbar\omega_0/E_z)\,|v_z| = n_I\, 4\pi f^2 (\hbar\omega_0/|P_z|). \qquad (11.134)$$

Since $E_z \sim \hbar/\tau \sim \Gamma$, we obtain

$$\Gamma \sim \left\{ 4\pi\hbar\, n_I f^2\, \hbar\omega_0 / \sqrt{2m^*} \right\}^{2/3}. \qquad (11.135)$$

By introducing the variables $E_z/k_0T \equiv \varepsilon$, $\zeta/k_0T \equiv z$, the integration of (11.132) is rewritten as

$$(8k_0T)^{-1}\int_{-\infty}^{+\infty}\frac{d\varepsilon}{\cosh^2\{(\varepsilon-z)/2\}}\;\frac{\varepsilon+[\varepsilon^2+(\Gamma/k_0T)^2]^{1/2}}{\varepsilon^2+(\Gamma/k_0T)^2}\,. \qquad (11.136)$$

If Γ/k_0T is much smaller than unity, (11.136) is approximated by

$$\int_{-\infty}^{+\infty}\frac{d\varepsilon}{\cosh^2\{(\varepsilon-z)/2\}}\left\{[\varepsilon^2+(\Gamma/k_0T)^2]^{-1/2}+\frac{\varepsilon}{\varepsilon^2+(\Gamma/k_0T)^2}\right\}\sim 8e^{-z}\ln\left(\frac{2k_0T}{\gamma\Gamma}\right), \qquad (11.137)$$

where $\gamma \sim O(1)$.

In the case (2) we should consider the multiple scattering due to single impurity center instead of the simultaneous collision by several scatterers in the case (1). The repeated scattering by the same scatterer produces an infinite number of scattered waves, which are coherent and interfere with each other and with the incident wave. In this case the Born approximation loses its validity and then the non-Born approximation is needed. Approximate solutions of this problem were obtained independently by Skobov,$^{143)}$ by Bychkov,$^{144)}$ and by Kahn.$^{145)}$

In the following we shall give a qualitative consideration.

Differential scattering cross section related to the scattering potential (11.133) is given by $d\sigma = f^2 d\Omega$ and f is the quantity which gives an order of magnitude of the force range of the potential.

The Born approximation becomes invalid, when the phase shift of the scattered wave relative to that of the incident wave is larger than about $\pi/4$: $|\delta| > O(1)$ (cf. Appendix 1). The phase shift δ is estimated as follows. The duration time due to the scattering by single scatterer is given by $\tau_d \sim f/|v_z| = f m^*/\hbar|k_z|$. During τ_d the phase shift is approximately given by

$$|\delta| \sim \tau_d \omega_0 \sim f/\ell^2|k_z| . \qquad (11.138)$$

Therefore, the Born approximation becomes very poor, when the following condition is satisfied :

$$1 \sim f/\ell^2|k_z| \quad \text{or} \quad E_z \lesssim \hbar^2 f^2/(2m^*\ell^4) . \qquad (11.139)$$

To obtain a reasonable value from the Born approximation, the integration limit should be cut off. In the non-degenerate semiconductors, we have

$$\int_{\hbar^2 f^2/(2m^*\ell^4)} \frac{dE_z}{E_z} \sim \ln\left[\frac{k_0 T}{\hbar^2 f^2/(2m^*\ell^4)}\right] . \qquad (11.140)$$

In consideration of the above results, we shall calculate σ_{zz} in the three cases : (I) degenerate system, $n =$ constant; (II) non-degenerate system, $n =$ constant; (III) degenerate semimetal.

(I). Degenerate system, $n =$ constant :

Since $-\partial f/\partial E_z \doteqdot \delta(E_z - \zeta + \hbar\omega_0/2)$, the divergence for $E_z = 0$ is immaterial. From (11.128), we have

$$\sigma_{xx} = \frac{e^2 n_I}{(2\pi)^4} \frac{s m^*}{\hbar^2} \frac{|v(0)|^2}{\zeta - \hbar\omega_0/2} . \qquad (11.141)$$

From the relations of $n = (s/\pi^2)(k_z)_\zeta$, $\zeta - \hbar\omega_0/2 = (\hbar^2/2m^*)(k_z^2)_\zeta$, we have

$$\sigma_{xx} \propto H^3 T^0, \quad \rho = \sigma_{xx}/(\sigma_{xx}^2 + \sigma_{xy}^2) \cong \sigma_{xx}/\sigma_{xy}^2 \propto H^5 T^0. \qquad (11.142)$$

where we employ

$$\sigma_{xy} = - \frac{ecn}{H} \quad \text{for } \omega_0 \tau \gg 1, \qquad (11.143)$$

and assume that $v(0)$ is field-independent.

(II). Non-degenerate system, $n =$ constant:

The cut-off energy $(E_z)_{min}$ is estimated in the cases (1) and (2):

$$(E_z)_{min} \simeq \begin{cases} \Gamma & : \text{Case (1)}, \\ \hbar^2 f^2/(2m^* \ell^4) & : \text{Case (2)}, \end{cases} \qquad (11.144)$$

From (11.128), σ_{xx} is given by

$$\sigma_{xx} \cong \frac{e^2 n_I}{(2\pi)^4} \frac{s m^*}{\hbar^2} |v(0)|^2 \xi \beta e^{\beta(\zeta - \hbar\omega_0/2)} \ln\left[\frac{k_0 T}{(E_z)_{min}}\right], \quad \xi \sim O(1). \qquad (11.145)$$

ζ is related to the carrier density n by

$$e^{\beta(\zeta - \hbar\omega_0/2)} = \frac{2\pi^2 n}{s} \sqrt{\frac{\hbar^2}{2\pi m^* k_0 T}} . \qquad (11.146)$$

Hence, if $|v(0)|^2$ does not depend on the field intensity, we have

$$\sigma_{xx} \propto H^0 T^{-3/2}, \quad \rho \propto H^2 T^{-3/2}. \qquad (11.147)$$

(III) Semimetals :

Consider the semimetal with effective masses m_e and m_h in the quantum limit. From (11.141), the electrical conductivity becomes

$$\sigma_{xx} = \frac{e^2 n_I}{(2\pi)^4} \frac{S|v(0)|^2}{\hbar^2} \times \left(\frac{m_e}{\zeta_e - \hbar\omega_e/2} + \frac{m_h}{\zeta_h - \hbar\omega_h/2} \right). \qquad (11.148)$$

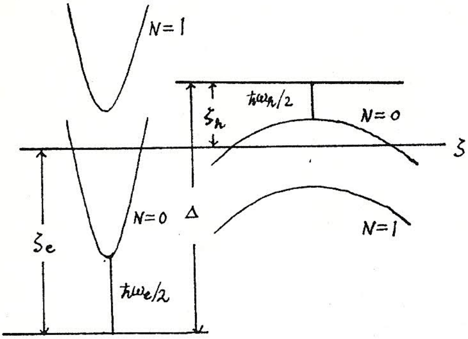


Fig. 11.4. Semimetal in the quantum limit. Δ is the overlapping energy.

Carrier densities n, p are related to the number of the Fermi pocket g_e and g_h as

$$n = \frac{S}{\pi^2} g_e k_\zeta^e \,, \quad p = \frac{S}{\pi^2} g_h k_\zeta^h .$$

If $g_e = g_h$ and $n \cong p$, $|n-p| \ll n, p$, we have

$$k_\zeta^e \fallingdotseq k_\zeta^h = k_\zeta . \qquad (11.149)$$

Condition of $\zeta_e + \zeta_h = \Delta =$ constant is rewritten in terms of k_ζ :

$$\frac{\hbar^2}{2}\left(\frac{1}{m_e} + \frac{1}{m_h}\right)(k_\zeta^2 + l^{-2}) = \Delta = \text{constant}. \qquad (11.150)$$

If the inequality $k_\zeta^2 \gg l^{-2}$ is satisfied (this condition usually holds), (11.150) shows that k_ζ is a constant which is independent of H.

Then, we have

$$\zeta_e - \hbar\omega_e/2\,,\quad \zeta_h - \hbar\omega_h/2 = \text{constant}. \qquad (11.151)$$

Thus, (11.148) leads to

$$\sigma_{xx} \propto H\ T^0, \qquad \rho \propto \begin{cases} H^3\,T^0 \;:\; \sigma_{xy}{}^2 \gg \sigma_{xx}\,\sigma_{yy}\,, \\ H^{-1}\,T^0 \;:\; \sigma_{xy}{}^2 \ll \sigma_{xx}\,\sigma_{yy}\,. \end{cases} \qquad (11.152)$$

If, $|n-p| \ll n, p$, $\sigma_{xy}{}^2$ is much smaller than $\sigma_{xx}\,\sigma_{yy}$.

More generally, we have

$$\begin{cases} \zeta_i - \hbar\omega_i/2 = \dfrac{\hbar^2}{2m_i}k_\zeta{}^2 = \dfrac{\mu}{m_i}\left(\Delta - \dfrac{\hbar^2}{2\mu l^2}\right), \quad i = e \text{ or } h, \\ 1/\mu = 1/m_e + 1/m_h \quad (\mu : \text{reduced mass}). \end{cases} \qquad (11.153)$$

Hence,

$$\sigma_{xx} \propto \frac{H}{\Delta - \hbar^2/(2\mu l^2)}\,, \quad \rho \propto \begin{cases} H^3/\{\Delta - \hbar^2/(2\mu l^2)\} \;:\; \sigma_{xy}{}^2 \gg \sigma_{xx}\,\sigma_{yy}\,. \\ H^{-1}/\{\Delta - \hbar^2/(2\mu l^2)\} \;:\; \sigma_{xy}{}^2 \ll \sigma_{xx}\,\sigma_{yy}\,. \end{cases}$$

$$(11.154)$$

(11.150) ~ (11.154) are valid as long as the inequality $\Delta > \hbar^2/(2\mu l^2)$ is satisfied. If this condition does not hold, semimetal – semiconductor transition appears.

Up to now we have assumed that $v(0)$ is independent of the magnetic field intensity. In the quantum limit the density of states of carriers at the Fermi level is proportional to H and the screening effect on the ionized impurity potential is enhanced with increasing magnetic field. The Fourier component of the screened Coulomb potential becomes

$$v(q) = \frac{4\pi Ze}{\varepsilon}\,\frac{1}{q^2+q_s^2}\,, \quad q_s^2 = \frac{4\pi e^2 N(\zeta)}{\varepsilon} \propto H\,, \qquad (11.155)$$

where Ze denotes the effective nuclear charge, ε the dielectric constant and $N(\zeta)$ the density of states at the Fermi level. Accordingly, we have $|v(0)|^2 \propto H^{-2}$ and (11.148) leads to

$$\sigma_{xx} \propto H^{-1}T^{0}. \qquad (11.156)$$

Fig. 11.5 represents the observed conductivity of the pyrolytic and single crystal graphite in the quantum limit. Graphite enters into the quantum limit for $H \simeq 7\,\mathrm{T}$. The experiment is performed at $T = 4.2\,\mathrm{K}$.[146)]

Observed data approximately obey (11.156). In compensated semi-metals ($n \cong p$, $|n-p| \ll n, p$) σ_{xy}^2 is much smaller than $\sigma_{xx}\sigma_{yy}$, then (11.156) leads to $\rho \propto H$.

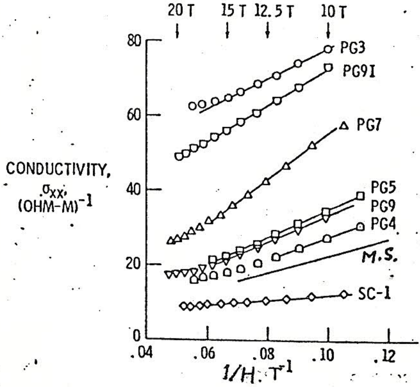


Fig. 11.5 Magnetoconductivity σ_{xx} of graphite in the quantum limit. M.S. indicates the measurement due to McClure-Spry.[147)] PG: pyrolytic graphite, SC: single crystal graphite. (1 T = 10 KOe)

In the next place we shall consider the case (B) in which the force range of the scattering potential is long range.

(B). Since the force range a satisfies the relation $a \gg l$, the uncertainty relation $\Delta X \Delta Y \cong 2\pi l^2$ (See. (11.92)) is essentially equivalent to $\Delta X \Delta Y \cong 0$. Therefore, it is permissible to consider that X and Y are the c-number. It is allowed to replace (x, y) in the scattering potential $V(x, y, z)$ by (X, Y). Then, (11.94) becomes

$$\dot{X} \cong \frac{c}{eH} \frac{\partial V(X, Y, Z)}{\partial Y}, \quad \dot{Y} \cong -\frac{c}{eH} \frac{\partial V(X, Y, Z)}{\partial X}, \tag{11.157}$$

and the displacement ΔX due to the collision is given by

$$\Delta X \sim \frac{c}{eH} \overline{\frac{\partial V}{\partial Y}} \tau_d , \tag{11.158}$$

where τ_d is the duration time of the scattering process and $-$ denotes the time average. In consideration of $\tau_d = a/|v_z|$ and $1/\tau = n_I \pi a^2 |v_z|$, (11.52) provides

$$\sigma_{xx} \cong \frac{e^2}{2} \left\langle n' \left(\frac{c}{eH} \overline{\frac{\partial V}{\partial Y}} \frac{a}{|v_z|} \right)^2 n_I \pi a^2 |v_z| \right\rangle , \tag{11.159}$$

where

$$n' = \begin{cases} dn/d\zeta & : \text{degenerate system}, \\ n/k_0T & : \text{non-degenerate system}. \end{cases} \tag{11.160}$$

Accordingly, we get

$$\sigma_{xx} \propto \frac{n'}{H^2} \left\langle \frac{1}{|p_z|} \right\rangle . \tag{11.161}$$

It should be minded that a does not mean the force range itself but it is a quantity related to the scattering cross section σ by $\sigma = \pi a^2$.

On making use of (11.161) we shall consider $(H \cdot T)$-dependence of σ_{xx} and ρ for (I), (II) and (III) cases.

(I). Degenerate system, n = constant :

Carrier density n is given by

$$n = 2 \left[\frac{S}{(2\pi)^2}\right] \int_{-k_\zeta}^{k_\zeta} dk_z = \frac{S k_\zeta}{\pi^2}, \qquad (11.162)$$

where the factor 2 denotes the spin degeneracy. (11.162) is valid only if the Zeeman splitting is negligible. g-factor in bismuth along a certain direction attains 260. In this case we should modify (11.162) in consideration of the Zeeman splitting.

From (11.162) and $k_\zeta = \sqrt{2m^*/\hbar^2\,(\zeta - \hbar\omega_c/2)}$, we have $n' = dn/d\zeta \propto H/k_\zeta \propto H^2$, $|p_z| = \hbar k_\zeta \propto H^{-1}$ and (11.161) gives

$$\sigma_{xx} \propto H T^0, \quad \rho \propto H^3 T^0. \qquad (11.163)$$

In Fig. 11.6 observed values of the magnetoresistance of n-InSb are shown.[148] The critical field intensity for the quantum limit is 8 kOe for No. 315 sample and 22 kOe for No. 116 sample. No. 116 exhibits $\rho \propto H^{3.3}$ at 4.2 K and 1.3 K in 30 ~ 90 kOe and No. 315 behaves similarly in 12 ~ 25 kOe. These behaviors support (11.163). Further increase of

ρ in strong magnetic fields is ascribed to the carrier freeze-out effect.[149]

In the case of Fig. 11.6 the scattering potential is the long range Coulomb potential.

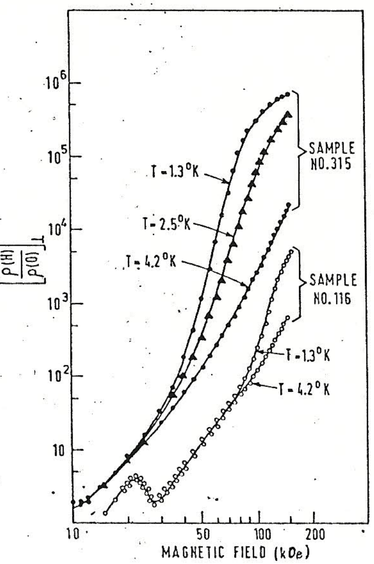


Fig. 11.6 Transverse magnetoresistance of n - InSb. In the exhaustion region the carrier density of NO.315 is 2.3×10^{15}/c.c. and that of NO.116 is 1.1×10^{16} /c.c.[148]

(II) Non-degenerate system, n = constant :

Since

$$\left\langle \frac{1}{|p_z|} \right\rangle \propto \left\langle \frac{1}{E_z^{1/2}} \right\rangle \propto T^{-1/2}, \qquad (11.164)$$

(11.161) yields

$$\sigma_{xx} \propto H^{-2} T^{-3/2}, \quad \rho \propto H^0 T^{-3/2}. \qquad (11.165)$$

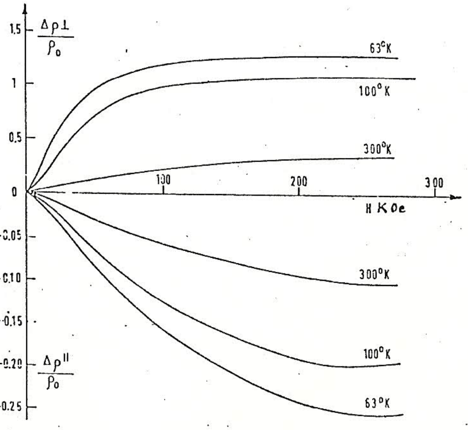


Fig. 11.7 Magnetoresistance of n - GaAs. Carrier density at 77K is $n = 2.4 \times 10^{15}$ /c.c. Sample is compensated and the ionized impurity scattering is dominant.[150]

In Fig. 11.7 transverse magnetoresistance $\Delta\rho^{\perp}/\rho_0$ and longitudinal magnetoresistance $\Delta\rho^{\parallel}/\rho_0$ of n-GaAs are shown.[150] Below 150K the ionized impurity scattering is dominant. At $T = 63$K and in 100 KOe, it is shown that $\hbar\omega_0/k_0T \approx 3$. In strong magnetic fields $\Delta\rho^{\perp}/\rho_0$ is field-independent. This accords with the theoretical prediction (11.165).

It is very interesting that Fig. 11.7 exhibits the negative longitudinal magnetoresistance. Argyres and Adams pointed out[151] that in the quantum limit non-degenerate carriers subjected to the ionized impurity scattering show the negative longitudinal magnetoresistance. Detailed account will be given in Section 12.4.

(III) Semimetals :

In consideration of (11.149) and (11.162), (11.161) yields

$$\sigma_{xx} \propto 1/(Hk_s^2) \propto 1/\{H[\Delta - \hbar^2/(2\mu l^2)]\}. \qquad (11.166)$$

If $\Delta \gg \hbar^2/(2\mu l^2)$, we have

$$\sigma_{xx} \propto H^{-1}T^0, \quad \rho \propto \begin{cases} H\ T^0 & : \sigma_{xy}^2 \gg \sigma_{xx}\sigma_{yy}. \\ H\ T^0 & : \sigma_{xy}^2 \ll \sigma_{xx}\sigma_{yy}. \end{cases} \qquad (11.167)$$

11.7 Phonon Scattering in Strong Magnetic Field

Total Hamiltonian is given by

$$\mathcal{H} = \mathcal{H}_e + \mathcal{H}_p + V; \quad \mathcal{H}_0 = \mathcal{H}_e + \mathcal{H}_p, \qquad (11.168)$$

where $\mathcal{H}_e$ and $\mathcal{H}_p$ respectively, denote the Hamiltonian of the electron system and of the phonon system. V is the electron-phonon interaction.

The following calculation is carried out in a similar way to the procedures employed in getting σ_{xx} related to the impurity scattering.

In the first place we shall consider the quantity $\langle \dot{\mathbb{X}}(0)\dot{\mathbb{X}}(t)\rangle$.

From (11.112) and (11.113), we have

$$\langle \dot{\mathbb{X}}(0)\,\dot{\mathbb{X}}(t)\rangle = \langle T_r\, f(\mathcal{H}_e)\dot{X}(0)\{1-f(\mathcal{H}_e)\}\, e^{it\mathcal{H}_0/\hbar}\,\dot{X}\, e^{-it\mathcal{H}_0/\hbar}\rangle . \qquad (11.169)$$

By taking into consideration the equation of motion for X (11.94) and

$$e^{it\mathcal{H}_p/\hbar}\, V\, e^{-it\mathcal{H}_p/\hbar} = \sum_q V_q(r)\, e^{i\omega_q t} . \qquad (11.170)$$

we obtain

$$\int_{-\infty}^{+\infty}\langle \dot{\mathbb{X}}(0)\,\dot{\mathbb{X}}(t)\rangle dt = \int_{-\infty}^{+\infty} dE\, f(E)\Big\langle T_r\Big(\delta(E-\mathcal{H}_e)\dot{X}\{1-f(\mathcal{H}_e)\}\int_{-\infty}^{+\infty} dt \sum_q e^{it\mathcal{H}_e/\hbar}$$

$$\times\ \frac{i}{\hbar}[V_q, X]\, e^{i\omega_q t}\, e^{-itE/\hbar}\Big)\Big\rangle = 2\pi\hbar \sum_q \int_{-\infty}^{+\infty} dE\, f(E)\{1-f(E-\hbar\omega_q)\}\Big\langle T_r\Big(\delta(E-\mathcal{H}_e)$$

$$\times\ \frac{i}{\hbar}[V, X]\,\delta(E-\hbar\omega_q-\mathcal{H}_e)\,\frac{i}{\hbar}[V_q, X]\Big)\Big\rangle . \qquad (11.171)$$

By inserting

$$\left\{\begin{aligned} & f(E)\{1-f(E-\hbar\omega_q)\} = \{f(E-\hbar\omega_q)-f(E)\}\, N_q , \\ & N_q = \{\exp(\hbar\omega_q/k_0 T)-1\}^{-1} \end{aligned}\right. \qquad (11.172)$$

into the above expression, the electrical conductivity becomes

$$\sigma_{xx} = \frac{e^2}{\Omega} \sum_q N_q \frac{\hbar\omega_q}{k_0 T} \int_{-\infty}^{+\infty} dE \; \frac{f(E-\hbar\omega_q) - f(E)}{\hbar\omega_q} \; \frac{1}{2} \frac{2\pi}{\hbar} \langle \mathrm{Tr} \big(\delta(E - H_e)[X, V]$$

$$\times \delta(E - \hbar\omega_q - H_e)[V_q, X] \big) \rangle . \tag{11.173}$$

In the limit of $\hbar\omega_q \to 0$ *(11.173) is equivalent to the expression of the conductivity limited by the impurity scattering.*

The electron-phonon interaction is assumed to be of the usual form

$$V(r) = \frac{1}{\sqrt{\Omega}} {\sum_q}' \{ C(q)\, b_q\, e^{iqr} + C^*(q)\, b_q^+ e^{-iqr} \}, \tag{11.174}$$

where the summation extends over q*'s inside one half of the unit cell of the reciprocal lattice.*

Thus, we have

$$e^{itH_p/\hbar}\, V(r)\, e^{-itH_p/\hbar} = \frac{1}{\sqrt{\Omega}} {\sum_q}' \{ C(q) b_q e^{i(qr-\omega_q t)} + C^*(q) b_q^+ e^{-i(qr-\omega_q t)} \}. \tag{11.175}$$

The equation of motion (11.94) is now written as

$$\dot{X} = {\sum_q}' \frac{i l^2}{\hbar\sqrt{\Omega}} q_y \{ C(q)\, b_q\, e^{iqr} - C^*(q)\, b_q^+ e^{-iqr} \}. \tag{11.176}$$

On making use of the well-known formulae

$$\langle b_q^+ b_{q'} \rangle = \delta_{qq'} N_q , \quad \langle b_q b_{q'}^+ \rangle = \delta_{qq'} (N_q + 1), \tag{11.177}$$

and (11.175), (11.176), we obtain the electrical conductivity limited by the phonon scattering as follows.

$$\sigma_{xx} = \frac{e^2}{\Omega^2}\int_{-\infty}^{+\infty} dE\, f(E) \sum_q{}' |C(q)|^2 \frac{(l^2 q_y)^2}{2k_0T}\frac{2\pi}{\hbar}\Big[(N_q+1)\, Tr\Big(\delta(E-H_e)e^{iqr}\{1-f(H_e)\}$$

$$\times\, \delta(E-\hbar\omega_q-H_e)e^{-iqr}\Big) + N_q\, Tr\Big(\delta(E-H_e)e^{-iqr}\{1-f(H_e)\}\delta(E+\hbar\omega_q-H_e)e^{iqr}\Big)\Big]$$

$$= \frac{e^2}{\Omega^2}\int_{-\infty}^{+\infty} dE \sum_q{}' |C(q)|^2 \frac{(l^2 q_y)^2}{2k_0T} N_q(N_q+1)\frac{2\pi}{\hbar}\Big[\{f(E-\hbar\omega_q)-f(E)\}$$

$$\times\, Tr\Big(\delta(E-H_e)e^{iqr}\delta(E-\hbar\omega_q-H_e)e^{-iqr}\Big) + \{f(E)-f(E+\hbar\omega_q)\}\, Tr\Big(\delta(E-H_e)\, e^{-iqr}$$

$$\times\, \delta(E+\hbar\omega_q-H_e)e^{iqr}\Big)\Big]. \qquad (11.178)$$

The last expression of (11.178) is valid only if the phonon system is in thermal equilibrium. By putting $E+\hbar\omega_q \to E$ in the second expression, (11.178) becomes

$$\sigma_{xx} = \frac{e^2}{\Omega^2}\sum_q\int_{-\infty}^{+\infty}\frac{f(E-\hbar\omega_q)-f(E)}{\hbar\omega_q}\frac{(l^2q_y)^2}{2}\frac{2\pi}{\hbar}|C(q)|^2 N_q(N_q+1)\frac{\hbar\omega_q}{k_0T}$$

$$\times\, Tr\{\delta(E-H_e)\,e^{iqr}\,\delta(E-\hbar\omega_q-H_e)\,e^{-iqr}\}, \qquad (11.179)$$

where $2\sum_q{}'$ is replaced by $\sum_q$. Using the $(N, p_z . X)$-representation, we get

$$\sigma_{xx} = \frac{2e^2}{\Omega^2}\sum_q\frac{(X-X')^2}{2k_0T}\frac{2\pi}{\hbar}|C(q)|^2 N_q(N_q+1)\sum_{N X p_z}\sum_{N'}\{f(E_N(p_z)-\hbar\omega_q)-f(E_N(p_z))\}$$

$$\times\, \delta(E_N(p_z)-\hbar\omega_q-E_{N'}(p_z-\hbar q_z))\,|J_{NN'}(X, q_x, X')|^2, \qquad (11.180)$$

where

$$X' - X = \ell^2 q_y \, , \quad J_{NN'}(X, q_x, X') = \int \phi_N^*(x - X) e^{i q_x x} \phi_{N'}(x - X') dx. \qquad (11.181)$$

Rewriting (11.180),

$$\sigma_{xx} = \frac{e^2}{\Omega^2} \sum_q \frac{(X - X')^2}{k_0 T} \frac{2\pi}{\hbar} | C(q) |^2 N_q \sum_{N p_z X} \sum_{N'} f(E_N(p_z)) \left\{ 1 - f(E_{N'}(p_z - \hbar q_z)) \right\}$$

$$\times \delta \left(E_N(p_z) - \hbar \omega_q - E_{N'}(p_z - \hbar q_z) \right) | J_{NN'}(X, q_x, X') |^2 . \qquad (11.182)$$

In the case of the acoustic phonon scattering (11.182) was in detail studied by Titeica.136) For simplicity we shall pay our attention to the quantum limit case.

Since,

$$| J_{00}(X, q_x, X') |^2 = e^{-q_\perp^2/2s} , \quad s = 1/\ell^2 , \qquad (11.183)$$

and

$$\sum_{X p_z} \cdots = \frac{s \Omega}{\hbar (2\pi)^2} \int d p_z \cdots , \quad E_0(p_z) = \frac{\hbar \omega_0}{2} + \frac{p_z^2}{2m^*} = \frac{\hbar \omega_0}{2} + E_z , \qquad (11.184)$$

(11.182) becomes

$$\sigma_{xx} = \frac{2e^2}{\Omega^2} \int \frac{\Omega}{(2\pi)^3} d\mathbf{q} \frac{(\ell^2 q_y)^2}{2 k_0 T} \frac{2\pi}{\hbar} | C(q) |^2 N_q (N_q + 1) \frac{s \Omega}{\hbar (2\pi)^2} \int d p_z \left\{ f(E_0(p_z) - \hbar \omega_q) \right.$$

$$\left. - f(E_0(p_z)) \right\} \delta \left[\frac{1}{2m^*} (2 p_z \hbar q_z - \hbar^2 q_z^2) - \hbar \omega_q \right] e^{-q_\perp^2/2s} . \qquad (11.185)$$

11.8 Acoustic Phonon Scattering

In this case $C(q)$ takes the form

$$C(q) = i D \sqrt{\frac{\hbar}{2 d \omega_q}} \, q \; . \qquad (11.186)$$

Now from (11.185)

$$\sigma_{xx} = \frac{e^2 \ell^2}{(2\pi)^3 k_0 T} \frac{D^2}{4 d v_s \hbar} \int dq_z \, dq_\perp \, q_\perp^3 \, q \, N_q (N_q + 1) e^{-q_\perp^2/2s} \int dp_z \{ f(E_0(p_z) - \hbar\omega_q) - f(E_0(p_z)) \}$$

$$\times \delta \left[\frac{1}{2m^*} (2 p_z \hbar q_z - \hbar^2 q_z^2) - \hbar\omega_q \right]. \tag{11.187}$$

If $E_z \gg \hbar\omega_q$, the δ-function yields

$$\hbar q_z = p_z \left\{ 1 \pm \sqrt{1 - \hbar\omega_q / E_z} \right\} \cong 2 p_z \text{ or } \hbar\omega_q / v_z . \tag{11.188}$$

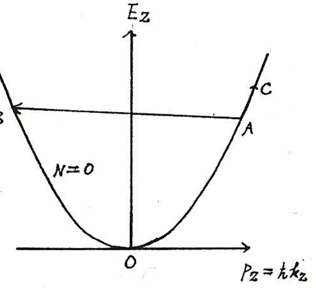


Fig. 11.8 acoustic phonon scattering in the quantum limit.

In Fig. 11.8 A → B is the backward scattering accompanied by a large momentum change $2p_z$, while A → C denotes the forward scattering with a small momentum change $\hbar\omega_q / v_z$.

If $2 p_z v_s = 2m^* v_z v_s \gg k_0 T$, the backward scattering is prohibited. On the other hand, if $2m^* v_z v_s \ll k_0 T$ the backward scattering occurs as the foward scattering does.

Two factors $N_q (N_q + 1)$ and $e^{-q_\perp^2/2s}$ limit the integration range of $q_\perp$ as

$$q_\perp \sim \begin{cases} k_0 T / \hbar v_s & : \; k_0 T / \hbar v_s \ll 1/\ell , \\ 1/\ell & : \; k_0 T / \hbar v_s \gg 1/\ell . \end{cases} \tag{11.189}$$

It is readily shown that if $2m^* v_z v_s \ll k_0 T$. q_z is much smaller than $q_\perp$.

Proof : In the case of $k_0 T/\hbar v_s \ll 1/l$, (11.189) leads to $q_\perp \sim k_0 T/\hbar v_s$.

From the assumption we obtain $k_0 T/\hbar v_s \gg 2k_z \sim q_z$ and then $q_z \ll q_\perp$.

From (11.189) $q_\perp \sim 1/l$ for $k_0 T/\hbar v_s \gg 1/l$. In the quantum limit the condition of $\hbar\omega_0 \gg p_z^2/2m^*$ is realized. This leads to $1/l \gg k_z$. Accordingly, we have $q_z \ll q_\perp$.

Integration of the δ-function in (11.187) over q_z-space is given by

$$\int dq_z\, \delta\left[(1/2m^*)(2p_z\hbar q_z - \hbar^2 q_z^2) - \hbar\omega_q\right] = (2m^*/\hbar^2)\int dq_z\, \delta\left[(q_z - q_z^+)(q_z - q_z^-)\right]$$

$$= (2m^*/\hbar^2)\,(q_z^+ - q_z^-)^{-1} = m^*/\hbar|p_z| , \qquad (11.190)$$

where $q_z^\pm$ denote the two roots of the argument of the δ-function being put zero.

In the degenerate system we may approximate : $f(E_0(p_z) - \hbar\omega_q) - f(E_0(p_z)) \cong -\hbar\omega_q\, \partial f(E_0(p_z))/\partial E_0(p_z) \cong \hbar\omega_q\, \delta(E_0(p_z) - \zeta)$ and then, σ_{xx} becomes

$$\sigma_{xx} \cong \frac{e^2 l^2 D^2 m^*}{2(2\pi)^3 k_0 T d \hbar (\zeta - (1/2)\hbar\omega_0)} \int_{-\infty}^{+\infty} dq_\perp\, q_\perp^5\, e^{-q_\perp^2/2s} \left\{N_q(N_q+1)\right\}_{q=q_\perp} , \qquad (11.191)$$

where we employ the relation $q_z \ll q_\perp$. We shall estimate σ_{xx} under the condition of $k_0 T/\hbar v_s \gg 1/l$. Of course this condition does not hold at low temperatures and in strong magnetic field. Since $q \cong q_\perp \sim 1/l$,

$$N_q(N_q+1) \cong (k_0 T/\hbar v_s q_\perp)^2 . \qquad (11.192)$$

Accordingly, (11.191) is given by

$$\sigma_{xx} \cong \frac{e^2 s D^2 m^* k_0 T}{(2\pi)^3 \hbar^3 d\, v_s^2 (\zeta - (1/2)\hbar\omega_0)} . \tag{11.193}$$

If the electron concentration n is constant, we have $1/\{\zeta - (1/2)\hbar\omega_0\} \propto H^2$ (See. (11.118)). Therefore, we obtain

$$\sigma_{xx} \propto H^3 T, \quad \rho \propto H^5 T. \tag{11.194}$$

In the non-degenerate system

$$f(E_0(p_z)) = A e^{-\beta E_z}, \quad A = \frac{2\pi^2 n}{S}\sqrt{\frac{\hbar^2}{2\pi m^* k_0 T}} , \tag{11.195}$$

and the electrical conductivity is given by

$$\sigma_{xx} \cong \frac{e^2 D^2 n}{2 d \hbar^2 v_s^2}\sqrt{\frac{m^*}{(2\pi)^3 k_0 T}} \left\{ - E_i(-x) \right\} , \tag{11.196}$$

where

$$E_i(-x) = - \int_x^\infty dt\, \frac{e^{-t}}{t} , \quad x = \hbar v_s / (l k_0 T) \ll 1 . \tag{11.197}$$

E_i is called exponential integral and for $x \ll 1$ $E_i(-x)$ is approximated by

$$E_i(-x) = \gamma + \log x + \sum_{n=1}^{\infty} \frac{(-1)^n x^n}{(n+1)!} \cong \gamma + \log x , \tag{11.198}$$

γ : Euler's constant (~ 0.577).

If the carrier concentration n is constant, we have

$$\sigma_{xx} \propto H^0 T^{-1/2} , \quad \rho \propto H^2 T^{-1/2}. \tag{11.199}$$

In the case of $k_0 T/\hbar v_s \ll 1/l$, the calculation is very complicated and the reader is referred to the review article 141).

In the following we shall calculate the electrical conductivity limited by the piezoelectric scattering under the condition of $E_z \gg \hbar\omega_q$, $k_0 T/\hbar v_s \gg 1/l$.

For definiteness we consider the zincblende lattice structure (See Section 7.10). The piezoelectric coupling is expressed by

$$V(r) = -e \sum_{q}{}' (\phi_q b_q e^{iqr} + \phi_q^* b_q^+ e^{-iqr}), \tag{11.200}$$

$$\left\{ \begin{aligned} \phi_q &= \frac{8\pi e_{14}}{\Omega^{1/2}\varepsilon} \{ \xi_x(q) n_y n_z + \text{cyclic terms} \}, \\ n &= q/q, \quad \xi(r) = \sum_q \xi(q) e^{iqr}. \\ \xi(q) &= \sum_\lambda \sqrt{\frac{\hbar}{2d\omega_{q\lambda}}}\, e_{q\lambda}, \quad \lambda : \text{suffix specifying polarization.} \end{aligned} \right. \tag{11.201}$$

Calculation can be performed in parallel with the procedures employed in getting (11.187).

$$\sigma_{xx} = \frac{e^2 l^2}{(2\pi)^3 \hbar^2 k_0 T} \left(\frac{8\pi e e_{14}}{\varepsilon} \right)^2 \sum_\lambda \frac{\hbar}{d v_\lambda} \int dq_z dq_\perp q_\perp^3 \frac{\Gamma_\lambda(q)}{q} N_q (N_q + 1) e^{-q_\perp^2/2s}$$

$$\times \int dp_z [f(E_0(p_z) - \hbar\omega_q) - f(E_0(p_z))] \delta[(1/2m^*)(2p_z\hbar q_z - \hbar^2 q_z^2) - \hbar\omega_q], \tag{11.202}$$

where

$$\Gamma_\lambda(q) = (e_{\lambda x} n_y n_z + \text{cyclic terms})^2, \quad v_\lambda : \text{sound velocity.} \tag{11.203}$$

$\Gamma_\lambda(q)$ is approximated by the quantity averaged over $n = q/q$, and

$$\langle \Gamma_l \rangle = 3/35\,,\ \langle \Gamma_{t_1} \rangle = \langle \Gamma_{t_2} \rangle = 2/35\,, \tag{11.204}$$

where l corresponds to the longitudinal mode and $t_{1,2}$ denotes the transverse wave.

From the condion of $E_z \gg \hbar\omega_g$ and $k_0T/\hbar v_\lambda \gg 1/l$, (11.202) in the degenerate system becomes

$$\sigma_{xx} = \frac{e^2 k_0 T}{2(2\pi)^3 \hbar^3} \left(\frac{8\pi e e_{14}}{\varepsilon}\right)^2 \frac{1}{\zeta - \hbar\omega_0/2} \sum_\lambda \frac{\langle \Gamma_\lambda \rangle}{d\, v_\lambda^2}\,. \tag{11.205}$$

Assuming $n =$ constant, we have

$$\sigma_{xx} \propto H^2 T, \qquad \rho \propto H^4 T. \tag{11.206}$$

Similarly, in the non-degenerate system

$$\sigma_{xx} = \frac{e^2 n}{2\hbar^2 S} \left(\frac{8\pi e_{14}}{\varepsilon}\right)^2 \sqrt{\frac{m^*}{(2\pi)^3 k_0 T}} \sum_\lambda \frac{\langle \Gamma_\lambda \rangle}{d\, v_\lambda^2} \left(-E_i(-x)\right). \tag{11.207}$$

If n is constant,

$$\sigma_{xx} \propto H^{-1} T^{1/2}, \quad \rho \propto H T^{-1/2}. \tag{11.208}$$

11.9 de Haas - van Alphn Effect

As stated briefly in Section 11.1, Landau discovered the very remarkable fact that the orbital motions of free electrons give a diamagnetic contribution in quantum mechanics, whereas as is well-known classically they are without such an effect (Miss van Leewen's theorem). This difference comes from the fact that the boundary electrons, which can not complete the cyclotron motion, have different quantized velocities than those which do not touch the walls of the vessel. Then the magnetic moments of these two types of electrons do not compensate each other as in classical theory.152)

In the following we shall see that the magnetic susceptiblity of the free-electron gas is a rapidly oscillating function of the magnetic field, so that its derivative with respect to H can exceed the nonoscillatory part of the magnetic moment at sufficiently low temperatures. This effect was originally predicted by Landau153) and first observed by de Haas and van Alphen154) (DHVA effect). Oscillations of the de Haas - van Alphen type have also been observed in transport properties, e.g., in the electrical conductivity (Shubnikov - de Haas effect), in the thermal conductivity and in the thermoelectric power.

In this Section we shall derive the expression of the DHVA effect for the electrons with arbitrary dispersion relation $E(k)$.155)

The magnetic moment M is related to the thermodynamic potential

Φ by

$$M = \chi H = -\frac{1}{\Omega}\frac{\partial \Phi}{\partial H}, \quad (\chi : \text{magnetic susceptibility}). \qquad (11.209)$$

Φ is given by

$$\Phi = -k_0 T \sum_i \ln\left[1 + \exp(S - E_i)/k_0 T\right]$$

$$= -\frac{\Omega k_0 T}{(2\pi)^2}\frac{s}{\hbar}\sum_{n,\sigma}\int dp_z \ln\left[1 + \exp\{(S - E_{n\sigma}(p_z))/k_0 T\}\right], \qquad (11.210)$$

where $s = eH/\hbar c$.. σ denotes the spin index and

$$E_{n\sigma} = E_n(p_z) \pm \mu H. \qquad (11.211)$$

In getting the oscillatory part of Φ, it is convenient to use the Poisson formula

$$\sum_{n_0}^{\infty}\phi(n) = \int_a^{\infty}\phi(n)\,dn + 2\,\mathrm{Re}\sum_{k=1}^{n}\int_a^{\infty}\phi(n)\,e^{2\pi i k n}\,dn, \qquad (11.212)$$

where a is a number which lies between $n_0 - 1$ and n_0. It can be readily proved by use of the relation

$$\sum_{n=-\infty}^{\infty}\delta(x-n) = \sum_{k=-\infty}^{\infty} e^{2\pi i k x}. \qquad (11.213)$$

(11.213) can be easily proved as follows. It is shown that if $x \neq n$ (n: integer) the right hand side of (11.213) vanishes. By changing $k \to k + k_1$ (k_1: integer), the right hand side becomes

$$\sum_{k=-\infty}^{\infty} e^{2\pi i k x} = e^{2\pi i k_1 x}\sum_{k=-\infty}^{\infty} e^{2\pi i k x}.$$

Since $e^{2\pi i k_1 x} \neq 1$, we obtain $\sum_{k=-\infty}^{\infty} e^{2\pi i k x} = 0$. Integrating $\sum_k e^{2\pi i k x}$ over an interval $(-\delta, \delta)$ and putting $\delta \to 0$, we obtain

$$\int_{-\delta}^{\delta} \sum_{k=-\infty}^{\infty} e^{2\pi i k x} dx = \sum_{k=-\infty}^{\infty} \frac{e^{2\pi i k \delta} - e^{-2\pi i k \delta}}{2\pi i k} = \sum_{k=-\infty}^{\infty} \frac{\sin 2\pi k \delta}{\pi k} = \int_{-\infty}^{\infty} \frac{\sin 2\pi k \delta}{\pi k} = 1.$$

Then, the right hand side of (11.213) behaves as the δ-function like in the vicinity of $x = 0$ and this function is a periodic function of x which vanishes for $x \neq n$. This proves (11.213). Multiplying a function $\phi(x)$ on both sides of (11.213) and integrating them over (a, ∞), one obtains the Poisson's sum formula. The first term in (11.212) comes from $k = 0$, while the contributions from k and $-k$ are grouped together in the second term.

Now apply (11.212) to (11.210). Two differnt terms appear. One is the non oscillarty part in H and the second the oscillating term $\Phi_{osc.}$ We are interested in $\Phi_{osc.}$, where it is given by

$$\Phi_{osc.} = -2 \,\mathrm{Re} \sum_{k,\sigma} I_{k\sigma}, \tag{11.214}$$

$$I_{k\sigma} = \frac{\Omega k_0 T}{(2\pi)^2} \frac{S}{\hbar} \int_0^{\infty} dn \int_{-\infty}^{\infty} dp_z \ln\left[1 + \exp\left(\frac{\zeta_\sigma - E_n(p_z)}{k_0 T}\right)\right] e^{2\pi i k n}, \tag{11.215}$$

where $\zeta_\sigma = \zeta + \mu H \sigma_z \quad (\sigma_z = \pm 1)$.

By changing the integration variable from n to E, (11.215) becomes

$$I_{k\sigma} = \frac{\Omega k_0 T}{(2\pi)^2} \frac{S}{\hbar} \int_0^{\infty} dE \ln\left[1 + \exp\left(\frac{\zeta_\sigma - E}{k_0 T}\right)\right] \int_{p_{z\,min}}^{p_{z\,max}} dp_z \frac{\partial n}{\partial E} e^{2\pi i k n}, \tag{11.216}$$

where $p_{z\max}$ and $p_{z\min}$ are the functions on E. $e^{2\pi i k n}$ is a rapidly oscillating function on p_z. Since $n \gg 1$, we can use the method of steepest descents. Assume that n takes an extremum value n_m at $p_z = p_{zm}$. The main contribution to the integral comes from the vicinity of p_{zm}.

$$n(E, p_z) \cong n_m(E) + \frac{1}{2}\left(\frac{\partial^2 n}{\partial p_z^2}\right)_m (p_z - p_{zm})^2 . \qquad (11.217)$$

The integration over p_z can be approximated by

$$\left(\frac{\partial n}{\partial E}\right)_m e^{2\pi i k n_m} \int_{-\infty}^{\infty} dz \exp\left[i\pi k \left(\frac{\partial^2 n}{\partial p_z^2}\right)_m z^2\right] . \qquad (11.218)$$

If $(\partial^2 n/\partial p_z^2)_m > 0$, by changing the variable from z to y defined by $z = e^{i\pi/4} y$, (11.218) becomes

$$\int dz \exp\left[i\pi k \left(\frac{\partial^2 n}{\partial p_z^2}\right)_m z^2\right] = e^{i\pi/4} \int \exp\left[-\pi k \left(\frac{\partial^2 n}{\partial p_z^2}\right) y^2\right] dy .$$

If $(\partial^2 n/\partial p_z^2) < 0$, we should put $z = e^{-i\pi/4} y$.

Thus,

$$\int dz \exp\left[i\pi k \left(\frac{\partial^2 n}{\partial p_z^2}\right)_m z^2\right] = e^{\pm i\pi/4} \left(k \left|\frac{\partial^2 n}{\partial p_z^2}\right|_m\right)^{-1/2} , \qquad (11.219)$$

By inserting (11.218) and (11.219) into (11.216), we obtain

$$I_{k\sigma} \cong \frac{\Omega k_0 T}{(2\pi)^2} \frac{S}{\hbar} \sum_m \int_0^{\infty} dE \ln\left[1 + \exp\left(\frac{\zeta_0 - E}{k_0 T}\right)\right] e^{\pm i\pi/4} \left(\frac{\partial n_m}{\partial E}\right) e^{2\pi i k n_m}$$

$$\times \left(k \left|\frac{\partial^2 n}{\partial p_z^2}\right|_m\right)^{-1/2} . \qquad (11.220)$$

$\sum_m$ is the summation over every extremum values $n_m(E.P_z)$.

In carrying out the partial integration we employ the relation that the term $|\partial^2 n/\partial P_z^2|_m^{-1/2}$ is slowly varying as compared with the logarithmic term and $e^{2\pi i k n_m}$. Accordingly, we have

$$I_{k\sigma} \cong \frac{\Omega S}{(2\pi)^2\hbar}\,\frac{1}{2\pi i k^{3/2}}\sum_m e^{\pm i\pi/4}\int_0^\infty \frac{e^{2\pi i k n_m}}{e^{(E-\zeta_\sigma)/k_0T}+1}\left|\frac{\partial^2 n}{\partial P_z^2}\right|_m^{-1/2} dE. \qquad (11.221)$$

The principal contribution comes from the vicinity of $E=\zeta_\sigma$, since around $E \cong \zeta_\sigma$ the Fermi function is strongly nonstationary. Expanding $n_m(E)$ near ζ_σ,

$$n_m(E) \cong n_m(\zeta_\sigma) + (\partial n_m/\partial E)_{\zeta\sigma}(E-\zeta_\sigma),$$

$$\int_0^\infty \frac{e^{2\pi i k n_m}}{e^{(E-\zeta_\sigma)/k_0P}+1}\,dE \cong e^{2\pi i k n_m(\zeta_\sigma)}\int_{-\infty}^{\infty}\frac{dx}{e^{x/k_0T}+1}\exp\left[2\pi i k x\left(\frac{\partial n_m}{\partial E}\right)_{\zeta\sigma}\right],$$

and using the relation

$$\int_{-\infty}^{\infty}\frac{e^{i\alpha y}\,dy}{e^y+1} = -\frac{i\pi}{\sinh \pi\alpha},$$

we obtain

$$I_{k\sigma} \cong -2\,\frac{\Omega k_0 T S}{(2\pi)^2\hbar k^{3/2}}\sum_m e^{\pm i\pi/4}\left|\frac{\partial^2 n}{\partial P_z^2}\right|_{m,\zeta_\sigma}^{-1/2}\frac{e^{2\pi i k n_m(\zeta_\sigma)}}{\sinh\left[2\pi^2 k_0 T k(\partial n/\partial E)_{\zeta\sigma}\right]}. \qquad (11.222)$$

In the terms except a rapidly oscillating term $\exp[2\pi i k n_m(\zeta_\sigma)]$, it is permissible to put $\zeta_\sigma = \zeta$.

Since $\mu H \ll \zeta$,

$$\sum_{\sigma} \exp\left[2\pi i k\, n_m(\zeta_\sigma)\right] \cong \exp\left[2\pi i k\, n_m(\zeta)\right] \sum_{\sigma} \exp\left[2\pi i k\, (\partial n/\partial E)_\zeta\, \mu H \sigma_z\right]$$

$$= 2 \exp\left[2\pi i k\, n_m(\zeta)\right] \cos\left[2\pi k\, (\partial n/\partial E)_\zeta\, \mu H\right]. \qquad (11.223)$$

n_m is related to the cross sectional area S_m at $P_z = P_{zm}$ and $E =$ constant:

$$n_m \cong (c/2\pi\hbar e H)\, S_m. \qquad (11.224)$$

Proof of it is easy.
From (11.88), we have

$$[\pi_x, \pi_y] = \frac{\hbar e}{ic} H. \qquad (11.225)$$

The Bohr's condition of the orbital quantization for the closed orbit is given by

$$\oint \pi_y \, d\pi_x = \frac{2\pi e\hbar}{c} H\left[n + \gamma(n)\right], \quad (0 < \gamma < 1). \qquad (11.226)$$

Then, the area of the cross section for $P_z =$ constant and $E =$ constant is given by

$$S(E, P_z) = (2\pi e\hbar H/c)\left[n + \gamma(n)\right]. \qquad (11.227)$$

If $n \gg 1$, (11.227) leads to (11.224).
From (11.222), (11.223) and (11.224), the oscillating part of the thermodynamic function Φ_{osc} is given by

$$\Phi_{osc} \cong \frac{\Omega}{2^{3/2}\pi^{7/2}\hbar^3}\left(\frac{eH\hbar}{c}\right)^{5/2} \sum_m \left|\frac{\partial^2 S}{\partial P_z^2}\right|_{m,\zeta}^{-1/2} m^*(\zeta, P_{zm})^{-1} \sum_k \frac{\psi(k\lambda)}{k^{5/2}}$$

$$\times \cos\left(k\frac{cS_m}{e\hbar H} \pm \frac{\pi}{4}\right) \cos\left(\pi k \frac{m^*}{m}\right), \qquad (11.228)$$

where

$$\psi(z) = z/\sinh z, \quad \lambda = 2\pi^2 k_0 T\, c m^*/e\hbar H, \quad m^* = (2\pi)^{-1}\partial S/\partial E.$$

We shall now obtain an expression for the oscillating component of the magnetic moment which is given by $M_{osc} = -(\partial \Phi_{osc}/\partial H)$.

Since $cS_m/e\hbar H \gg 1$, we should differentiate only the cosine term.

$$M_{osc} \cong -\frac{(e\hbar/c)^{3/2} H^{1/2}}{2^{3/2}\pi^{7/2}\hbar^3} \sum_m \left|\frac{\partial^2 S_m}{\partial P_z^2}\right|_m^{-1/2} \frac{S_m}{m^*} \sum_{k=1}^{\infty} \frac{\psi(k\lambda)}{k^{3/2}} \sin\left(k\frac{cS_m}{e\hbar H} \pm \frac{\pi}{4}\right) \cos\left(\pi k \frac{m^*}{m}\right). \tag{11.229}$$

At low temperatures $\psi \sim 1$, then

$$M_{osc} \sim \frac{H^{1/2}}{\hbar^3}\left(\frac{e\hbar}{c}\right)^{3/2} \frac{S_m}{m^*}, \tag{11.230}$$

while the nonoscillating part is given by

$$M_0 \sim (\bar{\mu}^2/\hbar^3) P_F m^* H, \; (\bar{\mu} = e\hbar/2m^*c) \tag{11.231}$$

where P_F is the Fermi momentum (See Appendix 10).
Therefore,

$$M_{osc}/M_0 \sim (S/\bar{\mu}H)^{1/2}. \tag{11.232}$$

At moderate temperatures only the first term remains in the summation over k:

$$M_{osc} \cong -\frac{2^{1/2} k_0 T (e\hbar/c)^{3/2}}{\pi^{3/2} H^{1/2}} \sum_m S_m \left|\frac{\partial^2 S}{\partial P_z^2}\right|_m^{-1/2} \exp\left(-\frac{2\pi^2 k_0 T c m^*}{e\hbar H}\right)$$

$$\times \sin\left(k\frac{cS_m}{e\hbar H} \pm \frac{\pi}{4}\right) \cos\left(\frac{\pi m^*}{m}\right). \tag{11.233}$$

M_{osc} is periodic in H^{-1} and its period is

$$\Delta\left(\frac{1}{H}\right) = \frac{2\pi e\hbar}{c\,S_m}\,. \tag{11.234}$$

Until now, we have not taken into consideration the scattering effect. If this effect is taken into account, the factor

$$\exp(-2\pi c m^*/e\tau H) = \exp(-2\pi/\omega_0\tau), \tag{11.235}$$

should be multiplied. This is called the Dingle factor and the Dingle temperature T_D is defined by

$$k T_D = \hbar/\tau. \tag{11.236}$$

By analyzing the oscillation periods of the DHVA effect, we get the information on the extremal cross-sectional areas of the Fermi surfaces. A systematic study of the variation of these areas as a function of magnetic field orientation enables one to reconstruct the Fermi surface itself with fairly good accuracy. Bismuth is the first substance whose Fermi surface was determined by using the DHVA effect.$^{153)}$

Chapter 12 Conduction in Strong Magnetic Field (II)

12.1 Conduction with Non-equilibrium Phonon Distribution [156)]

In Section 11.7 we have calculated the electrical conductivity assuming the phonon distibution being in thermal equilibrium. However, it is expected that the deviation of the distribution function from thermal equilibrium will affect the transport coefficients.

Under the combined action of the electric and magnetic fields ($\mathcal{E} \perp H$), carriers acquire the drift velocity $\mathbb{V}_d = c(\mathcal{E} \times \mathbb{H})/H^2$ and the phonons are dragged by carriers along $\mathbb{V}_d$. This causes the phonon deviation.

If an electron makes a transition $(N.P_z.X) \rightarrow (N'.P_z'.X')$, the phonon system receives the momentum $q_y = s(X'-X)$.

If the dissipative processes in the phonon system are sufficiently active and then, the momentum transferred from the electron system rapidly disappears (namely, restores the thermal equilibrium very rapidly), the electron transitions can consecutively occur. Hence, the electric current flows.

On the contrary if the momentum relaxation processes in the phonon system are sufficiently slow, the phonon distributions deviate along the y-direction (parallel to $\mathcal{E} \times \mathbb{H}$) and their drift velocities approach to $\mathbb{V}_d$. In this case the phonons no longer scatter the electrons and then the electric current does not flow.

In the following we shall formulate it.

The current density related to the equilibrium phonon distribution is given by

$$j_1 = \frac{2\pi e}{\Omega^2 \hbar k_0 T} \sum_{\alpha,\beta} \sum_{q}{}' |J_{\beta\alpha}|^2 |C(q)|^2 N_q^0 f_\alpha (1-f_\beta) \delta(E_\alpha - E_\beta + \hbar\omega_q) X_{\beta\alpha}^2 \, e\mathcal{E} , \qquad (12.1)$$

where $J_{\beta\alpha} = \langle \beta | e^{iqr} | \alpha \rangle$, $X_{\beta\alpha} = X_\beta - X_\alpha$. The above expression is same as (11.182).

Equation of motion for the phonon q is expressed by

$$\left(\frac{\partial N_q}{\partial t}\right)_{\text{carrier}} + \left(\frac{\partial N_q}{\partial t}\right)_{\text{relaxation}} = 0 , \qquad (12.2)$$

the first term represents the contribution from the interaction with carriers and the second one is related to the all relaxation processes except the electron-phonon scattering.

Explicitly, $(\partial N_q / \partial t)_{\text{carrier}}$ is expressed by

$$\left(\frac{\partial N_q}{\partial t}\right)_{\text{carrier}} = \sum_{\alpha,\beta} \left\{ W^{(em)}(\alpha \to \beta) f_\alpha (1-f_\beta) - W^{(ab)}(\alpha \to \beta) f_\alpha (1-f_\beta) \right\} , \qquad (12.3)$$

where $W^{(em)}$ and $W^{(ab)}$ represent the transition probability corresponding to the phonon emission and absorption, respectively.

$$W^{(em),(ab)} = \frac{2\pi}{\hbar} (N_q + 1 \text{ or } N_q) \frac{|C(q)|^2}{\Omega} |J_{\beta\alpha}|^2 \delta(E_\alpha - E_\beta \mp \hbar\omega_q) . \qquad (12.4)$$

In the δ-function a quantity $e\mathcal{E}(X_\alpha - X_\beta)$ is included. Retaining the terms of $O(\mathcal{E})$, we have

$$\left(\frac{\partial N_q}{\partial t}\right)_{\text{carrier}} = -\frac{2\pi}{\hbar k_0 T}\frac{|C(q)|^2}{\Omega}N_q^\circ \sum_{\alpha,\beta} e\mathscr{E}X_{\alpha\beta}f_\alpha(1-f_\beta)|J_{\beta\alpha}|^2\delta(E_\alpha - E_\beta + \hbar\omega_q)$$

$$-\frac{g(q)}{t^{(c)}(q)}, \quad N_q = N_q^\circ + g(q), \qquad (12.5)$$

where

$$1/t^{(c)}(q) = \frac{2\pi}{\hbar}\sum_{\alpha,\beta}{}' \frac{|C(q)|^2}{\Omega}|J_{\beta\alpha}|^2 f_\alpha(1-f_\beta)\frac{\delta(E_\alpha - E_\beta + \hbar\omega_q)}{N_q^\circ + 1}, \quad (X_{\beta\alpha} = q_y/s). \qquad (12.6)$$

Assuming

$$\left(\frac{\partial N_q}{\partial t}\right)_{\text{relaxation}} = -\frac{g(q)}{t^{(r)}(q)}, \qquad (12.7)$$

and inserting (12.5), (12.6) and (12.7) into (12.2), we obtain

$$\left\{\begin{aligned} g(q) &= -\frac{\hbar V_d q_y}{k_0 T}N_q^\circ(N_q^\circ+1)\frac{t(q)}{t^{(c)}(q)}, \\ 1/t(q) &= 1/t^{(r)}(q) + 1/t^{(c)}(q), \quad V_d = c\mathscr{E}/H. \end{aligned}\right. \qquad (12.8)$$

Thus, number of the carriers which make transition $\alpha \to \beta$ per unit time through the interaction with the phonon q, is given by

$$-\frac{2\pi}{\hbar}\frac{|C(q)|^2}{\Omega}|J_{\beta\alpha}|^2\left\{f_\alpha(1-f_\beta)(N_q^\circ + g(q) + 1) - f_\beta(1-f_\alpha)(N_q^\circ + g(q))\right\}$$

$$\times\ \delta(E_\alpha - E_\beta - \hbar\omega_q). \qquad (12.9)$$

Since the terms including N_q° vanish, (12.9) becomes

$$-\frac{2\pi}{\hbar}\frac{|C(q)|^2}{\Omega}|J_{\alpha\beta}|^2(f_\alpha - f_\beta)\delta(E_\alpha - E_\beta - \hbar\omega_q)g(q). \qquad (12.10)$$

Thus, the current density due to the deviation of the phonon distribution from the thermal equilibrium is given by

$$j_2 = \frac{2\pi e}{\hbar \Omega^2} \sum_{\alpha,\beta,q} |C(q)|^2 |J_{\beta\alpha}|^2 f_\beta (1-f_\alpha)\, \delta(E_\alpha - E_\beta - \hbar\omega_q)\, X_{\alpha\beta}\, \frac{g(q)}{N_q^\circ + 1} \quad . \qquad (12.11)$$

By adding (12.1) and (12.11), the total current density is

$$j = \frac{2\pi e}{\Omega^2 \hbar k_0 T} \sum_{\alpha,\beta,q} |C(q)|^2 |J_{\beta\alpha}|^2 N_q^\circ f_\alpha (1-f_\beta)\, \delta(E_\alpha - E_\beta + \hbar\omega_q)\, X_{\beta\alpha}$$

$$\times \left\{ e\,\mathcal{E} X_{\beta\alpha} + \frac{k_0 T\, g(q)}{N_q^\circ (N_q^\circ + 1)} \right\} \quad . \qquad (12.12)$$

From (12.8) and (12.6), (12.12) leads to

$$\sigma_{xx} = \frac{\hbar^2 c^2}{\Omega k_0 T H^2} \sum_q q_y^2 N_q^\circ (N_q^\circ + 1) / \{ t^{(c)}(q) + t^{(r)}(q) \} \quad . \qquad (12.13)$$

If the phonon relaxation rate is very slow ($t^{(r)} \to \infty$), σ_{xx} becomes zero, while σ_{xx} is given by $j_1 / \mathcal{E}$ for $t^{(c)} \gg t^{(r)}$ (equilibrium phonon distribution). We can obtain an equivalent expression to (12.13) by solving the Boltzmann equation.

In the abscence of a magnetic field the deviation of the phonon distribution from the thermal equilibrium, enhances σ_{xx}. It will be discussed in Chapter 14.

12.2 Thermomagnetic Coefficients in Strong magnetic Field and the Onsager Relation

If an electric field and a temperature gradient are set up in the sample, an electric current j and a heat current w are expressed by

$$j = \sigma \mathcal{E} - \beta \nabla T, \quad w = \chi \mathcal{E} - \lambda \nabla T. \qquad (12.14)$$

If $H \parallel z$ and $\mathcal{E}, \nabla T \perp z$, the Onsager relation gives

$$T\beta_{xy}(H) = \chi_{yx}(-H). \qquad (12.15)$$

However, as will be shown in this Section a naive calculation does not provide (12.15), and some investigators arrived at an erroneous conclusion that the Onsager relation is invalid in strong magnetic fields. Such a mistake comes from a neglect of the surface current. We shall consider this in detail.157)

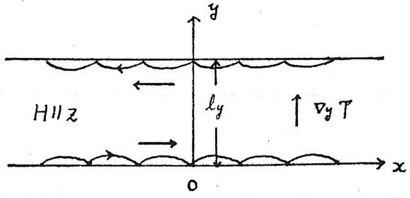


Fig. 12.1 Surface current induced by a magnetic field.

Let consider a sample whose length along the y-direction is l_y and the extension in the zx-plane is infinite (See Fig. 12.1). Surface current density along the z-direction per unit length is related to the magnetic moment per unit area by

$$J_{Mx} = c M_z. \qquad (12.16)$$

If the temperature gradient $\nabla_y T$ is set up, the surface currents at $y=0$ and $y=l_y$ do not cancel out. The total surface current density flowing across the cross section parallel to the yz-plane, is given by

$$[J_{Mx}(0) + J_{Mx}(l_y)]\, l_z = c\, l_z\, [M_z(T_0) - M_z(T_{l_y})] = -c\, \frac{dM_z}{dT}\frac{dT}{dy}\, l_z l_y . \qquad (12.17)$$

Then, the contribution to the macroscopic current is given by

$$\Delta j_x = -c\, \frac{dM_z}{dT}\frac{dT}{dy} . \qquad (12.18)$$

(12.18) yields the correction to the tensor component β_{xy}

$$\Delta \beta_{xy} = c\, \frac{dM_z}{dT} . \qquad (12.19)$$

In the next place we consider the case of $\nabla_y T = 0$ and $\mathcal{E}_y \neq 0$. In this case the surface currents at $y=0$ and $y=l_z$ cancel each other but the surface flow of the electrostatic energy remains finite. At $y=0$ the surface flow density of the electrostatic energy is given by

φ: electrostatic potential

$$J_{Mx}(0)\, \varphi(0) = c\, M_z\, \varphi(0) . \qquad (12.20)$$

Thus, the total flow density becomes

$$c\, M_z\, l_z\, [\varphi(0) - \varphi(l_y)] = -c\, M_z\, \frac{d\varphi}{dy}\, l_z l_y = c\, M_z\, \mathcal{E}_y\, l_y l_z . \qquad (12.21)$$

The correction to the macroscopic heat current density is

$$\Delta w_x = c\, M_z\, \mathcal{E}_y . \qquad (12.22)$$

Accordingly, we have

$$\Delta \chi_{xy} = c M_z . \qquad (12.23)$$

By evaluating the microscopic current which does not include the boundary effect,[158] we obtain

$$\beta_{xy}^{(0)} = \frac{c\mathcal{S}}{H} - c\,\frac{dM_z}{dT} , \quad \mathcal{S} : \text{entropy density}. \qquad (12.24)$$

Therefore,

$$\beta_{xy} = \beta_{xy}^{(0)} + \Delta\beta_{xy} = \frac{c\mathcal{S}}{H} . \qquad (12.25)$$

Similarly, we obtain (see Appendix 11)

$$\chi_{xy}^{(0)} = \frac{c}{H}\left(-M_z H + \mathcal{S} T\right) , \qquad (12.26)$$

hence,

$$\chi_{xy} = \chi_{xy}^{(0)} + \Delta\chi_{xy} = \frac{c\mathcal{S}T}{H} . \qquad (12.27)$$

(12.25) and (12.27) lead to the Onsager relation $T\beta_{xy}(H) = \chi_{yx}(-H)$. It should be noted that $T\beta_{xy}^{(0)}(H) \neq \chi_{yx}^{(0)}(-H)$.

In the following we shall consider the same problem by a different approach.[159] In Fig. 12.2 we shall ~~assume~~ the potential as follows:

$$U(y) = \begin{cases} \infty : & y \to 0 \text{ or } y \to l_y , \\ 0 : & Y_1 < y < l_y - Y_1 . \end{cases}$$

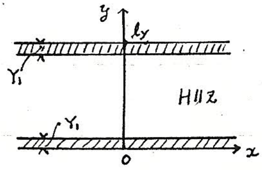


Fig. 12.2 $(l_x = l_z = 1)$

Here, we assume $l \ll Y_1 \ll l_y$ ($l = \sqrt{c\hbar/eH}$) and take the vector potential $\mathbb{A} = (-Hy, 0, 0)$.

The Hamiltonian and the eigenfunction are given by

$$\mathcal{H} = \frac{1}{2m}\left(P_y{}^2 + P_z{}^2\right) + \frac{1}{2m}\left(P_x - \frac{eH}{c}y\right)^2 + U(y), \tag{12.28}$$

$$\psi = e^{i(P_x x + P_z z)/\hbar}\,\varphi(y). \tag{12.29}$$

$\varphi(y)$ obeys the equation

$$\left\{\begin{aligned} &\frac{\hbar^2}{2m}\frac{d^2\varphi}{dy^2} + \left[E - \frac{P_z{}^2}{2m} - U(y) - \frac{m\omega_0^2}{2}(y-y_0)^2\right]\varphi = 0, \\ &\omega_0 = \frac{eH}{mc}, \quad y_0 = \frac{cP_x}{eH} = \frac{l^2 P_x}{\hbar}. \end{aligned}\right. \tag{12.30}$$

In the region of $Y_1 < y_0 < l_y - Y_1$, the energy values are

$$E^{(0)}_{n,P_z} = \hbar\omega_0(n + 1/2) + \frac{P_z{}^2}{2m}. \tag{12.31}$$

If, however, y_0 is located outside this interval, the energy values depend on three quantum numbers n, P_z and y_0; in this case the quantum number y_0 no longer has the meaning of the center of a Landau oscillator and y_0 varies from $-\infty$ to $+\infty$.

The current density is

$$\begin{aligned} j_{x\nu} &= -\frac{e\hbar}{2mi}\left(\psi_\nu^* \frac{\partial\psi_\nu}{\partial x} - \psi_\nu \frac{\partial\psi_\nu^*}{\partial x}\right) - \frac{e^2 A_x}{mc}\psi_\nu^*\psi_\nu \\ &= e\,\omega_0(y - y_0)\,|\varphi_\nu(y)|^2, \end{aligned} \tag{12.32}$$

where $\nu \equiv (n, p_x, y_0)$.

The total current through the cross section parallel to the yz-plane is

$$J_\nu = \int_0^{l_y} j_{x\nu}(y)dy = e\omega_0 \int_0^{l_y} (y-y_0)|\varphi_\nu(y)|^2 dy \,, \qquad (12.33)$$

The Hamiltonian H includes p_x as a parameter, then

$$\frac{\partial E_\nu}{\partial p_x} = \left\langle \frac{\partial H}{\partial p_x} \right\rangle_\nu \,, \qquad (12.34)$$

(see Appendix 12). Since $\partial H/\partial p_x = \omega(y-y_0)$, (12.33) leads to

$$J_\nu = e\frac{\partial E_\nu}{\partial p_x} \,. \qquad (12.35)$$

The mean current density averaged over the statiscal ensemble is

$$J = \sum_\nu \rho_{\nu\nu} J_\nu \,, \qquad (12.36)$$

where ρ denotes the density matrix.

Now, the integration over y_0 is separated into three regions $(-\infty, Y_1)$, $(Y_1, l_y - Y_1)$, $(l_y - Y_1, \infty)$. If y_0 is in the interval $(Y_1, l_y - Y_1)$, we see at once that J_ν vanishes, since φ_ν is an even function of $y - y_0$.

If y_0 is located in the interval $(-\infty, Y_1)$ or in $(l_y - Y_1, \infty)$, electrons move in the narrow layers close to the boundary with a thickness of order $Y_1 \ll l_y$. In these layers the temperature variation is negligibly small, then $\rho_{\nu\nu}$ is considered to be the thermal equilibrium Fermi distribution. The contribution from the interval $(-\infty, Y_1)$ is written in the form

$$J_1 = \sum_{y_0=-\infty}^{Y_1} \sum_{n, p_z} f_0(E_\nu) J_\nu \, . \tag{12.37}$$

Inserting (12.35) into (12.37) and putting $\sum_{y_0} \to 2/(2\pi\hbar) \int dp_x \cdots$, and $\eta = E_\nu - E_\nu^{(0)}$, we obtain

$$J_1 = \frac{e}{\pi\hbar} \sum_{n, p_z} \int_0^\infty f_0(E^{(0)}_{n, p_z} + \eta)\, d\eta = - \frac{c\, \Phi(T)}{H} \, , \tag{12.38}$$

where Φ denotes the thermodynamic potential which is given by (11.210). Namely, Φ is given by

$$\Phi(T, \zeta . H) = -k_0 T \sum_i \ln\left[1 + e^{(\zeta - E_i)/k_0 T}\right] = -k_0 T \frac{eH}{\pi\hbar c} \sum_{n . p_z} \ln[1 + e^{(\zeta - E)/k_0 T}] , \tag{12.39}$$

The relation (12.38) is proved as follows:

$$\int_0^\infty d\eta\, f_0(E_\nu^{(0)} + \eta) = \sum_{n=1}^{\infty} \int_0^\infty d\eta\, (-1)^{n-1} e^{-n\beta(E_\nu^0 + \eta - \zeta)} = k_0 T \ln[1 + e^{\beta(\zeta - E_\nu^{(0)})}] ,$$

$$(\beta = 1/k_0 T) . \tag{12.40}$$

In the differential from Φ is written by

$$d\Phi = -S\, dT - N\, d\zeta - M\, dH \, . \tag{12.41}$$

where S is the entropy, N the concentration and M denotes the magnetization.

Let denote the temperature in the interval $(l_y - Y_1, \infty)$ by $T + \Delta T$.

The current density due to this region is

$$J_2 = c\,\frac{\Phi(T+\Delta T)}{H} = c\,\frac{\Phi(T)}{H} + \frac{c}{H}\frac{d\Phi}{dT}\frac{dT}{dy}\,l_y\,. \qquad (12.42)$$

Then, the total macroscopic current density becomes

$$j_x = \frac{J_1 + J_2}{l_y} = \frac{c}{H}\frac{d\Phi}{dT}\frac{dT}{dy}\,. \qquad (12.43)$$

In the first equation of (12.14) we put $\mathcal{E} = (0, (1/e)\,d\zeta/dy, 0)$, $\nabla T = (0, \partial T/\partial y, 0)$ and $d\zeta/dy = (d\zeta/dT)(dT/dy)$. From (12.43), we get

$$\beta_{xy} = \frac{\sigma_{xy}}{e}\frac{d\zeta}{dT} - \frac{c}{H}\frac{d\Phi}{dT}\,, \qquad (12.44)$$

while (12.41) yields

$$\frac{d\Phi}{dT} = -\mathcal{S} - N\frac{d\zeta}{dT}\,. \qquad (12.45)$$

Then,

$$\beta_{xy} = \frac{c\mathcal{S}}{H}\,, \qquad (12.46)$$

where the relation $\sigma_{xy} = -Nec/H$ is employed. Thus, we again obtain (12.25).

The discussions are limited to the collisionless case.

The thermoelectric power S is given by

$$S = \frac{\mathcal{E}_y}{\nabla_y T} = \frac{\beta_{xy}}{\sigma_{xy}} = -\frac{\mathcal{S}}{Ne} = -\frac{s}{e}\,, \qquad (12.47)$$

where s is the entropy per electron.

In some cases it may be possible that (12.47) plays a dominant role in the thermoelectric phenomena in the quantum limit.

It is easy to directly verify (12.24). The total microscopic density is given by

$$j_x = \sum_\nu f(E_\nu)\, j_{x\nu}, \qquad \nu \equiv (n, p_z, y_0). \tag{12.48}$$

$f(E_\nu)$ depends on y_0 through the temperature $T(y_0)$, where $T(y_0)$ is

$$T(y_0) = T(0) + y_0 \nabla_y T. \tag{12.49}$$

Then,

$$f(E_\nu) = f_0(E_\nu) - \left(\frac{E_\nu - \zeta}{T} + \frac{d\zeta}{dT} \right) \frac{\partial f_0}{\partial E_\nu} \frac{dT}{dy}\, y_0\,, \tag{12.50}$$

Since j_x does not depend on y, we can put $y=0$ in (12.32).

Therefore,

$$j_x = \sum_\nu f(E_\nu)\, j_{x\nu} = e\omega_0 \sum_{n p_z y_0} y_0^2\, |\varphi_n(y_0)|^2 \left(\frac{E_\nu - \zeta}{T} + \frac{d\zeta}{dT} \right) \frac{\partial f_0}{\partial E_\nu} \frac{dT}{dy}. \tag{12.51}$$

By using the relations

$$\sum_{n p_z y_0} \cdots = \frac{2}{(2\pi\hbar)^2} \sum_n \int dp_z \int dp_x \cdots = \frac{eH}{2\pi^2\hbar^2 c} \sum_n \int dp_z \int dy_0 \cdots, \tag{12.52}$$

$$\int_{-\infty}^{\infty} y_0^2\, |\varphi_n(y_0)|^2\, dy_0 = l^2 (n + 1/2), \tag{12.53}$$

(12.51) is expressed by

$$j_x = \frac{e\omega_0}{2\pi^2\hbar}\sum_n \int dp_z\,(n+1/2)\left(\frac{E_{np_z}-\zeta}{T} + \frac{d\zeta}{dT}\right)\frac{\partial f_0}{\partial E_{np_z}}\,\frac{dT}{dy}. \qquad (12.54)$$

From (12.14), we have

$$j_x = \left(\frac{\sigma_{xy}}{e}\frac{d\zeta}{dT} - \beta_{xy}^{\circ}\right)\frac{dT}{dy}. \qquad (12.55)$$

Accordingly,

$$\beta_{xy}^{\circ} = \frac{\sigma_{xy}}{e}\frac{d\zeta}{dT} - \frac{e\omega_0}{2\pi^2\hbar}\sum_n \int dp_z\,(n+1/2)\left(\frac{E_{np_z}-\zeta}{T} + \frac{d\zeta}{dT}\right)\frac{\partial f_0}{\partial E_{np_z}}. \qquad (12.56)$$

On the other hand, (12.41) gives

$$cH\frac{d}{dT}\left[\frac{\partial}{\partial H}\left(\frac{\Phi}{H}\right)_{\zeta,T}\right] = \frac{c\mathcal{S}}{H} + \frac{cN}{H}\frac{d\zeta}{dT} - c\frac{dM_z}{dT}, \qquad (12.57)$$

and (12.39) leads to

$$cH\frac{d}{dT}\left[\frac{\partial}{\partial H}\left(\frac{\Phi}{H}\right)_{\zeta,T}\right] = \frac{e\omega_0}{2\pi^2\hbar}\sum_n \int dp_z\,(n+1/2)\frac{\partial f_0}{\partial T}$$

$$= -\frac{e\omega_0}{2\pi^2\hbar}\sum_n \int dp_z\left(\frac{E_{np_z}-\zeta}{T} + \frac{d\zeta}{dT}\right)\frac{\partial f_0}{\partial E_{np_z}}(n+1/2). \qquad (12.58)$$

In consideration of (12.57) and (12.58), (12.56) is given by

$$\beta_{xy}^{\circ} = \frac{c\mathcal{S}}{H} - c\frac{dM_z}{dT}. \qquad (12.59)$$

Thus, (12.24) is verified. Similary, we can prove (12.26)

In this Section we arrived at the important results that the microscopic flow densities $j^{(0)}$ and $w^{(0)}$ are related to the macroscopic ones by

$$j = j^{(0)} - c\,\mathrm{curl}\,M\,, \quad w = w^{(0)} - c\,\mathrm{curl}\,(\varphi M)\,, \tag{12.60}$$

and the flux flows are not $j^{(0)}$, $w^{(0)}$ but j, w. In the case where the eigenstates are specified by the Landau levels, the terms including M become very important.

12.3 A Note on the Diffusion Term of the Thermopower in Strong Magnetic Field

In the previous Section we payed our attention to the non-diagonal thermomagnetic coefficients β_{xy}, X_{xy} in the collision free case.

If we do not consider the scattering processes, β_{xx} and X_{xx} disappear in strong magnetic fields.

The thermoelectric power is composed of the two contributions — the phonon drag term and the diffusion term. The phonon drag effect will be treated in detail in Chapter 14. Here, let consider the diffusion term. The thermopower S and the Nernst coefficient A_{NE} are expressed by

$$\left\{\begin{aligned} S &= \frac{\mathcal{E}_x}{\nabla_x T} = \frac{\sigma_{yy}\beta_{xx} - \sigma_{xy}\beta_{yx}}{\sigma_{xx}\sigma_{yy} - \sigma_{xy}\sigma_{yx}} = \frac{\sigma_{yy}X_{xx}(-H) - \sigma_{xy}X_{xy}(-H)}{T(\sigma_{xx}\sigma_{yy} - \sigma_{xy}\sigma_{yx})}\,, \\ A_{NE} &= \frac{\mathcal{E}_y}{H\nabla_x T} = \frac{\sigma_{yy}\beta_{yx} - \sigma_{yx}\beta_{xx}}{H(\sigma_{xx}\sigma_{yy} - \sigma_{xy}\sigma_{yx})} = \frac{\sigma_{xx}X_{xy}(-H) - \sigma_{yx}X_{xx}(-H)}{HT(\sigma_{xx}\sigma_{yy} - \sigma_{xy}\sigma_{yx})}\,, \end{aligned}\right. \tag{12.61}$$

where $H \parallel z$, $\nabla_y T = 0$ and $\nabla_x T \neq 0$. Here, we use the Onsager relation

$$T\beta_{ij}(H) = \chi_{ji}(-H). \tag{12.62}$$

Ansel'm and Askerov calculated β_{xx} and obtained the result that β_{xx} becomes infinity with $T \to 0$.[160] This is in contradiction to the third law of thermodynamics. Ono pointed out[161] that such a contradiction comes from the neglect of the interaction energy transfer. Ono treated the problem in which the electron phonon scattering is a predominant process by using the Green's function technique. Here, we shall employ an elementary method and consider the impurity scattering.

In the case of $\nabla T = 0$ the heat current density w is given by

$$w = \frac{1}{2}\mathrm{Tr}\,\rho\{v(\mathcal{H} - \zeta N) + (\mathcal{H} - \zeta N)v\}, \tag{12.63}$$

where $\mathcal{H}$ is the total Hamiltonian composed of the Hamiltonian of the electron system and the impurity potential:

$$\mathcal{H} = \mathcal{H}_0 + V, \tag{12.64}$$

v is the velocity operator and N the electron number operator. Ansel'm and Askerov took $\mathcal{H}_0$ instead of $\mathcal{H}$.

In calculating (12.63) we employ the method developed by Adams and Holstein in Section 11.2. In the approximation of he order in $O(V^2)$, w_x is expressed by

$$w_x = \frac{1}{2}\sum_{\mu\mu'}\left\{ D_{\mu\mu'}(\varepsilon_\mu + \varepsilon_{\mu'} - 2\zeta)\, v_{\mu'\mu} + \sum_\nu G_{\mu\nu}\left(V_{\nu\mu'} v_{\mu'\mu} + v_{\nu\nu'} V_{\nu'\mu}\right)\right\}$$

$$= \frac{1}{2}\sum_{\mu\mu'}\left\{ D_{\mu\mu'}(\varepsilon_\mu + \varepsilon_{\mu'} - 2\zeta) + \sum_\nu \left(G_{\mu\nu} V_{\nu\mu'} + V_{\mu\nu} G_{\nu\mu'}\right)\right\} v_{\mu'\mu}. \qquad (12.65)$$

$D_{\mu\mu'}$ and $G_{\mu\nu}$ are defined by (11.42):

$$\begin{cases} G_{\mu\nu} = i\pi f_{\mu\nu} V_{\mu\nu}\, \delta(\varepsilon_{\mu\nu} + e\mathcal{E}X_{\mu\nu}), \\ D_{\mu\mu'} = \dfrac{i\pi}{\varepsilon_{\mu\mu'}} \displaystyle\sum_\nu V_{\mu\nu} V_{\nu\mu'} \left\{ f_{\mu\nu}\, \delta(\varepsilon_{\mu\nu} + e\mathcal{E}X_{\mu\nu}) + f_{\mu'\nu}\, \delta(\varepsilon_{\mu'\nu} + e\mathcal{E}X_{\mu'\nu})\right\}, \end{cases}$$

(12.66)

where we take the representation (N, p_z, X) and (μ', μ) or (ν, ν') represents $N \neq N'$, $(p_z, X) = (p_z', X')$.

In consideration of $v_{\mu\mu'} = -v_{\mu'\mu}$ and $V_{\mu\nu} V_{\nu\mu'} = V_{\mu'\nu} V_{\nu\mu}$, w_x is rewritten in the form

$$w_x = 2\pi i \sum_{\mu\mu'} \sum_\nu \left(\frac{\varepsilon_\mu - \zeta}{\varepsilon_{\mu\mu'}}\right) v_{\mu'\mu} V_{\mu\nu} V_{\nu\mu'} f_{\mu\nu}\, \delta(\varepsilon_{\mu\nu} + e\mathcal{E}X_{\mu\nu}). \qquad (12.67)$$

Retaining the terms linear in $\mathcal{E}$, we obtain

$$w_x = 2\pi i \mathcal{E} \sum_{\mu\mu'} \sum_\nu \left(\frac{\varepsilon_\mu - \zeta}{\varepsilon_{\mu\mu'}}\right) v_{\mu'\mu} V_{\mu\nu} V_{\nu\mu'} X_{\nu\mu} \frac{\partial f}{\partial \varepsilon_\nu}\, \delta(\varepsilon_{\mu\nu}). \qquad (12.68)$$

(12.68) approaches zero with $T \to 0$. ~~Accordingly~~, $X_{xx} \to 0$ with

with $T \to 0$. After carrying out the calculations similar to (11.46) ~ (11.49), (12.68) yields

$$\chi_{xx} = e \sum_{\mu\nu} (\mathcal{E}_\mu - \zeta) \frac{1}{2} X_{\mu\nu}^2 \frac{2\pi}{\hbar} |V_{\mu\nu}|^2 \frac{\partial f}{\partial \mathcal{E}_\nu} \delta(\mathcal{E}_{\mu\nu}). \qquad (12.69)$$

It is readily shown that w_x remains finite at $T = 0\,°K$ if we disregard the terms with $\mathfrak{G}$ in (12.65).

Examples of Sections 12.2 and 12.3 show that we should be careful to deal with the thermomagnetic effects in strong magnetic fields.

12.4 Negative Longitudinal Magnetoresistance in the Quantum Limit

Up to now we focussed our attention on the transverse effects. Now we discuss the longitudinal magnetoresistance and the associated negative magnetoresistance in the quantum limit.

In Figs. 12.3 and 12.4 observed curves of the longitudinal magnetoresistance in n-InSb are illustrated.[162] Argyres and Adams pointed out[163] that non-degenerate semiconductors in the quantum limit may exhibit the negative magnetoresistance if the ionized impurity scattering is predominant. Figs. 12.3 and 12.4 for n-InSb and Fig. 11.7 related to n-GaAs just correspond to such situation.

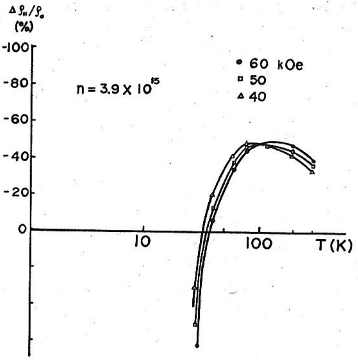


Fig. 12.3 Temperature dependence of $\Delta\rho_{11}/\rho_0$ of n-InSb with $n = 3.9 \times 10^{15}$ cm^{-3}.

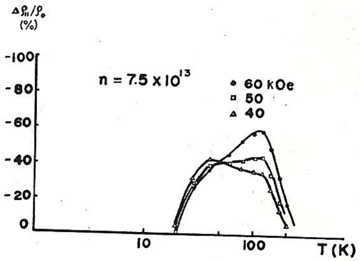


Fig. 12.4 Temperature dependence of $\Delta\rho_{11}/\rho_0$ of n-InSb with $n = 7.5 \times 10^{13}$ cm^{-3}.

The following calculation is limited to the case in which the acoustic phonon and ionized impurity scatterings are predominant. Since $m^* = 0.014\, m_0$, the Landau splitting is

$$\hbar\omega_0 = 1.324 \times 10^{-18} H, \qquad (12.70)$$

and (12.70) becomes $\hbar\omega_0/k_0 = 384$ K for $H = 40$ kOe. Therefore, at the temperature below 100 K all electrons can be considered to be populated in the lowest Landau level $N = 0$.

Perturbed Hamiltonian is composed of the following two parts:

$$\left\{\begin{aligned} \mathcal{H}_I &= \pm \frac{4\pi e^2}{\Omega \varepsilon} \sum_i \sum_q \frac{e^{iq(r-R_i)}}{q^2 + q_D^2}, \\ q_D{}^2 &= \frac{4\pi n e^2}{\varepsilon k_0 T}, \ (\varepsilon : \text{dielectric constant}) \end{aligned}\right. \qquad (12.71)$$

where R_i denotes the ionized center coordinate, and

$$\mathcal{H}_A = -i\,D\sqrt{\frac{\hbar}{2d\Omega\omega_q}}\;q\left(b_q e^{iqr} - b_q^{+} e^{-iqr}\right). \qquad (12.72)$$

q_D values for the two n values corresponding to Figs. 12.3 and 12.4 are listed in Table 12.1.

T (K)	40	60	80	100	120
$q_D\,(\mathrm{cm}^{-1})$ $n = 3.9\times10^{15}\,\mathrm{cm}^{-3}$	3.41×10^5	2.78×10^5	2.41×10^5	2.15×10^5	1.97×10^5
$q_D\,(\mathrm{cm}^{-1})$ $n = 7.5\times10^{13}\,\mathrm{cm}^{-3}$	4.72×10^4	3.86×10^4	3.34×10^4	2.99×10^4	2.73×10^4

Table 12.1 Values of the screening constant q_D.
$q_D = (\text{Debye length})^{-1}$ $(\varepsilon = 17.64)$

If we only consider H_I, the scattering processes which contribute to the resistivity is restricted to the backward scattering shown in Fig. 11.8 (A → B process) and the forward scattering (A → C) is prohibited due to the violation of the energy conservation law.

Momentum change associated with the A → B process is given by

$$q_z = 2k_z \simeq 2\sqrt{\frac{2m^* k_0 T}{\hbar^2}} = 1.13\times10^5\sqrt{T}. \qquad (12.73)$$

From (12.73) and Table 12.1 we have

$$q_z^2 \gg q_D^2 \quad \text{for } T \gtrsim 40\,\mathrm{K}, \qquad (12.74)$$

while in the quantum limit $q_\perp^2 \sim s = eH/\hbar c = 1.52\times10^7 H$.

Then, in the field intensity $H \gtrsim 40$ KOe

$$q_\perp^2 \sim s >> q_D^2 . \qquad (12.75)$$

Accordingly, it is concluded that q-dependence of H_I severely limits the backward scattering specified by $A \to B$.

On the other hand in the absence of magnetic field the forward scattering is allowed, since the constant energy surface is spherical, and this scattering process limits the conductivity. Therefore, we have

$$\sigma_z(0) < \sigma_z(H), \qquad (12.76)$$

where $\sigma_z(H)$ denotes the longitudinal conductivity in the quantum limit. This explains the negative magnetoresistance. Fig. 12.3 indicates that at low temperatures $\Delta\rho_{\parallel}/\rho_0$ becomes positive. This behavior can be explained in consideration of the condition $q_D^2 \sim q_z^2 + q_\perp^2$ at low temperatures. Transition from the negative magnetoresistance to the positive one shifts to higher temperature side with increasing the carrier density n. It is consistent with Figs. 12.3 and 12.4.

Apperance of a maximum in the $\Delta\rho_{\parallel}/\rho_0$ vs T curve is due to the LO-phonon scattering which plays an important role at high temperatures.[162] Since the Boltzmann equation is valid in the longitudinal magnetoresistance,

$$-\frac{e\mathcal{E}}{\hbar}\frac{\partial f_0(\alpha)}{\partial k_z} = \sum_{\alpha'}\left[W(\alpha,\alpha')f(\alpha') - W(\alpha',\alpha)f(\alpha)\right], \qquad (12.77)$$

where $W(\alpha,\alpha')$ denotes the transition probability from α' to α.

We write

$$f = f_0 + \varphi, \quad f_0 = Ae^{-\beta E}, \quad A = \frac{2\pi^2 n}{s}\sqrt{\frac{\hbar^2}{2\pi m^* k_0 T}}\,. \qquad (12.78)$$

In the regions of H and T we are interested $q_\perp \sim \sqrt{s} \sim q_z$, and the phonon system participated in the scattering process has a typical energy ~ $\hbar v_s \sqrt{s}$. As an example, let insert $v_s = 3.7\times 10^5$ cm/sec and $H = 50$ kOe. We have $\hbar v_s\sqrt{s}/k_0 = 2.46$ K. Then, it is permitted to consider the acoustic phonon scattering to be elastic in the temperature range where the negative magnetoresistance appears.

By defining the relaxation time, the deviation of the distribution function becomes

$$\begin{cases} \varphi(\alpha) = e\mathcal{E}\, v_z\, \tau(\alpha)\dfrac{\partial f_0}{\partial E(\alpha)}, \\[2ex] 1/\tau(\alpha) = 1/\tau_I + 1/\tau_A, \end{cases} \qquad (12.79)$$

$$\begin{cases} \nu_I = 1/\tau_I = \dfrac{a_I}{2}\dfrac{\hbar^2}{2m^*}\dfrac{1 + x\,E_i(-x)}{E^{3/2}\left(1 + q_D^2/q_z^2\right)}, \\[2ex] a_I = \dfrac{2\pi}{\hbar}\left(\dfrac{e^2}{\varepsilon}\right)^2 N_I\sqrt{\dfrac{2m^*}{\hbar^2}}, \quad N_I : \text{impurity concentration.} \\[2ex] x = (q_z^2 + q_D^2)/2s, \quad q_z = 2k_z. \end{cases} \qquad (12.80)$$

E_i is the exponential integral defined by (11.197).

$$\nu_A = 1/\tau_A = \frac{a_A S}{\sqrt{E}}, \quad a_A = \frac{D^2 k_0 T}{2\pi\hbar d v_s^2}\sqrt{\frac{2m^*}{\hbar^2}}. \tag{12.81}$$

Since $\hbar\omega_0 \gg k_0 T$, the electrical conductivity is

$$\sigma_z(H) = -\frac{2e^2 S}{(2\pi)^2}\,\frac{2m^*}{\hbar^2}\int_0^\infty \frac{dE}{\sqrt{E}}\,\tau(E)\,v_z^2(E)\,\frac{\partial f_0}{\partial E}. \tag{12.82}$$

In the absence of a magnetic field the relaxation rates corresponding to ν_I and ν_A are given by (see Sections 7.1 and 7.8)

$$\begin{cases} \omega_I = 1/\tau_I = \dfrac{a_I}{2}\,\dfrac{\hbar^2}{2m^*}\,E^{-3/2}\left\{\ln(1+b) - b/(1+b)\right\}, \\ b = (2k/q_D)^2, \end{cases} \tag{12.83}$$

$$\omega_A = 1/\tau_A = a_A\,\frac{2m^*}{\hbar^2}\,E^{1/2}, \tag{12.84}$$

and the corresponding conductivity becomes

$$\sigma_z(0) = -\frac{e^2}{6\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2}\int_0^\infty dE\sqrt{E}\;\tau(E)\,v_z^2(E)\,\frac{\partial f_0}{\partial E}. \tag{12.85}$$

As mentioned already, in order to explain the observed curves in Figs. 12.3 and 12.4 it is needed to take into consideration the interaction with the LO-phonons. In this case the Boltzmann equation is composed of infinite number of the difference equation. In the temperature region $T \lesssim 200\,\mathrm{K}$ the Boltzmann equation is approximated by restricting the energy range as $E < 2\hbar\omega_\ell$ $(2\hbar\omega_\ell/k_0 = 566\ \mathrm{K})$.

By solving the Boltzmann equation which is composed of two coupled equations we can explain fairly well the experimental results shown in Figs. 12.3 and 12.4.[162] In this section we ignore the LO-phonon scattering and give an qualitative explanation on the negative magneto-resistance.

At low temperatures ν_A and ω_A can be neglected as compared with ν_I and ω_I. From (12.82) and (12.85) we obtain

$$\frac{\sigma_z(H)}{\sigma_z(0)} \sim \left(\frac{\hbar^2 S}{2m^*} \Big/ \tilde{E}\right)\left\langle\frac{\omega_I}{\nu_I}\right\rangle . \qquad (12.86)$$

In the (H, T) region we are interested it is shown that $\hbar^2 S/2m^* > \tilde{E} \sim k_0 T$ and (12.80) and (12.83) lead to

$$\frac{\omega_I}{\nu_I} = \frac{\ln(1+b) - b/(1+b)}{1 + x e^{x} E_i(-x)} . \qquad (12.87)$$

Since $b \gg 1$, we obtain $\ln(1+b) - b/(1+b) > 1$. Moreover, as is shown in Fig. 12.5 the denominator of (12.87) is always smaller than unity. Then, we obtain the result

$$\frac{\sigma_z(H)}{\sigma_z(0)} > 1, \quad \frac{\Delta\rho_{\parallel}}{\rho_0} < 0 . \qquad (12.88)$$

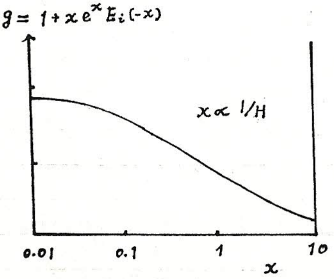


Fig. 12.5 Behavior of the function $g(x)$.

For example, let insert $T = 77K$, $H = 60\,KOe$ and $n = 4\times10^{15}\,cm^{-3}$ into (12.87), we have $\omega_I/\nu_I \cong 3.57 > 1$. This result explains an apperance of the negative magnetoresistance. However, inclusion of the acoustic phonon and LO-phonon scatterings makes $\Delta\rho_{11}/\rho_0$ less negative.

12.5 Esaki Kink Effect

I-V characteristic of bismuth exhibits a sharp kink at a certain voltage, when the specimen is subjected to a transverse magnetic field. This remarkable effect was first observed by Easaki.[164] His result is shown in Fig. 12.6. Similar phenomenon was observed in graphite.[165] The threshold electric field $\mathcal{E}_{kink}$ is related to the magnetic field by

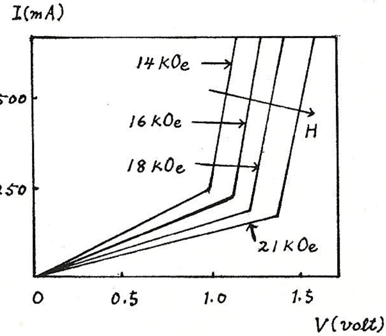


Fig. 12.6 Esaki kink effect of Bi. H is parallel to the trigonal axis.[164]

$$\mathcal{E}_{kink} = \alpha H, \qquad (12.89)$$

where α is a constant which is very sensitive to the magnetic field direction.

In the configuration of $\mathcal{E} \parallel x$, $H \parallel z$ electrons and holes flow along the direction $\mathcal{E}\times H$ ($\parallel$ y-direction) with a constant drift velocity $V_d = c\,\mathcal{E}/H$. Inserting the observed values of $\mathcal{E}_{kink}$

we obtain $V_d \sim 10^5$ cm/sec which is same order of magnitude as the sound velocity. In the bismuth sample employed in the experiment the acoustic phonon scattering is still active at the helium temperatures.

These results suggest us that the kink effect may be closely related to the electron-phonon interaction.

The Landau wave function is given by (see Section 11.1)

$$\psi_{N,k_z,X} = (L_y L_z)^{-1/2} \phi_N(x-X) e^{i(k_y y + k_z z)}, \quad X = -\frac{\hbar k_y}{m\omega_0} - \frac{e\mathcal{E}}{m\omega_0^2}. \qquad (12.90)$$

Consider a process in which electron makes a transition $k_y \to k_y'$ and simultaneously a phonon q_y is emitted ($q_y = k_y' - k_y$). Then, the center of the Landau orbit changes from X to $X + \delta X$, where $\delta X = \hbar q_y / m\omega_0$. Energy change of the electron is $e\mathcal{E}\delta X$. If the condition

$$e\mathcal{E}\delta X = e\mathcal{E}\frac{\hbar q_y}{m\omega_0} \geq \hbar v_s q_y \qquad (12.91)$$

is realized, energy of the electric field is transfered from the electron system to the phonon system and the phonons are excited. Rewriting (12.91), one obtains

$$\frac{c\mathcal{E}}{H} > v_s, \qquad (12.92)$$

and $v_s = V_d$ for $\mathcal{E} = \mathcal{E}_{kink}$. Scattering of electrons by phonons is enhanced with increase of the phonon number and this induces the electric current increase. Kink effect is essentially a nonlinear effect. In this effect amplification of the acoustic phonons can not be directly observed. However, it is possible to observe the amplification of an ultrasonic wave propagating in crystal, if ultrasonic gain rather ultrasonic attenuation is realized.[166)]

12.6 Magnetic Breakdown [167)]

Magnetic breakdown (or Magnetic breakthrough) which occurs in strong magnetic field, is analogous to Zener breakdown. Consider the two-dimensional free electron states modified by a one-dimensional periodic potential $V_0 \cos Gy$. Hamiltonian, then becomes

$$\mathcal{H} = \frac{\hbar^2 k^2}{2m} + V_0 \cos Gy. \qquad (12.93)$$

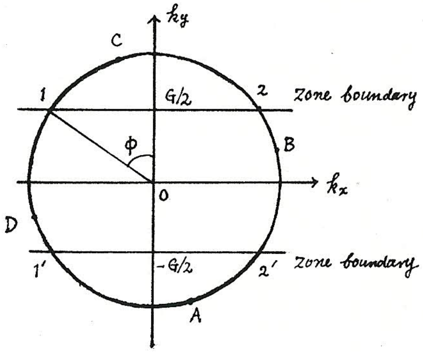


Fig. 12.7 Two-dimensional Fermi surface and zone boundary.

At the points 1, 1', 2 and 2' band gap appears. In the presence of a magnetic field H ($\perp$ xy-plane) the Hamiltonian is:

$$\mathcal{H} = \frac{1}{2m}\left(p + \frac{e}{c}A\right)^2 + V_0 \cos Gy. \qquad (12.94)$$

Let us consider the case $\mathcal{E} = 0$.

By integrating the equation of motion $\hbar \dot{k} = -(e/c)\, v \times H$, we get

$$k_x = -s(y - y_0), \quad k_y = s(x - x_0), \quad s = eH/\hbar c. \qquad (12.95)$$

(12.95) shows that the trajectories of the electrons in r-space normal to the magnetic field are equal to the trajectories in k-space after a rotation by $\pi/2$ and a multiplication by a scal factor S^{-1}.

It is easy to see that for non-vanishing potential $V_0 \neq 0$ two types of electron trajectories are possible : (a) represents an open orbit,

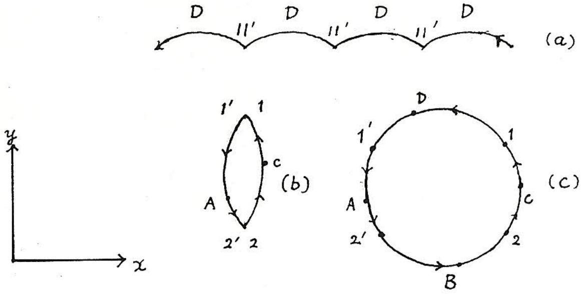


Fig. 12.8 Electron trajectories in xy-plane,
(a) open orbit, (b) closed orbit, (c) free electron orbit

while (b) corresponds to a closed orbit. 11'-point is the Bragg reflection point in (a), while (b) orbit has two Bragg reflection points 11' and 22'.

If the field intensity is strong enough, electrons move along the free electron like orbit (c) in Fig. 12.8 without the Bragg reflection at 1, 2, 1', 2' as if the band gap does not exist.

Transition from (a) or (b) to (c) is called "magnetic breakdown"[68] or "magnetic breakthrough." Hereafter, we shall abbreviate it MB.

At first glance we might expect that MB could occur in the

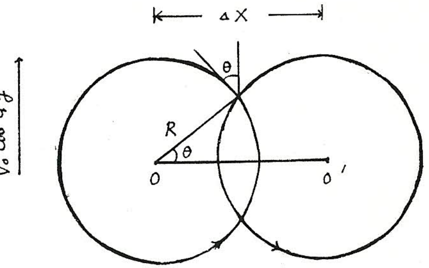


Fig. 12.9 Transition from an orbit O to a neighboring orbit O′. These circles represent classical electron orbits in real space. $\Delta X = \hbar G / m\omega_0$.

field satisfying the condition $\hbar\omega_0 \sim E_g$ (E_g : band gap). However, it is not the case but the threshold field is given by

$(\hbar\omega_0 E_F)^{1/2} \sim E_g$ .169) (12.96)

Then, we can observe MB by applying a magnetic field whose intensity is attainable in our laboratory.

Consider an electron circulating along the classical orbit O and calculate the transition probability to a neighboring orbit O′ induced by the perturbing potential $V_0 \cos Gy$.

Initial state is given by

$$\begin{cases} \psi_{N,k_z.k_y} = (L_y L_z)^{-1/2}\,\phi_N(x-X)\,e^{i(k_y y + k_z z)}, \quad X = -\dfrac{\hbar k_y}{m\omega_0} = -\dfrac{k_y}{s}, \qquad (12.97) \\ E_{N,k_z.k_y} = \hbar\omega_0 (N + 1/2) + \hbar^2 k_z^2/2m. \end{cases}$$

The perturbing potential $\frac{1}{2}V_0(e^{iGy} + e^{-iGy})$ induces the transition $(N, k_z, k_y) \rightarrow (N, k_z, k_y')$, where $k_y' = k_y \pm G$. In the classical limit $(N \gg 1)$ change in k_y not only represents the shift in orbit center, but also gives the change in wave number of the electron resulting from the transition from one cyclotron orbit to another with same energy.

This is clearly shown in Fig. 12.9. From (12.97) and the classical relation $R = v/\omega_0$, where v denotes the electron velocity, we get

$$\begin{aligned}\Delta k_y &= -(m\omega_0/\hbar)\,\Delta X = -(m\omega_0/\hbar)\,2R\cos\theta \\ &= (m/\hbar)(v'-v)\cos\theta = (m/\hbar)(v_y'-v_y). \qquad (12.98)\end{aligned}$$

Transition probability per unit time from $(N.k_z.k_y)$-state to the final states f is given by

$$W = \frac{2\pi}{\hbar}\sum_f |V_{Nk_zk_y,f}|^2\,\delta(E_f - E_{Nk_zk_y}). \qquad (12.99)$$

The quantity we are interested in is the transition probability per one period of the cyclotron motion W/ω_0. Let consider one Fourier component $\frac{1}{2}V_0 e^{iGy}$ of the perturbing potential. Other component gives rise to the same contribution.

Matrix element of the perturbing potential is

$$\begin{aligned}V_{N,k_z,k_y,f} &= \int dx\,\phi_N^*(x)\,\phi_{N'}(x+G/s)\,L_y^{-1}\int dy\,e^{i(k_y-k_y')y}\,\frac{1}{2}V_0 e^{iGy}\,\delta_{k_z,k_z'} \\ &= f_{NN'}(\xi)\,\frac{1}{2}V_0\,\delta_{k_y',k_y+G}\,\delta_{k_z,k_z'}, \qquad (12.100)\end{aligned}$$

where

$$\begin{aligned}f_{NN'}(\xi) &\equiv \int_{-\infty}^{\infty} dx\,\phi_N(x)\,\phi_{N'}(x+G/s), \\ \xi &= G^2/2s = \hbar^2G^2/2m\hbar\omega_0. \qquad (12.101)\end{aligned}$$

$\sum_f \cdots$ includes $\sum_{N'}\cdots$. In the case of $N' \gg 1$, we may replace this summation by $\int dE\,(dN'/dE) = \int dE/\hbar\omega_0$, and integrate out the δ-function. (12.99) then becomes

$$W = \frac{2\pi}{\hbar}\, 2\,|V_{N,k_z,k_y',\,N,k_z,k_y'}|^2 (\hbar\omega_0)^{-1}. \qquad (12.102)$$

and f_{NN} is given by

$$f_{NN}(\xi) \equiv \int_{-\infty}^{\infty} dx\, \phi_N(x)\,\phi_N(x+G/s) = \exp\left(-\frac{1}{2}\xi\right) L_N(\xi), \qquad (12.103)$$

where L_N is the Laguerre polynomial of n-th order. Therefore,

$$W/\omega_0 = (\pi^{1/2} V_0/\hbar\omega_0)^2\,|f_{NN}(\hbar^2 G^2/2m\hbar\omega_0)|^2. \qquad (12.104)$$

Asymptotic formula of f_{NN} $(N \gg 1)$ is given by

$$f_{NN}(\xi) \xrightarrow[N\to\infty]{} (-1)^N (\pi N \sin 2\phi)^{-1/2} \sin\left[N(2\phi - \sin 2\phi) + \pi/4\right], \qquad (12.105)$$

where

$$\xi = 4N\cos^2\phi. \qquad (12.106)$$

Angle ϕ has the following meaning. From (12.101) and (12.106) we have

$$\hbar^2 G^2/8m = N\hbar\omega_0 \cos^2\phi = E_\perp \cos^2\phi,$$

where $E_\perp = N\hbar\omega_0 = E_F - \hbar^2 k_z^2/2m$. Then, ϕ is the angle shown in Fig. 12.7. Since the asymptotic formula (12.105) is only valid for the case in which two classical orbits with different centers overlap, then we shall consider only electron "orbits in k-space" which intersect the Brillouin zone boundary, so that (12.101) is appropriate.

Substituting (12.105) into (12.104), one obtains

$$W/\omega_0 = (V_0/\hbar\omega_0)^2 (N\sin 2\phi)^{-1} \sin^2[N(2\phi - \sin 2\phi) + \pi/4] . \qquad (12.107)$$

We are interested in the semiclassical case ($N \gg 1$). Then, we must average (12.107) over the orbits which participate in MB. Though the portion of the Fermi surface related to MB is a small part, it involves a large number of different quantum levels.

With $N \gg 1$ and $\Delta N/N \ll 1$, we obtain

$$\left\langle N^{-1} \sin^2[N(2\phi - \sin\phi) + \pi/4] \right\rangle_{\text{average}} = \frac{1}{2} N^{-1} . \qquad (12.108)$$

Thus, we get the average transition probability per cyclotron period :

$$\overline{W}/\omega_0 = E_g^2/2E_\perp \hbar\omega_0 \sin 2\phi , \qquad (12.109)$$

where $E_g = V_0$ is the band gap at the Brillouin zone boundary and $E_\perp = N\hbar\omega_c$.

The unperturbed state in the present calculation is represented by Fig. 12.8 (c), which corresponds to the free electron case. If (12.109) is much smaller than unity, electrons continue the cyclotron motion and they do not feel the presence of the band gap E_g. On the other hand, if

$$E_g^2/2E_\perp \hbar\omega_0 \sin 2\phi \gg 1 , \qquad (12.110)$$

MB does not appear. Since $E_\perp \sim E_F$, we obtain the condition f MB (12.96).

Until now we focused our attentions to the case in which the periodic potential is perpendicular to the magnetic field. However, other configurations are also of experimental interest, we consider the case where the periodic potential makes an angle α with the field direction. In this case the perturbing potential $\frac{1}{2} V_0 e^{i\mathbb{G}\mathbb{r}}$ induces the transitions $k_z k_y N \rightarrow k_z' k_y' N'$, where $k_z' = k_z + G_z$ and $k_y' = k_y + G_y$. The calculation can be carried out essentially as before.

If α is very small, then all of the "orbits" involved in MB have essentially the same N, and the angle ϕ is close to $\pi/2$. Since $\sin\alpha = G_y/G$ and $\cos\phi = \hbar G_y/\sqrt{8mE_\perp}$. We obtain

$$\overline{W}/\omega_0 = E_g^2/2E_\perp \hbar\omega_c\left(\hbar G/\sqrt{2mE_\perp}\right)\sin\alpha, \quad (\alpha \ll 1). \qquad (12.111)$$

A semiclassical approach for calculating the galvanomagnetic tensor with magnetic breakdown will be presented in Chapter 15.

Chapter 13 Surface and Size Effects, Electron-Sound Wave Interaction

High frequency electromagnetic wave propagating perpendiculary to the metal surface, is screened by mobile carriers and the amplitude of the wave remains finite only in the small region close to the surface. This is the phenomenon called "skin effect." Penerating distance δ of the wave is called "skin depth." As will be given in Section 13.2, δ is expressed by

$$\delta = c(2\pi\omega\sigma)^{-1/2}. \tag{13.1}$$

In pure specimen mean free path of the electrons l at enough low temperatures will satisfy the condition:

$$l \gg \delta . \tag{13.2}$$

In this case the assumption that the electric field may be regarded as spatially constant cannot be valid and the spatial variation of the electric field must then be taken into account. Local relation $j(r) = \sigma \mathcal{E}(r)$ is no longer correct but the following non-local relation should be employed:

$$\mathbf{j}(\mathbf{r}) = \int \Sigma(\mathbf{r}-\mathbf{r}')\,\mathcal{E}(\mathbf{r}')\,d\mathbf{r}'. \tag{13.3}$$

The region $l \gg \delta$ is called the region of the anomalous skin effect. A long mean free path has a profound effect on the propagation characteristics of the medium. Azbel'-Kaner cyclotron resonance is closely related to the anomalous skin effect. The geometry in the cyclotron resonance experiment in metals is as follows. The static field **H** lies in the plane of the sample ; the rf electric field also lies in the plane of the surface and may be either parallel or perpendicular to **H**. If the relaxation time is sufficiently long, the carriers spiral about H, going in and out of the rf field localized in the skin depth once each cycle ~~of~~ the cyclotron motion. Resonant absorption of energy will occur if a carriers sees the rf electric field in the same phase every time the carrier is in the thin layer of the skin effect.

This is an example of the non-local effect.

The path integral method suggested by Chambers$^{170)}$ is a powerful tool for dealing with the problems above-mentioned.

The purpose of this Chapter is to discuss the effects related to surface and sample dimension, the ultrasonic attenuation due to electrons and the conduction electron spin resonance.

13.1 Chambers' Theory

Let denote the solution of the Boltzmann equation by $f = f_0 + g$.

Let the relaxation time for electron collision be τ, and assume that the distribution function of electrons immediately after collision corresponds to $g = 0$ (randomization of the velocity).

After their last collision at $P'(r, v, t')$ electrons move along the trajectory T (See Fig. 13.1). The value of the distribution function f at $P(\mathbf{r}.\mathbf{v}.t)$ is found simply by integrating the number scattered into the trajectory at previous points along it with energy $E-\Delta E$, (where ΔE is the energy acquired from the applied fields before reaching $\mathbf{r}$), by multiplying their probability reaching $\mathbf{r}$:

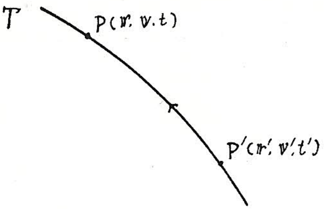


Fig. 13.1 Trajectory of electrons in phase space.

$$f(\mathbf{r}.\mathbf{v}.t) = \int_{-\infty}^{t} (dt'/\tau)\, f_0(E-\Delta E)\, e^{-(t-t')/\tau}, \tag{13.4}$$

where E is the energy at $P(\mathbf{r}.\mathbf{v}.t)$.

On writing $f_0(E-\Delta E) = f_0(E) - \Delta E\, df_0/dE$ and integrating by parts, we obtain

$$g(\mathbf{r}.\mathbf{v}.t) = -\frac{df_0}{dE}\int_{-\infty}^{t}(dt'/\tau)\,\Delta E\, e^{-(t-t')/\tau} = \frac{df_0}{dE}\int_{-\infty}^{t} dt'\left(\frac{d\Delta E}{dt'}\right) e^{-(t-t')/\tau}. \tag{13.5}$$

$\Delta E\,(t')$ is given by $\Delta E(t') = e\int_{t'}^{t} \mathcal{E}(r.s)\,v(s)\,ds$, where $\mathcal{E}(r.t)$ is the applied electric field (magnetic field, if present, has no direct effect on ΔE, but alter $v(t)$) and $d\Delta E/dt = -e\,\mathcal{E}(r.t)\,v(t)$.

If $\tau = \tau(v) = \tau(t)$, $\exp\{-(t-t')/\tau\}$ should be replaced by $\exp\left\{-\int_{t'}^{t} ds/\tau(s)\right\}$. Thus, $g(\mathbf{r}.\mathbf{v}.t)$ is given by

$$g(\mathbf{r},\mathbf{v}.t) = -\frac{df_0}{dE}\int_{c}^{t} dt'\,(-e)\,\mathcal{E}(r'.t')\,v(r'.t')\exp\left\{-\int_{t'}^{t} dt''/\tau(t'')\right\}. \tag{13.6}$$

Finally, we obtain the expression of the current density 170)

$$j(r.t) = -\frac{2e^2}{(2\pi)^3}\int dk\, v\,\frac{df_0}{dE}\int_c^t dt'\,\mathcal{E}(r'.t')\,v(r'.t')\exp\left\{-\int_{t'}^{t} dt''/\tau(t'')\right\}. \qquad (13.7)$$

(13.7) involves the velocity correlation $v(r.t)\,v(r'.t')$. Then, it may be considered to be a kind of the Kubo-type formula (11.83).

Chambers obtained (13.6) by using the intuitive method mentioned above. However, in view of the generality and usefulness of the result as a starting point for the study of many transport phenomena, it seems worthwhile confirming its validity by showing that is is also an exact solution of the Boltzmann equation 171)

$$\frac{\partial f}{\partial t} + v.\nabla_r f - e\left(\mathcal{E} + \frac{1}{c}v\times H\right).\nabla_p f = -\frac{f-f_0}{\tau(P)}. \qquad (13.8)$$

The lower limit c of the integration over t' in Figs.(13.6) and (13.7) is an integration constant which is determined by the boundary condition.

In (13.6) independent variables are $(t, \mathbf{r}, P, t'. t'')$ and $\mathbf{r}'$ takes the form

$$\mathbf{r}' = \mathbf{r} + \mathbf{G}(T, P), \quad (T = t - t'). \qquad (13.9)$$

$\mathbf{G}$ is a function of P and T.

Therefore,

$$\partial\mathbf{r}'/\partial\mathbf{r} = \mathbf{1} \ \text{ and } \ \partial\mathbf{r}'/\partial t = \partial\mathbf{G}/\partial T, \qquad (13.10)$$

where $\mathbf{1}$ is the unit tensor. Since $\mathbf{r}'$ represents the trajectory of an electron, the function $\mathbf{G}$ is determined by the law of force acting on the electron. Consider an electron with momentum $\mathbf{p}$ arriving at $\mathbf{r}$ at time t, and denote the variation of $(\mathbf{r}.\ \mathbf{p})$ in a time interval δt by $(\delta\mathbf{r}.\ \delta\mathbf{p})$.

From (13.9), we obtain

$$\mathbf{r}' = \mathbf{r} + \mathbf{G}(t-t',\ \mathbf{p}) = \mathbf{r} + \delta\mathbf{r} + \mathbf{G}(t+\delta t - t',\ \mathbf{p}+\delta \mathbf{p}),$$

where $\delta\mathbf{r} = \mathbf{v}(\mathbf{r}.t)\,\delta t$, and $\delta \mathbf{p} = -e\left[\mathcal{E}(\mathbf{r}.t) + \frac{1}{c}\mathbf{v}\times\mathbf{H}\right]\delta t$.

Then,

$$\mathbf{v}(\mathbf{r}, t)\,\delta t + \frac{\partial \mathbf{G}}{\partial T}\,\delta t - e\left[\mathcal{E}(\mathbf{r}.t) + \frac{1}{c}\mathbf{v}\times\mathbf{H}\right]\cdot\frac{\partial \mathbf{G}}{\partial \mathbf{p}}\,\delta t = 0.$$

From (13.9) and (13.10), we obtain

$$\frac{\partial \mathbf{r}'}{\partial t} = -\,\mathbf{v}(\mathbf{r}.t)\cdot\frac{\partial \mathbf{r}'}{\partial \mathbf{r}} + e\left[\mathcal{E}(\mathbf{r}.t) + \frac{1}{c}\mathbf{v}\times\mathbf{H}\right]\cdot\frac{\partial \mathbf{r}'}{\partial \mathbf{p}}. \qquad (13.11)$$

For simplicity, we assume $\tau(\mathbf{p}) =$ constant and replace $\int dt''/\tau(t'')$ by $(t-t')/\tau$. The extension of the proof to the more general case is straightforward.

Thus, by differentiating (13.6) we obtain

$$\frac{\partial g}{\partial t} = -\,\frac{df_0}{dE}(-e)\,\mathcal{E}(\mathbf{r}.t)\,\mathbf{v}(\mathbf{r}.t) - \frac{g}{\tau}$$
$$-\,\frac{df_0}{dE}\int dt'\left\{\frac{\partial \mathbf{r}'}{\partial t}\cdot\frac{\partial}{\partial \mathbf{r}'}\left[-e\,\mathcal{E}(\mathbf{r}'.t')\cdot\mathbf{v}(\mathbf{r}'.t')\right]\exp\left[-(t-t')/\tau\right]. \qquad (13.12)$$

If we make substitution (13.11) in the last term of (13.12), it becomes

$$-\,\mathbf{v}\cdot\frac{\partial g}{\partial \mathbf{r}} + e\left(\mathcal{E} + \frac{1}{c}\mathbf{v}\times\mathbf{H}\right)\cdot\frac{\partial g}{\partial \mathbf{p}}, \qquad (13.13)$$

where we utilized that g depends on $(\mathbf{r}, \mathbf{p})$ only through $\mathbf{r}'$.

In consideration of

$$\frac{\partial f_0}{\partial t} = \frac{\partial f_0}{\partial \mathbf{r}} = 0 , \quad \frac{\partial f_0}{\partial p} = \frac{d f_0}{d E} \mathbf{v} , \quad \frac{\partial f_0}{\partial P}(v \times H) = 0 , \tag{13.14}$$

and by substituting (13.12), (13.13), (13.14) into (13.8), it is readily verified that the Boltzmann equation is satisfied if in (13.6) we neglect the effect of the electric field on the trajectory of an electron.

The path-integral expression for $g(\mathbf{r}, \mathbf{v}, t)$ forms a convenient starting point for the discussion of size effect and skin effect problems.

The major assumption in deriving (13.6) is that every scattering process is 'catastrophic', in the sense that the electron is equally likely to be scattered to any point on the Fermi surface at each collision.172) In the Boltzmann equation this is equivalent to assuming that the collision term can be written in the form $(\partial f_k/\partial t)_{coll} = -g_k/\tau_k$, with a relaxation time τ_k which is independent of the form of g_k.

However, Richards193) pointed out that the path-integral formulation of transport problems is rigorously valid for general scattering in any material for which the Boltzmann equation is valid.

13.2 Normal Skin Effect

Consider a semi-infinite metal sample ($z>0$) in a high frequency electromagnetic field. Let us assume that the wave is incident normal to its surface with $\mathcal{E}$ polarized along the x axis and H along the y axis. By ignoring the displacement current $\dot{D}/4\pi$, the relevant Maxwell's equations are

$$\mathrm{curl}\, H = \frac{4\pi}{c}\, j, \quad \mathrm{curl}\, \mathcal{E} = -\frac{1}{c}\frac{\partial H}{\partial t}. \quad (\mu = 1) \qquad (13.15)$$

We shall assume the usual Ohm's law $j = \sigma \mathcal{E}$ and substituting $\mathcal{E}_x,\ H_y \propto \exp\{i(kz-\omega t)\}$ into (13.15), we obtain

$$\frac{4\pi}{c}\sigma \mathcal{E}_x = -ik\, H_y, \quad ik\, \mathcal{E}_x = \frac{i\omega}{c} H_y. \qquad (13.16)$$

From (13.16)

$$k^2 = \frac{4\pi i\omega}{c^2}\sigma, \qquad (13.17)$$

and

$$k = k_1 + i k_2 = \left(\frac{2\pi\omega\sigma}{c^2}\right)^{1/2}(1+i). \qquad (13.18)$$

Therefore, the electromagnetic wave decays inside metal as $\exp(-k_2 z)$. This is the so-called skin effect and the skin depth δ is

$$\delta = k_2^{-1} = c\,(2\pi\omega\sigma)^{-1/2}. \qquad (13.19)$$

The condition for the local relation $j = \sigma\mathcal{E}$ being valid is given by

$$l \ll \delta. \qquad (13.20)$$

This corresponds to the normal skin effect. As an example we shall estimate δ and l for copper.

Inserting $\omega/2\pi = 1\,\mathrm{GHz}$, $\sigma = 5.85 \times 10^5\,(\Omega\,\mathrm{cm})^{-1}$ at room temperature, we obtain

$$\delta \cong 2 \times 10^{-4}\,\mathrm{cm}, \quad l \doteqdot 3 \times 10^{-6}\,\mathrm{cm}, \quad (l \ll \delta).$$

The observable electrodynamic properties of a metal surface are described completely by the surface impedance Z defined as

$$Z = \mathcal{E}_x(0) \Big/ \int_0^\infty j_x(z)\,dz = R - iX, \qquad (13.21)$$

The real part R of Z is called the surface resistance; R determines the power absorption by the metal. The imaginary part X is called the surface reactance; it determines the frequency shift of a resonant cavity bounded by the metal.

On making use of (13.15) Z is rewritten in the form:

$$Z = R - iX = \mathcal{E}_x(0) \Big/ \left| -\frac{c}{4\pi} H_y(z) \right|_0^\infty = \frac{4\pi}{c} \frac{\mathcal{E}_x(0)}{H_y(0)} = \frac{4\pi i \omega}{c^2} \frac{\mathcal{E}_x(0)}{\mathcal{E}_x'(0)}. \qquad (13.22)$$

From (13.16) and (13.18) the surface impedance in the normal skin effect is

$$\left\{ \begin{aligned} Z &= \frac{4\pi}{c^2} \frac{\omega}{k} = \left(\frac{2\pi\omega}{\sigma c^2} \right)^{1/2} (1 - i), \\ R = X &= \left(\frac{2\pi\omega}{\sigma c^2} \right)^{1/2}. \end{aligned} \right. \qquad (13.23)$$

13.3 Anomalous Skin Effect

The skin depth δ decreases with lowering temperature, while the mean free path l becomes large and then the opposite relation $l \gg \delta$ to (13.20) will be realized at low temperatures. In this case $j-\mathcal{E}$ relationship is expressed by the non-local relation as (13.3) or (13.7).

In the case of high purity copper at the helium temperature we obtain $l \sim 0.1\,\mathrm{cm}$, $\delta \sim 10^{-6}\,\mathrm{cm}$ for $\omega/2\pi = 1\,\mathrm{GHz}$ and accordingly $l \gg \delta$. This is the anomalous skin effect.

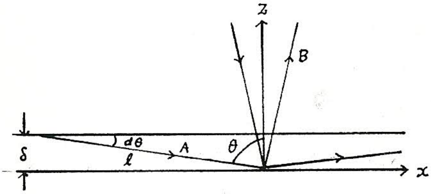


Fig. 13.2 Effective path A and ineffective path B in the anomalous skin effect region.

Electrons moving nearly parallel to the surface (path A in Fig. 13.2) are accerlated by the electric field associated with the electromagnetic wave and can effectively absorb the wave energy. On the other hand electrons which are incident on the surface with large angle (path B), do not have enough time feeling the electromagnetic field and pass by rapidly the skin depth.

Accordingly, effective number of the electrons which contribute to the conduction is given by

$$n_{eff} \sim n\, d\Omega/4\pi \sim n(\delta/l),$$

where $d\Omega \simeq \sin\theta\, d\theta \sim d\theta \sim \delta/l$ (See Fig. 13.2).

The effective conductivity then becomes

$$\sigma_{eff} \sim \sigma(\delta/l). \tag{13.24}$$

By making substitution σ_{eff} in (13.19) instead of σ, the skin depth is given by

$$\delta \simeq (c^2 l/2\pi\omega\sigma)^{1/3}. \tag{13.25}$$

Since (13.22) gives $Z = (4\pi/c^2)(\omega/k)$, $k_1 \sim k_2 \simeq \delta^{-1}$ and (13.25) lead to the surface resistance

$$R \simeq \left(\frac{2\pi\omega}{c^2}\right)^{2/3}\left(\frac{l}{\sigma}\right)^{1/3}. \tag{13.26}$$

(13.24) is the 'ineffectiveness concept' introduced by Pippard.[174)]

Apart from the factor with order one (13.26) is in agreement with the result obtained by the rigorous calculation. In consideration of $\sigma/l \sim ne^2/m v_F$ we find that (13.26) is temperature independent and depends only on the property of the Fermi surface. Pippard carefully analized the variation of surface resistance components of Cu with angle of cut on single crystal and determined the shape of the Fermi surface which is currently accepted.[175)]

In the following we shall present a more detailed theory on the basis of the ineffectiveness concept.[172)] By generalizing (6.20) and (6.28) the conductivity tensor σ_{ij} is given by

$$\sigma_{ij} = \frac{e^2}{4\pi^3 \hbar} \int dS\,(n_i n_j l), \quad (i,j = x.y.z), \qquad (13.27)$$

where the integration is performed over the Fermi surface and $n_i = v_i/v$, $n_j = v_j/v$. In Fig. 13.3 the surface element dS specified by the principal radii of curvature R_1, R_2 is shown. The normal n to the surface element dS is parallel to the velocity v. As already mentioned, dS effectively contributes to the surface impedance if n is nearly to the sample surface.

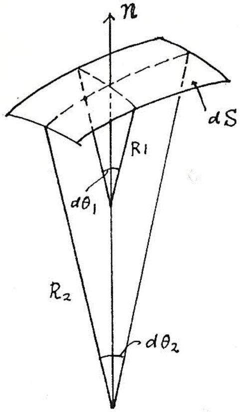


Fig. 13.3 Surface element dS and principal radii of curvature of the Fermi surface.

From Fig. 13.3 the surface element is

$$dS = R_1 R_2\, d\theta_1 d\theta_2 .$$

Consider the polar coordinate (θ, φ) with polar axis n and θ_1 is measured in the plane $\varphi =$ constant. Then, we have $d\theta_1 = d\theta$, $d\theta_2 = \sin\theta\, d\varphi$ and

$$dS = R_1 R_2\, d\Omega = \frac{d\Omega}{K(\theta.\varphi)}, \quad (d\Omega = \sin\theta\, d\theta\, d\varphi), \qquad (13.28)$$

where $K(\theta.\varphi)$ is the so-called Gaussian curvature of the surface. Since we are interested in the effective electrons, we can put $K(\theta, \varphi) \doteqdot K(\frac{1}{2}\pi, \varphi)$. In the coordinate system of Fig. 13.2 the velocity components are $v_x = v\sin\theta\cos\varphi$, $v_y = v\sin\theta\sin\varphi$, $v_z = v\cos\theta$. Consider the electrons with θ lying in the region $\pi/2 - (\beta/2)/al < \theta < \pi/2 + (\beta/2)/al$, where a is defined by $\mathcal{E}(z) = \mathcal{E}(0)\,e^{-az}$. β is an adjustable paramter of order unity and called the fudge factor.

Substituting $d\Omega = (\beta/al)\,d\varphi$ into (13.27), we obtain

$$\sigma_{ij,\mathrm{eff}} = \frac{e^2}{4\pi^3\hbar}\,\frac{\beta}{a}\oint d\varphi\, n_i n_j \sum K^{-1}(\tfrac{1}{2}\pi,\varphi), \tag{13.29}$$

where $n_x = \cos\varphi$, $n_y = \sin\varphi$. Unless the Fermi surface is a single closed convex surface, there may be several different points on it at which v has the same direction $(\theta.\varphi)$. $\sum$ in (13.29) means the summation over all such points.

The Maxwell's equation yield

$$a_x^2\,\mathcal{E}_x(z) = -\frac{4\pi i\omega}{c^2}\,\sigma_{xx,\mathrm{eff}}\,\mathcal{E}_x(z). \tag{13.30}$$

Combining with (13.29),

$$a_x^3 = -i\beta S_{xx}^3/\pi, \tag{13.31}$$

where

$$S_{xx}^3 = \frac{e^2\omega}{c^2\pi\hbar}\oint d\varphi\cos^2\varphi\sum K^{-1}(\tfrac{1}{2}\pi,\varphi),\quad S_{yy}^3 = \frac{e^2\omega}{c^2\pi\hbar}\oint d\varphi\sin^2\varphi\sum K^{-1}(\tfrac{1}{2}\pi,\varphi). \tag{13.32}$$

Since $\mathcal{E}_x(0)/\mathcal{E}_x'(0) = -1/a_x$, (13.22) leads to

$$Z_{xx} = -\frac{4\pi i\omega}{c^2\gamma_x} = \frac{4\pi\omega}{c^2}\left(\frac{\pi}{\beta}\right)^{1/3} S_{xx}^{-1}\,e^{-\pi i/3}. \tag{13.33}$$

Similarly, Z_{yy} is obtained. The surface impedance is determined by the Gaussian curvature of the Fermi surface at which the velocity is nearly parallel to the sample surface. By choosing an appropriate value for β we can obtain the same result as the rigorous one.

In the extreme anomalous skin effect ($\delta \ll l$), we can obtain exact formulas for the impedance in the case of purely specular and completely diffuse scattering of electrons by the surface.[176] It is shown that the nature of the reflection has little effect on the impedance: in the diffuse scattering case $\beta = 8\pi/3\sqrt{3}$, whereas in the specular reflection case $\beta = (8\pi/3\sqrt{3}) \times 8/9$. In the following we shall treat the specular reflection case.

Since the sample is bounded by $z = 0$, the Maxwell's equation

$$\frac{d^2 \mathcal{E}_x}{d z^2} = -\frac{4\pi i \omega}{c^2} j_x , \qquad (13.34)$$

should be modified by introducing the boundary condition. For the mathematical convenience we consider the sample extended from $z = -\infty$ to $z = +\infty$. The electric field $\mathcal{E}(z)$ then has a mirror symmetry as shown in Fig. 13.4. Therefore, $d\mathcal{E}_x/dz$ exhibits a discontinuous jump at $z = 0$. In consideration of this point, (13.34) is modified as follows:

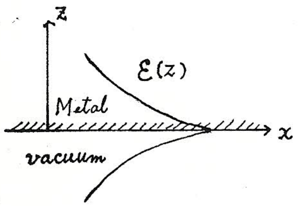


Fig. 13.4 Form of the electric field in the case of specular reflection.

$$\frac{d^2 \mathcal{E}_x}{d z^2} = -\frac{4\pi i \omega}{c^2} j_x + 2\left(\frac{d \mathcal{E}_x}{d z}\right)_{+0} \delta(z) . \qquad (13.35)$$

This modification is equivalent to the existence of the current sheet $i c^2 \mathcal{E}_x'(0)\,\delta(z)/2\pi\omega$ on the metal surface $\left(\mathcal{E}_x'(0) = (d\mathcal{E}_x/dz)_{+0}\right)$.

By expanding $\mathcal{E}_x$, j_x into the Fourier integrals

$$\mathcal{E}_x = \int_{-\infty}^{+\infty} \mathcal{E}_x(q)\, e^{-iqz}\, dq , \quad j_x = \int_{-\infty}^{+\infty} j_x(q)\, e^{-iqz}\, dq , \qquad (13.36)$$

we obtain from (13.35)

$$\left[q^2 - \frac{4\pi i \omega}{c^2} \sigma_{xx}(q) \right] \mathcal{E}_x(q) = -\frac{\mathcal{E}_x'(0)}{\pi} , \qquad (13.37)$$

where $j_x(q) = \sigma_{xx}(q)\,\mathcal{E}_x(q)$. From (13.36) and (13.37) the surface impedance is given by

$$Z_{xx} = \frac{4\pi i \omega}{c^2} \frac{\mathcal{E}_x(0)}{\mathcal{E}_x'(0)} = -\frac{4 i \omega}{c^2} \int_{-\infty}^{+\infty} \frac{dq}{q^2 - \frac{4\pi i \omega}{c^2} \sigma_{xx}(q)} . \qquad (13.38)$$

In the next place we must calculate $\sigma_{xx}(q)$. In the abscence of a magnetic field $\mathbf{v}$ and τ are both time-independent. Then, we can put $\mathbf{r}' = \mathbf{r} - \mathbf{v}(t-t')$ in (13.6). In the presence of an electric field $\mathcal{E}(\mathbf{r}, t) = \mathcal{E}(q)\, e^{i(\omega t - \mathbf{q}\mathbf{r})}$, $\mathcal{E}(\mathbf{r}', t')$ is related to $\mathcal{E}(\mathbf{r}, t)$ by

$$\mathcal{E}(\mathbf{r}', t') = \mathcal{E}(\mathbf{r}, t) \exp\left\{ i(\omega - \mathbf{q}\mathbf{v})(t' - t) \right\} . \qquad (13.39)$$

Hence, (13.6) becomes

$$g(r, v, t) = e \frac{df_0}{dE} \frac{v \mathcal{E}(r,t) \tau}{1 + i(\omega - q \cdot v)\tau} . \qquad (13.40)$$

If the condition of $\omega\tau \gg 1$ or $ql \gg 1$ holds, g becomes smaller than the d.c.-value $e(df_0/dE) v \cdot \mathcal{E} \tau$. The electrons move through a rapidly varying field in the course of one mean free path, and absorb little net energy from the electromagnetic field. However, the electrons with the velocity v given by $\omega \cong q v$ significantly contribute to the electric current (surf-riding effect). If $\omega/q \ll v$ the condition $\omega \cong q v$ is essentially equivalent to $q \cdot v \cong 0$. This means that the electrons effectively contribute to the current move along the direction perpendicular to the wave propagation vector. By following the same procedures employed in getting (13.29), we obtain

$$\sigma_{ij}(q) = \frac{e^2}{4\pi^3 \hbar} \oint d\varphi \int_0^{\pi} \frac{d\theta \sin\theta \, n_i n_j}{K(\theta, \varphi)} \frac{v\tau}{1 + i(\omega - q v \cos\theta)\tau} . \qquad (13.41)$$

If $ql \gg |1 + i\omega\tau|$, the major contribution to the integral over θ comes from $\theta \cong \pi/2$. Then, we can put $K(\theta, \varphi) \cong K(\frac{1}{2}\pi, \varphi)$, $n_x \cong \cos\varphi$ and $n_y \cong \sin\varphi$. By integrating over θ, (13.41) becomes

$$\sigma_{ij}(q) = \frac{e^2}{4\pi^2 \hbar |q|} \oint d\varphi \, n_i n_j \sum K^{-1}(\tfrac{1}{2}\pi, \varphi) . \qquad (13.42)$$

Accordingly,

$$\sigma_{xx}(q) = c^2 S_{xx}{}^3 / 4\pi\omega|q|, \quad \sigma_{yy}(q) = c^2 S_{yy}{}^3 / 4\pi\omega|q|. \qquad (13.43)$$

On making substitution (13.43) into (13.38), the surface impedance takes the form:

$$Z_{xx} = \frac{16\pi\omega e^{-\pi i/3}}{3^{3/2}\, c^2 S_{xx}}, \qquad (13.44)$$

where the following formula is employed:

$$\int_0^\infty \frac{x\,dx}{x^3 - ia} = \frac{2\pi e^{\pi i/6}}{3^{3/2}\, a^{1/3}}. \qquad (13.45)$$

If the energy is given by $E_k = \hbar^2 k^2/2m$, the surface impedance is given by[176)]

$$Z = \frac{8}{9}\left(3^{1/2}\pi\omega^2 l/c^4\sigma\right)^{1/3}(1 - i\sqrt{3}), \quad (\sigma = ne^2 l/mv_F), \qquad (13.46)$$

which is in agreement with (13.44). In the diffuse scattering case 8/9 should be replaced by unity.

In closing this Section we shall summarize the main results in the anomalous skin effect.

(1). $Z \propto \omega^{2/3}$,

(2). $X = \sqrt{3}\, R$,

(3). Z is independent of temperature and is only determined by the shape of the Fermi surface.

13.4 Azbel'-Kaner Cyclotron Resonance

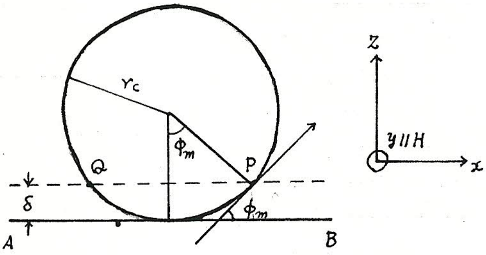


Fig. 13.5 Orbit of an electron through the skin depth at the surface AB. magnetic field is parallel to the y-axis pointing into the plane of the paper.

Azbel' and Kaner(177) have shown that a cyclotron resonance phenomenon is possible in a metal under extreme anomalous skin effect conditions when the magnetic field is parallel to the metal surface.

This resonance is somewhat different from the cyclotron resonance in semiconductors in that a resonance is in general expected when the oscillating electric field $\mathcal{E}$ is parallel to H as well as when it is perpendicular (See Fig. 13.5). Under the anomalous skin effect conditions the skin depth is usually two orders of magnitude smaller than the rdius of carrier orbits ($r_c \gg \delta$). During each cyclotron period an electron interacts with the rf field for a time short compared with either the cyclotron period or the rf period. Thus, additional subsidiary resonances are expected to occur if $\omega = n\omega_0$ $(n = 1, 2, \cdots)$ is satisfied, where $\omega_0 = eH/m^*c$. Hence, resonances observed at constant ω will appear at a field $H = m^* c\omega/e$ and also at fields H/n.

By putting $\tau(t'') = \tau$ and $df_0/dE = -\delta(E - \zeta)$ in (13.7), α- component of the electric current is given by

$$j_\alpha(r,t) = \frac{2e^2}{(2\pi)^3\hbar}\int\frac{dS}{v}\,v_\alpha\int_c^t v(r',t')\cdot\mathcal{E}(r',t')\exp[-(t-t')/\tau]\,dt', \qquad (13.47)$$

where dS means the integral over the Fermi surface. Magnetic field is included in (13.47) through the electron trajectory.

If we assume that an electron undergoes diffuse scattering by the surface, the limit of integration c is the latest time prior to t that the trajectory cuts the surface.

In Fig. 13.5

$$\delta = r_c - r_c\cos\phi_m\,, \quad \delta \cong r_c\,\phi_m^2\,. \quad \phi_m \cong (\delta/r_c)^{1/2}. \qquad (13.48)$$

The time spent by an electron within the skin depth is roughly given by $2r_c\phi_m/v_x$. During this time interval $\mathcal{E}$ and v almost remain constant. Every revolution the electron returns to the skin depth, and the integrand in (13.47) changes by a factor

$$e^{-W} = \exp\left[-\frac{2\pi}{\omega_0\tau} - i\,\frac{2\pi\omega}{\omega_0}\right], \qquad (13.49)$$

so that the t' integration can be approximated by

$$\frac{2r_c\phi_m}{v_x}\,v\cdot\mathcal{E}\,(1+e^{-W}+e^{-2W}+\cdots) = \frac{2r_c\,\phi_m\,v\cdot\mathcal{E}}{v_x(1-e^{-W})}. \qquad (13.50)$$

Using (13.28), we obtain $\int dS\cdots = \int d\Omega/K(\theta,\varphi)\cdots$, where θ is measured from the polar axis z in Fig. 13.5.

Since the integration over θ is given by

$$\int_{\pi/2-\phi_m}^{\pi/2} \sin\theta \, d\theta \doteqdot \phi_m ,$$

j_α takes the form

$$j_\alpha \cong \frac{2e^2}{(2\pi)^3\hbar} \int_0^{2\pi} d\varphi \, \frac{2 r_c \phi_m \, v \cdot \mathcal{E}}{v_x \, (1-e^{-W})} \, \frac{\phi_m \, v_\alpha}{v K(\pi/2 . \varphi)} . \qquad (13.51)$$

We obtain the conductivity tensor $\sigma_{\alpha\beta}$, using (13.48)

$$\sigma_{\alpha\beta} \cong \frac{2e^2}{(2\pi)^3\hbar} \int_0^{2\pi} d\varphi \, \frac{\delta}{1-e^{-W}} \, \frac{n_\alpha n_\beta}{K(\pi/2 . \varphi)} , \quad (n_\alpha = v_\alpha/v) . \qquad (13.52)$$

Aside from a factor of order one and $(1-e^{-W})^{-1}$, (13.52) is equal to (13.42) if δ is replaced by $|\delta|^{-1}$. Considering (13.43) and (13.44) and multiplying a factor 9/8 corresponding to the diffuse scattering, we obtain the expression of the surface impedance :

$$Z_{\alpha\beta} = (1-i\sqrt{3})\sqrt{3}\, \pi^{4/3} \omega^{2/3} c^{-4/3} e^{-2/3} \hbar^{1/3} (B_{\alpha\beta})^{-1/3} , \qquad (13.53)$$

$$B_{\alpha\beta} = \int_0^{2\pi} d\varphi \, \frac{n_\alpha n_\beta}{K(\pi/2 . \varphi)} \, \frac{1}{1-e^{-W(\varphi)}} .$$

If $\omega_c \tau \gg 1$, $1-e^{-W} \cong 1-e^{-2\pi i \omega/\omega_0}$ and then, the resonance condition becomes $\omega = n\omega_0$. In general ω_0 depends on φ and so we should be careful in treating the integral over φ.[178)]

The cyclotron mass m^* is given by

$$\omega_0 = \frac{eH}{m^* c}\ , \quad m^* = \frac{\hbar^2}{2\pi}\left[\frac{\partial S(k_H, E)}{\partial E}\right]_{E=\zeta}\ , \qquad (13.54)$$

where $S(k_H, E)$ is the cross sectional area of the constant energy surface at $k_z = k_H$ ($H \parallel z$-axis). (See Appendix 13).

The main contribution to the integral in (13.53) comes from values of φ around φ_0 at which m^* takes extremum value.

In actual experiments, the frequency ω is fixed, and H is varied. Suppose that the resonance condition

$$\omega = n\omega_0(\varphi_0) \qquad (13.55)$$

is satisfied at $H = H_n$. Then, the resonance condion for $\varphi \simeq \varphi_0$ and $H \simeq H_n$ becomes

$$\omega_0(\varphi) \cong (\omega/n)\,[\,1+ \qquad + a(\varphi-\varphi_0)^2\,]\ , \qquad (13.56)$$

where $\quad \Delta = (H - H_n)/H_n, \ a \sim 1.$

a is negative if m^* takes a maximum value at φ_0, while a is positive if m^* becomes minimum. We can expand $1 - e^{-W}$ in powers of Δ, $(\varphi-\varphi_0)^2$ and $(\omega_0\tau)^{-1}$, using $W(\varphi) \cong -2\pi i\, n$ and $\omega_0\tau \gg 1$:

$$1 - e^{-W} \cong \frac{2\pi n}{\omega\tau} - 2\pi i n\Delta - 2\pi i n a(\varphi-\varphi_0)^2 . \qquad (13.57)$$

Thus, $B_{\alpha\beta}$ is written as

$$B_{\alpha\beta} \cong - \frac{n_\alpha(\varphi_0)\, n_\beta(\varphi_0)}{K(\pi/2, \varphi_0)} \int_{-\infty}^{\infty} \frac{dx}{2\pi i\, n a \left(x^2 + \frac{\Delta}{a} + \frac{i}{a\omega\tau}\right)} . \qquad (13.58)$$

In general there are several points of φ_0 at which m^* becomes extremum. Fig. 13.6 illustrates an example in which two extremum points φ_1 and φ_2 are found. In this case we must replace

$n_\alpha n_\beta / K$ by

$$\frac{n_\alpha(\varphi_1)\, n_\beta(\varphi_1)}{K(\pi/2, \varphi_1)} + \frac{n_\alpha(\varphi_2)\, n_\beta(\varphi_2)}{K(\pi/2, \varphi_2)}$$

$$\equiv - B_{\alpha\beta}^{(0)} . \qquad (13.59)$$

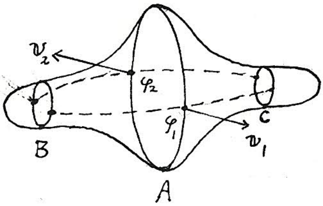


Fig. 13.6 Three cross sections of the Fermi surface are normal to the magnetic field. Velocities v_1 at φ_1 and v_2 at φ_2 are parallel to the metal surface.

Let consider the case of $|\Delta| \gg \omega\tau$. According to i) $a > 0$ and ii) $a < 0$, $B_{\alpha\beta}$ are expressed as follows ;

i) $a > 0$:

$$B_{\alpha\beta} \cong B_{\alpha\beta}^{(0)} \begin{cases} -i/[2n(\Delta a)^{1/2}] & : \Delta > 0 , \\ 1/[2n(|\Delta| a)^{1/2}] & : \Delta < 0 . \end{cases} \qquad (13.60)$$

ii) $a < 0$:

$$B_{\alpha\beta} \cong B_{\alpha\beta}^{(0)} \begin{cases} 1/[2n(\Delta |a|)^{1/2}] & : \Delta > 0 , \\ i/[2n(\Delta a)^{1/2}] & : \Delta < 0 . \end{cases} \qquad (13.61)$$

The above results indicate that the surface impedance behaves differently according to the sign of a being positive or negative.

(13.53), (13.60) and (13.61) lead to $Z_{\alpha\beta} \propto n^{1/3} |\Delta|^{1/6}$.

dZ/dH is more sensitive to H than Z. Since dZ/dH is proportional to $n^{1/3}|\Delta|^{-5/6}/H_n$, it exhibits a peak with $\Delta \to 0$. and the peak height is proportional to $n^{1/3}(\omega\tau)^{5/6}/H_n$.

Absorption derivative curves (dR/dH) for various $\omega\tau$ are shown in Fig. 13.7,[179] where

$$H_c = \omega m^* c/e. \qquad (13.62)$$

With $\tau \to \infty$, dR/dH exhibits maxima at $nH = H_c$ ($n = 1.2, \cdots$).

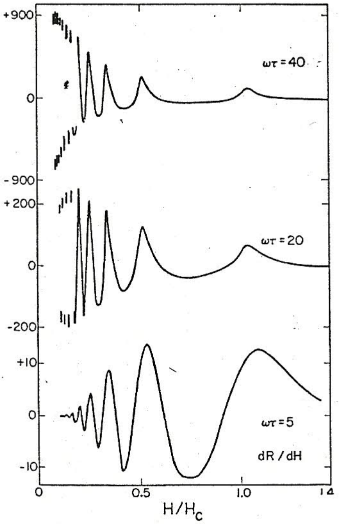
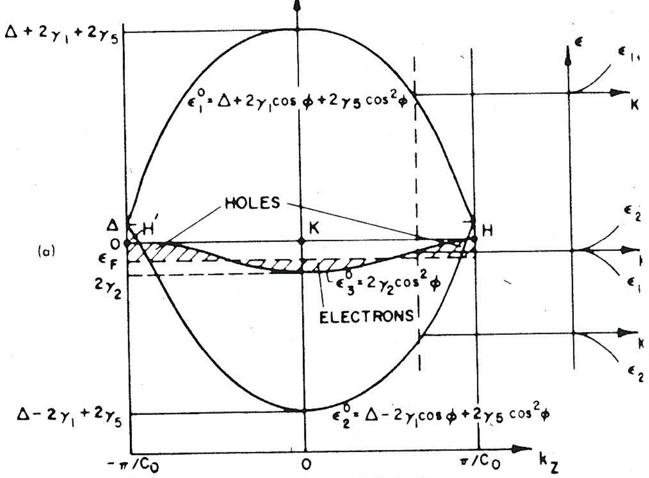


Fig. 13.7 Calculated absorption derivate curves (dR/dH) for finite relaxation times as indicated. Ordinate in arbitrary units.[179]


(a)
Δ + 2γ₁ + 2γ₅
ε₁⁰ = Δ + 2γ₁cos φ + 2γ₅ cos²φ
HOLES
Δ
H′
K
H
0
ε_F
2γ₂
ε₃⁰ = 2γ₂cos²φ
ELECTRONS
Δ − 2γ₁ + 2γ₅
ε₂⁰ = Δ − 2γ₁cos φ + 2γ₅ cos²φ
−π/C₀
0
π/C₀
k_z
ε
ε₁
K
ε₂
ε₁
K
ε₂

13.5 Surface State induced by Magnetic Field

Sharp oscillatory surface impedance in weak magnetic field was observed in metals and semimetals. Fig. 13.8 presents an example observed in bismuth. 180)

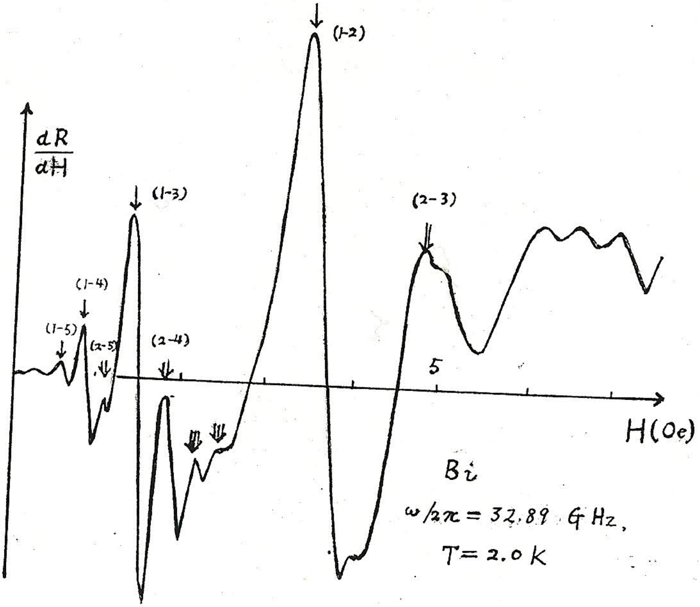


Fig. 13.8 Oscillations of the surface impedance of bismuth. 180)
Structures observed in the region $H > 5$ Oe are due to the Azbel'-Kaner resonance. Peaks for $H < 5$ Oe are induced by the transitions between the magnetic surface levels. H is applied parallel to the binary axis and the sample surface is tilted 56° from the trigonal axis to the binary axis direction. Explanation of this Figure will be given in the text.

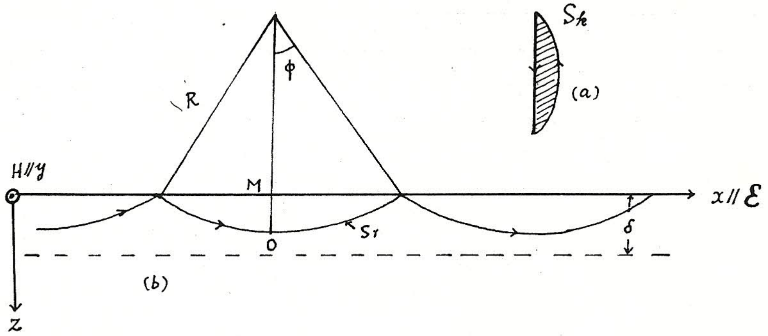


Fig. 13.9 Trajectory of an electron skipping over a reflecting metal surface in a weak magnetic field H. a: in momentum space, b: in coordinate space.

It was recognized that these oscillations come from the electrons skipping along arcs of small curvature ending on the metal surface as shown in Fig. 13.9. The spectrum of these states exhibits the oscillatory behavior of the surface impedance on the magnetic field strength due to resonance absorption of microwave quanta.(81)

Analysis of the magnetic field induced surface states provides a useful method for studying the velocity and relaxatime of electrons on the Fermi surface.

If the wavelength of an electron associated with the motion normal to the surface, is sufficiently larger than the average dimension of surface inhomogeneities, it is expected that the electron undergoes the specular reflection at the metal surface. This situation is realized if the relevant electrons move at a small angle at the surface. Since the motion of an electron travelling along a skipping trajectory is periodic in the direction normal to the surface, it must be quantized and quantum transitions between these levels, accompanied by absorption of photons, are possible. Although the physics is similar to that of cyclotron resonance, there is a big difference. In cyclotron resonance relevant number of the Landau levels is very large ($\hbar\omega_0 \ll \zeta$). It allows us to treat it as a quasi classical problem. In the case of resonant absorption by the skipping electrons one deals with transitions between the levels with small quantum numbers and it is necessary to calculate the energy levels quantummechanically.

In k-space the trajectory shown in Fig. 13.9 corresponds to the closed orbit represented by the shadea area in Fig 13.9 (a) and its area is given by (See Appendix 13)

$$S_k = \frac{2\pi e H}{\hbar c}\left[n + \gamma(n) \right], \qquad (13.63)$$

where γ depends on n and is restricted to $0 < \gamma < 1$. In the case of $n \gg 1$ (for example, DHVA-effect in Section 11.9) information on γ is unimportant, while in the present case $n \sim 1$, then detailed form of $\gamma(n)$ is essentially important. In the latter part of this Section it will be proved that $\gamma(n) \cong -1/4$.

Let denote $n + \gamma = n - 1/4 = n_1$. In Fig. 13.9 since $\phi \ll 1$, we have

$$z = R(1 - \cos\phi) \cong R\,\phi^2/2, \qquad (13.64)$$

where $z = OM$ and R is related to the radius of curvature in k-space by $R = k_c/s$, $s = eH/\hbar c$. Since z is comparable to the skin depth δ, by putting $k_c \sim k_F$ ϕ is estimated as follows:

$$\phi \sim \left(\frac{\delta}{R}\right)^{1/2} \sim \left(\frac{\delta s}{k_F}\right)^{1/2} = 2.46 \times 10^{-2} << 1 , \tag{13.65}$$

where we employed $H = 2\,\mathrm{Oe}$, $k_F = 5 \times 10^6\,\mathrm{cm}^{-1}$, $\delta = 10^{-4}\,\mathrm{cm}$.

Area of the segment S_r in Fig. 13.9 is given by

$$(2\phi/2\pi)\pi R^2 - R^2 \sin\phi \cos\phi \cong \frac{2}{3} R^2 \phi^3 \cong \frac{4}{3}(2z^3 R)^{1/2} .$$

Area of the segment S_k in k-space is related to S_r by $S_r(eH/\hbar c)^2$, and the Bohr-Sommerfeld quantization rule (13.63) leads to

$$\begin{aligned} S_k(n) &= s^2 \frac{4}{3}(2Z_n^3 R)^{1/2} = 2\pi s\, n_1 , \\ Z_n &= \frac{(9\pi^2)^{1/3}}{2}\left(\frac{\hbar c}{eHk_c}\right)^{1/3} n_1^{2/3} . \end{aligned} \tag{13.66}$$

On making use of the above expression we can obtain the quantized energy levels. Since the velocity v is almost parallel to the sample surface, the Lorentz force is directed along $-z$-axis and its magnitude is given by $-(e/c)\, v_x H$. This is equivalent to introduce an effective potential

$$V(z) = \frac{e}{c} v_x H z , \quad (z > 0) . \tag{13.67}$$

Substituting (13.66) into (13.67), we obtain

$$E_n = \frac{e}{c} v_x H Z_n . \tag{13.68}$$

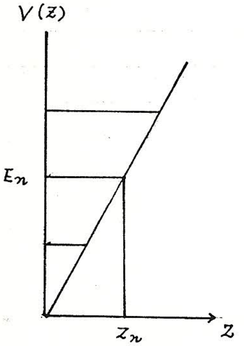


Fig. 13.10 Effective potential energy for an electron trapped in skipping orbit.

Resonance frequency is

$$\omega_{nm} = \frac{E_n - E_m}{\hbar}$$

$$= \frac{(9\pi^2)^{1/3}}{2}\left(\frac{eH}{\hbar c}\right)^{2/3}\frac{v_x}{k_c^{1/3}}\left(n_1^{2/3} - m_1^{2/3}\right). \quad (13.69)$$

In actual experiments ω is fixed and H is varied. Then, from (13.69)

$$H_{nm} = \frac{2^{3/2}}{3\pi}\,\frac{\hbar c}{e}\left(\frac{k_c}{v_x^3}\right)^{1/2}\omega^{3/2}\left(n_1^{2/3} - m_1^{2/3}\right)^{-3/2}. \quad (13.70)$$

The factor $(k_c/v_x^3)^{1/2}$ is associated with the region of the Fermi surface on which v_z is nearly zero. Since it depends on k_H, the observed values H_{nm} are mainly determined by extremal values of k_c/v_x^3. Strong resonance absorption is expected from the portion of the Fermi surface over which k_c/v_x^3 varies little. This is realized if parts of the Fermi surface are cylindrical.

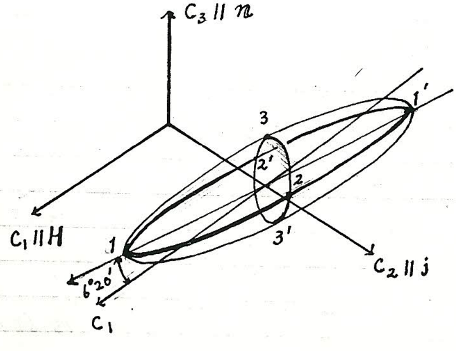


Fig. 13.11 Arrangement of one of three ellipsoids of the electron Fermi surface of bismuth.

C_1 : bisectrix axis, C_2 : binary axis, C_3 : trigonal axis. n : normal to the sample surface, j : microwave current. 1-1, 2-2, 3-3 : principal axes of ellipsoid.

The electrons contributing to the resonant absorption are located at the central cylindrical part of the ellipsoid around the points 2 and 2' in Fig. 13.11.

Let us assume that $n_1 - m_1 = \Delta n \ll n_1$. From (13.70)

$$H \cong \frac{\sqrt{3}}{\pi} \frac{\hbar c}{e} \omega^{3/2} \left(\frac{k_c}{v_x^3} \right)^{1/2} \frac{n_1^{1/2}}{\Delta n^{3/2}} . \tag{13.71}$$

Combining with (13.66), one obtains

$$z_n = \frac{\pi\sqrt{3}}{2} \left(\frac{v_x}{k_c \omega} \right)^{1/2} (n_1 \Delta n)^{1/2} . \tag{13.72}$$

To estimate n_1, we take a following set of parameters :

$z_n \doteqdot \delta = 10^{-4}\,\mathrm{cm}$, $v_x = 10^8\,\mathrm{cm/sec}$, $\omega/2\pi = 10\,\mathrm{GHz}$,
$k_c = 5 \times 10^6\,\mathrm{cm}^{-1}$, $\Delta n = 1$.

Thus, we obtain

$$n_1 \sim 4 . \tag{13.73}$$

Actually, values of n_1 are at most $\lesssim 10$ or 50. In Fig. 13.8 ↓ indicates the resonance series ($n = 1 \rightarrow m = 2, 3. 4, \cdots$), ↓ the series ($n = 2 \rightarrow m = 3. 4, \cdots$), and ⤋ corresponds to ($n = 3 \rightarrow m = 4. 5, \cdots$).

Finally, we shall prove $\gamma = 1/4$ in the following.[182)]

Take the vector potential as $\mathbf{A} = (Hz, 0, 0)$. Hamiltonian becomes

$$\mathcal{H} = \frac{1}{2m} \left(p_x + \frac{e}{c} H z \right)^2 + \frac{p_z^2}{2m} + \frac{p_y^2}{2m} . \tag{13.74}$$

Since p_z is very small and $p_x \cong p_F$ (p_F : Fermi momentum), let denote p_x as

$$p_x = p_F + \delta p_x . \qquad (13.75)$$

By substituting (13.75) into (13.74), we obtain

$$\mathcal{H} = \frac{p_F^2}{2m} + \delta p_x \frac{p_F}{m} + \frac{\delta p_x^2}{2m} + p_F \frac{eHz}{mc} + \delta p_x \frac{eH}{mc} z$$

$$+ \frac{1}{2m}\left(\frac{eHz}{c}\right)^2 + \frac{p_z^2}{2m} + \frac{p_y^2}{2m} . \qquad (13.76)$$

Neglecting the third, fith and sixth terms as small quantities, we obtain

$$\mathcal{H} = \frac{p_F^2}{2m} + \frac{p_y^2}{2m} + \delta p_x v_F + \frac{eH}{c} v_F z + \frac{p_z^2}{2m} , \qquad (13.77)$$

where $p_F = m v_F$.

In (13.77) $p_y^2/2m$ and $\delta p_x v_F$ commute with $\mathcal{H}$ and they can be considered to be c-number.

By introducing a parameter $z(E, p_x, p_y)$ defined by

$$\frac{e}{c} H v_F z(E, p_x, p_y) = E - \frac{p_F^2}{2m} - \frac{p_y^2}{2m} - \delta p_x v_F . \qquad (13.78)$$

the Schrödinger equation $(\mathcal{H} - E)\psi = 0$, $\psi \sim \exp[i(k_x x + k_y y)]\phi(z)$

takes the form

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dz^2} + \frac{eH}{c} v_F (z - z_n) \right] \phi_n(z) = 0 , \qquad (13.79)$$

where n is a suffix associated with the eigenvalue E_n. Accordingly, the energy ε_n measured from the Fermi level is

$$\mathcal{E}_n = \frac{eH}{c} v_F Z_n . \tag{13.80}$$

This is just the same expression as (13.68).

Boundary condition satisfied by ϕ_n is

$$\phi_n(0) = 0. \tag{13.81}$$

Solution of the differential equation (13.79) is called the Airy function. The airy function which disappears at $z \to \infty$ is given by

$$\phi_n(z) = N_n Ai(\zeta - \zeta_n) , (N_n : \text{normalization constant}) , \tag{13.82}$$

where $\zeta \equiv (2eHk_F/c\hbar)^{1/3} z$, $k_F = mv_F/\hbar$.

Since $\phi_n(0) = 0$, ζ_n is the root of $Ai(-\zeta_n) = 0$. $Ai(\zeta - \zeta_n)$ behaves as follows:

$$\begin{cases} \frac{1}{2}\pi^{-1/2} (\zeta - \zeta_n)^{-1/4} \exp\left[-\frac{2}{3}(\zeta - \zeta_n)^{3/2}\right] & : \zeta > \zeta_n , \\ \pi^{-1/2} (\zeta_n - \zeta)^{-1/4} \sin\left[\frac{2}{3}(\zeta_n - \zeta)^{3/2} + \frac{1}{4}\pi\right] & : \zeta < \zeta_n . \end{cases} \tag{13.83}$$

If $|\zeta_n| > 1$, roots of the equation $Ai(-\zeta_n) = 0$ are approximately given by

$$\zeta_n = \left[\frac{3\pi}{2}(n - \gamma)\right]^{2/3}, \ (\gamma = 1/4), \ n = 1, 2, 3, \cdots . \tag{13.84}$$

Hence, (13.66) is verified:

$$Z_n = \frac{(9\pi^2)^{1/3}}{2} \left(\frac{\hbar c}{eHk_F}\right)^{1/3} \left(n - \frac{1}{4}\right)^{2/3}. \tag{13.85}$$

13.6 Electron - Sound Wave Interaction [183)]

Study of the electron - ultrasonic wave interaction is a powerful tool for analysing the electronic structures of solids. Utilizing ultrasonic wave has two meritts : 1) it is possible to study the interaction between electrons and the sound wave whose wave length is much longer than those of the thermal phonons ; 2) we can extract the interaction between electrons and a monochromatic lattice vibration.

In this Section we shall present a general theory of conduction electron - sound wave interaction in the presence of a magnetic field. On the basis of this theory the geometric resonance observed by Bömmel[184)] and the Pippard's theory[185)] on the sound attenuation will be discussed.

Ultrasonic wave exerts two effects on the conduction electrons.

The first is the collision drag effect. Electrons instantaneously follow the motion of the lattice system induced by the ultrasonic wave, and attain to the displaced distribution around the local velocity $u(r.t)$.

Therefore, the collision drag effect is represented by[183)]

$$\left\{ \begin{aligned} &\left(\frac{\partial f}{\partial t}\right)_{coll} = - \frac{f - f_s}{\tau} , \\ &f_s = f_0 (v - u(r.t), E_F (r.t)) , \end{aligned} \right. \tag{13.86}$$

where v denotes the electron velocity and $u(r.t)$ is the velocity field associated with the sound wave. $E_F(r.t)$ represents the

Fermi energy at $(\mathbf{r}, t)$. (13.86) corresponds to the case with free electron mass. In general f_s is expressed by[186]

$$f_s = f_0\left(E(k - m\,u(\mathbf{r},t)/\hbar),\ E_F(\mathbf{r},t)\right) \doteqdot f_0\left(E(k) - m\,\mathbf{v}_k\cdot u(\mathbf{r},t),\ E_F(\mathbf{r},t)\right), \qquad (13.87)$$

where m is the free electron mass of an electron.

The second is the effect of the electric field associated with the sound wave. The sound wave of wave number q and frequency ω manifests itself as a velocity field $u(\mathbf{r},t) \propto \exp[i(q\mathbf{r} - \omega t)]$ in the positive background which has the same density as the electron gas.

The interaction between the acoustic wave and the electrons can be represented partly through the means of a self-consistent internal electromagnetic field and partly by means of a deformation potential.

The self-consistent electromagnetic field is derived from Maxwell's equations as follows.

$$\mathcal{E}_{\parallel} = \frac{4\pi}{i\omega\kappa}\, j_{\parallel}, \quad \mathcal{E}_{\perp} = \frac{(4\pi i/\omega)(v_s/c)^2}{1 - \kappa(v_s/c)^2}\, j_{\perp}, \qquad (13.88)$$

where $\mathcal{E}$ is the electric field and j is the total current density accompanying the sound wave. κ is the dielectric constant of the neutral background. The subscripts $\parallel$ and $\perp$ refer to components parallel and perpendicular to q, respectively, and v_s is the sound velocity.

The total current density $\mathbf{j}$ is composed of two contributions, one is from the electrons, $\mathbf{j}_e$, and one from the positive background, Neu,

$$\mathbf{j} = \mathbf{j}_e + Neu. \qquad (13.89)$$

The Boltzmann equation becomes

$$\frac{\partial f}{\partial t} - e(\mathcal{E}\cdot v)\frac{\partial f_0}{\partial E} - \frac{e}{c}(v\times \mathbb{H})\cdot\nabla_k f + v\cdot\nabla_r f = \left(\frac{\partial f}{\partial t}\right)_{coll}. \qquad (13.90)$$

In semiconductors or semimetals we must take into account the modulation of the energies of the carriers by the passing sound wave in terms of deformation potential energies proportional to the local dilation in the lattice.

In the case of semimetals, the electron and hole energies are then respectively

$$E_e = E_e^{\circ} + D_e\cdot \mathbf{e}, \quad E_h = E_h^{\circ} + D_h\cdot \mathbf{e}, \qquad (13.91)$$

where E_e° and E_h° are the electron and hole energies in the unstrained crystal and $\mathbf{e}$ is the strain associated with the sound wave. D_e and D_h are the deformation potential tensors (See Sections 3.1 and 3.2). Since $\mathbf{e}$ is given by $-\mathbf{q}u/\omega$, additional effective electric fields are

$$\mathcal{E}_d^{(e)} = \frac{\mathbf{q}\,\mathbf{q}}{ie\omega}\cdot D_e\cdot u, \quad \mathcal{E}_d^{(h)} = -\frac{\mathbf{q}\,\mathbf{q}}{ie\omega}\cdot D_h\cdot u. \qquad (13.92)$$

In the case of metals, the corresponding field to (13.92) does not appear and instead of it the modulation of the Fermi level appears. In the following we shall focus our attention to the case of metals.

Solution of (13.90) is given by the Chambers' formula (13.4)

$$f(\mathbf{r}, v, t) = \int_{-\infty}^{t} f_s(\mathbf{r}', v', t')\, e^{-(t-t')/\tau}\, dt'/\tau. \qquad (13.93)$$

It should be noted that (13.93) includes f_s instead of the thermal equilibrium distribution f_0.

Expanding f to first order in $\mathbf{u}$ and quantities proportional to $\mathbf{u}$,

$$f = f_0(\mathbf{v}, E_F^{\circ}) + f_1, \qquad N = N_0 + N_1, \tag{13.94}$$

$$\left\{\begin{aligned} f_1 &= -\frac{\partial f_0}{\partial E}\int_{-\infty}^{t}[\mathbf{v}'\cdot(-e\mathcal{E}' + m\mathbf{u}'/\tau) + \delta E_F'/\tau]\, e^{-(t-t')/\tau}\, dt', \\ \delta E_F' &= E_F(\mathbf{r}', t') - E_F^{\circ} = \left(\frac{\partial E_F}{\partial N}\right)_0 N_1', \end{aligned}\right. \tag{13.95}$$

where $'$ indicates $(\mathbf{r}', t')$. If $E(k) = (\hbar^2/2m)k^2$, we have

$$\delta E_F' = \frac{2}{3} E_F^{\circ}\left(\frac{N_1'}{N_0}\right). \tag{13.96}$$

Hereafter, we employ (13.96). The quantities $\mathcal{E}'$, $\mathbf{u}'$ and N_1' are all proportional to $\exp[i(\mathbf{q}\mathbf{r}' - \omega t')]$ so that f_1 becomes

$$\left\{\begin{aligned} f_1(\mathbf{r}, \mathbf{v}, t) &= -\frac{\partial f_0}{\partial E}\left[\mathbf{J}(\mathbf{v})\cdot\left(\mathcal{E} - \frac{m\mathbf{u}}{e\tau}\right) + \frac{2E_F^{\circ}}{3N_0\tau}K(\mathbf{v})N_1\right], \\ \mathbf{J}(\mathbf{v}) &= -e\int_{-\infty}^{t}\mathbf{v}'\exp\{i[\mathbf{q}(\mathbf{r}'-\mathbf{r}) - \omega(t'-t)] - (t-t')/\tau\}\, dt', \\ K(\mathbf{v}) &= \int_{-\infty}^{t}\exp\{i[\mathbf{q}(\mathbf{r}'-\mathbf{r}) - \omega(t'-t)] - (t-t')/\tau\}\, dt'. \end{aligned}\right. \tag{13.97}$$

By substituting (13.97) into $\mathbf{j}_e = -e\sum_{\mathbf{v}}\mathbf{v} f_1(\mathbf{r}, \mathbf{v}, t)$, we obtain

$$\mathbf{j}_e = \boldsymbol{\sigma}\cdot(\mathcal{E} - m\mathbf{u}/e\tau) - \mathbf{R}N_1 e v_s, \tag{13.98}$$

$$\boldsymbol{\sigma} = \sum_{\mathbf{v}}(-e\mathbf{v})\cdot\mathbf{J}(\mathbf{v})\left(-\frac{\partial f_0}{\partial E}\right), \quad \mathbf{R} = \frac{2E_F^{\circ}}{3N_0\tau v_s}\sum_{\mathbf{v}}\mathbf{v}K(\mathbf{v})\left(-\frac{\partial f_0}{\partial E}\right). \tag{13.99}$$

$\sigma\cdot(-mu/e\tau)$ is the collision-drag term and $-\mathbf{R}N_1 e v_s$ denotes the diffusion term accompanied by the electron density deviation from the thermal equilibrium value.

(13.98) and (13.99) give the non-local expressions of the electric current and conductivity. After integration over t', we obtain

$$i\,\mathbf{J}\cdot\mathbf{q} = -e\left\{1-[(1-i\omega\tau)/\tau]K\right\}. \qquad (13.100)$$

From (13.100) we can derive a useful relation between σ and $\mathbf{R}$,

$$i\,\sigma\cdot\mathbf{q} = -[3N_0 e^2 v_s(1-i\omega\tau)/2E_F^0]\cdot\mathbf{R}. \qquad (13.101)$$

Let rewrite (13.98). From the equation of continuity $-e\,\partial N_1/\partial t + \mathrm{div}\,\mathbf{j}_e = 0$, N_1 is expressed by

$$N_1 = -\mathbf{j}_e\,\mathbf{q}/e\omega = j_{e\parallel}/e v_s. \qquad (13.102)$$

Defining a tensor $\tilde{\mathbf{R}}$ by

$$\mathbf{R}\,j_{e\parallel} = \tilde{\mathbf{R}}\,\mathbf{j}_e, \qquad (13.103)$$

we obtain

$$\tilde{R}_{ij} = R_i\,\delta_{ij}, \qquad (13.104)$$

where we consider the configuration of $\mathbf{q}\parallel$ 1-axis and H in the 1-2 plane. By substituting (13.102) and (13.103) into (13.98), we can rewrite $\mathbf{j}_e$ and σ as

$$\mathbf{j}_e = \sigma_0\,\sigma'\cdot(\mathcal{E} - mu/e\tau),\quad \sigma' = (1-\tilde{\mathbf{R}})^{-1}\cdot\sigma/\sigma_0, \qquad (13.105)$$

where σ_0 is the dc-conductivity $N_0 e^2 \tau / m$. Similar expressions of j_e and σ in the presence of a constant external field was derived by Spector in connection the amplification of acoustic waves.[187)]

Net power dissipation of the sound wave per unit volume is given by

$$Q = \frac{1}{2}\left[j_e^* \cdot \mathcal{E} - u^* N_0 m (\langle v \rangle - u)/\tau \right]. \tag{13.106}$$

The first term corresponds to the average rate of loss of electronic kinetic energy via collisions. Not all of this kinetic energy transfer is irreversibly dissipated as heat; a part of it is coherently fed back into the sound wave. After the collision with the sound wave. the electron before $\langle v \rangle$ before the collision becomes u and the force exterted by the electrons is $N_0 m (\langle v \rangle - u)/\tau$. It should be noted that m is the true electron mass. Thus, energy is coherently returned to the sound wave per unit time is given by $\langle u N_0 m (\langle v \rangle - u)/\tau \rangle_{AV}$ and so (13.106) is proved.

(13.88) is rewritten in the form

$$j = -\sigma_0 B \cdot \mathcal{E}. \tag{13.107}$$

where $B_{ij} = B_{ii}\delta_{ij}$,

$$B_{11} = -\frac{i\omega}{4\pi\sigma_0}, \quad B_{22} = B_{33} = \frac{i\omega}{4\pi\sigma_0}\left(\frac{c}{v_s}\right)^2, \tag{13.108}$$

where $\varkappa (v_s/c)^2$ is neglected as compared with unity.

The correction to the $\mathbf{j}_e^* \mathcal{E}$ term in Q is related to the collision drag effect considered by Holstein.[186] This collision drag term is important chiefly at high frequencies or high magnetic fields.

(13.88) leads to $\mathrm{Re}(\mathbf{j}^* \cdot \mathcal{E}) = 0$. In consideration of this relation and from (13.89) and (13.107), (13.106) is rewritten as

$$Q = -\frac{1}{2} \mathrm{Re}\left[N_0 e \mathbf{u}^* (\mathbb{1} + \mathbf{B}) \cdot \mathcal{E} \right]. \tag{13.109}$$

Introducing a tensor $\mathbf{W}$ by

$$\mathcal{E} = \mathbf{W} N_0 e \mathbf{u} / \sigma_0 , \tag{13.110}$$

we obtain

$$Q = N_0 \left(\frac{1}{2} m |\mathbf{u}|^2 / \tau \right) \hat{\mathbf{u}} \cdot \mathbb{S} \cdot \hat{\mathbf{u}} , \tag{13.111}$$

where $\hat{\mathbf{u}}$ is a unit vector parallel to $\mathbf{u}$ and $\mathbb{S}$ is related to $\mathbf{W}$ by

$$\mathbb{S} = -\mathrm{Re}\left[(\mathbb{1} + \mathbf{B}) \cdot \mathbf{W} \right]. \tag{13.112}$$

On making use of the relations (13.89), (13.105), (13.107) and (13.110) $\mathbf{W}$ is expressed by

$$\mathbf{W} = -\left[\boldsymbol{\sigma}' + \mathbf{B} \right]^{-1} \cdot (\mathbb{1} - \boldsymbol{\sigma}'). \tag{13.113}$$

Then,

$$\mathbb{S} = \mathrm{Re}\left\{ [\mathbb{1} + \mathbf{B}] \cdot (\boldsymbol{\sigma}' + \mathbf{B})^{-1} \cdot (\mathbb{1} + \mathbf{B}) \right\} - \mathbb{1} . \tag{13.114}$$

or, in components

$$S_{ii} = \mathrm{Re}\left\{ (1+B_{ii})^2 \left[(\sigma'+B)^{-1}\right]_{ii} \right\} - 1. \qquad (13.115)$$

If u is parallel to i-direction, (13.111) gives

$$Q_i = N_0 \frac{m|u|^2}{2\tau} S_{ii} . \qquad (13.116)$$

The attenuation coefficient α is related to Q by

$$\alpha = Q \Big/ \left\{\tfrac{1}{2} N_0 M |u|^2 v_s\right\} , \qquad (13.117)$$

where M is the atomic mass of the metal. From (13.118), we get

$$\alpha_i = \frac{m v_F}{M v_s} \frac{S_{ii}}{l} , \quad l = v_F \tau \qquad (13.118)$$

Since α is comparable to the reciprocal of the mean free path L of the sound wave, we obtain for copper ($M v_s / m v_F \approx 100$)

$$L_i \approx 100 l / S_{ii} . \qquad (13.119)$$

In the case of longitudinal wave we have $|B_{11}| \ll 1$ (See (13.108)). Thus,

$$S_{11} = \mathrm{Re}\left[(\sigma'+B)^{-1} \right]_{11} - 1. \qquad (13.120)$$

Using the above relation we can calculate S_{ii}. If we can obtain the expression of σ, S is readily calculated by (13.114) and (13.105). After carring out a little algebra, σ is expressed as follows. (Detailed derivation is given by Appendix 14)

$$\sigma = \frac{3\sigma_0}{2} \sum_{n=-\infty}^{\infty} \int_0^{\pi} \begin{pmatrix} n/X \\ i\partial/\partial X \\ \cos\theta \end{pmatrix} J_n(X\sin\theta) \begin{pmatrix} n/X \\ -i\partial/\partial X \\ \cos\theta \end{pmatrix} J_n(X\sin\theta) \frac{\sin\theta\, d\theta}{1+i(n\omega_0-\omega+q_z v_F\cos\theta)\tau} \tag{13.121}$$

where $X = q_x v_F/\omega_0$. J_n denotes the n-th order Bessel function.

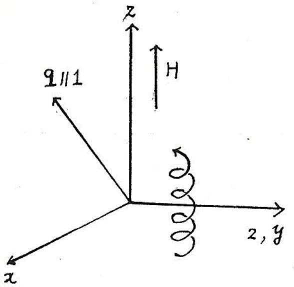


Fig. 13.12 (a) z-axis is in the (q, H)-plane.

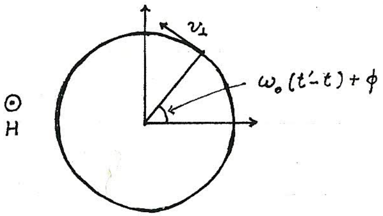


Fig. 13.12 (b) Electron orbit in magnetic field.

(13.121) is a useful formula which gives the conductivity tensor corresponding to the field $\mathcal{E} \propto \exp[i(qr-\omega t)]$.

In the following we consider the two different configurations : (A) $q \perp H$ and (B) $q \parallel H$.

(A) $q \perp H$:

In this case the coordinate system is given by $1 \leftrightarrow x$, $2 \leftrightarrow y$ and $3 \leftrightarrow z$. Non-zero conductivity tensor components are as follows.

$$\left\{\begin{aligned}
\sigma_{11} &= \frac{3\sigma_0}{(q l)^2}(1-i\omega\tau)\left[1-\sum_{n=-\infty}^{\infty}\frac{(1-i\omega\tau)\,g_n(X)}{1+i(n\omega_0-\omega)\tau}\right],\\
\sigma_{22} &= 3\sigma_0\sum_{n=-\infty}^{\infty}\frac{S_n(X)}{1+i(n\omega_0-\omega)\tau},\\
\sigma_{12} = -\sigma_{21} &= \frac{3\sigma_0}{2ql}\sum_{n=-\infty}^{\infty}\frac{(1-i\omega\tau)\,g_n'(X)}{1+i(n\omega_0-\omega)\tau},\\
\sigma_{33} &= 3\sigma_0\sum_{n=-\infty}^{\infty}\frac{r_n(X)}{1+i(n\omega_0-\omega)\tau},
\end{aligned}\right. \tag{13.122}$$

where

$$\left\{\begin{aligned}
&g_n(X) = \int_0^{\pi/2} J_n^{\,2}(X\sin\theta)\sin\theta\,d\theta; \quad g_n'(X) = (d/dX)\,g_n(X);\\
&S_n(X) = \int_0^{\pi/2}[J_n'(X\sin\theta)]^2\sin^3\theta\,d\theta; \quad r_n(X) = \int_0^{\pi/2} J_n^{\,2}(X\sin\theta)\cos^2\theta\sin\theta\,d\theta.
\end{aligned}\right. \tag{13.123}$$

Expressions of σ_{22} and σ_{33} can be readily obtainable from (13.121), and σ_{11} and σ_{12} are obtained by using the relations of $\sum_{n=-\infty}^{\infty} g_n(X) = 1$, $g_n(X) = g_{-n}(X)$ and $X\omega_0\tau = ql$ combining with (13.121).

Concrete expressions of $g_n(X)$, $g_n'(X)$, $S_n(X)$ and $r_n(X)$ are given by Appendix 14. From (13.115) S_{ii} takes the following form

$$\begin{aligned}
S_{11} &= \mathrm{Re}\left\{\frac{(1+B_{11})^2(\sigma_{22}'+B_{22})}{(\sigma_{11}'+B_{11})(\sigma_{22}'+B_{22})+\sigma_{12}'^{\,2}}\right\}-1\\
&\doteqdot \mathrm{Re}\left\{\frac{\sigma_{22}'+B_{22}}{\sigma_{11}'\sigma_{22}'+\sigma_{12}'^{\,2}+B_{22}\sigma_{11}'}\right\}-1.
\end{aligned} \tag{13.124}$$

$$S_{22} = \mathrm{Re}\left\{ \frac{(1+B_{22})^2(\sigma_{11}'+B_{11})}{(\sigma_{11}'+B_{11})(\sigma_{22}'+B_{22})+\sigma_{12}'^2} \right\} - 1$$

$$\doteqdot \mathrm{Re}\left\{ \frac{\sigma_{11}'(1+B_{22})^2}{\sigma_{11}'\sigma_{22}' + \sigma_{12}'^2 + B_{22}\sigma_{11}'} \right\} - 1, \qquad (13.125)$$

$$S_{33} = \mathrm{Re}\left\{ \frac{(1+B_{33})^2}{\sigma_{33}'+B_{33}} \right\} - 1. \qquad (13.126)$$

In deriving the above expressions the relations of $|B_{11}| \ll |B_{22}| = |B_{33}|$, σ_{ij}' are employed.

Bömmel revealed that the ultrasonic attenuation exhibits oscillatory dependence on magnetic field in tin at helium temperatures under the condition of $\omega_0\tau \gg 1$. 184) This effect is striking in the configuration of $q \perp H$. Pippard pointed out 188) that strong attenuation of the sound wave is expected if the radius R of the cyclotron motion is related to the wave length λ of the sound wave by the following relation

$$2R = (n+1)(\lambda/2), \quad n = 0, 1, 2, \ldots \qquad (13.127)$$

This relation is utilized in determination of the diameter of the Fermi surface. This is so called the geometric resonance (magneto-acoustic resonance). At A and B in Fig. 13.13 electrons are accerlated by the electric field of the sound wave. There is a relation between $2ky$ and $2R$,

$$2R = \frac{\hbar c}{eH} 2k_y . \qquad (13.128)$$

The quantity X in (13.121) is related to R by $X = Rq$.

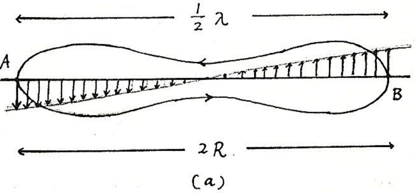


Fig. 13.13 (a). Electron orbit in real space. Arrows in Figure indicates the electric field induced by the sound wave.

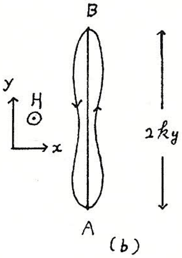


Fig. 13.13(b). Electron trajectory in k-space. The geometric resonance experiment determines the diameter $2k_y$ of the Fermi surface.

The attenuation coefficient α_i is proportional to S_{ii} (cf. (13.118)) and S_{ii} is calculated by using (13.124) ~ (13.126). As shown in (13.122) σ_{ii} which is included in S_{ii}, contains the Bessel function and its derivative. Accordingly, it is unexpected that S_{ii} takes maximum values at $X = (n+1)\pi/2$ which is equivalent to the intuitive relation (13.127). This is understood from the following simple consideration. Let consider a circular orbit. Namely,

$$v_y(t) = v_F \sin \omega_0 t , \quad x = R \sin \omega_0 t . \qquad (13.129)$$

In the expression of the electric field $\mathcal{E}_y = \mathcal{E}_y^\circ \exp[i(qx - \omega t)]$, it is permissible to approximate $\omega \to 0$ since $\omega_0 \gg \omega$. Absorbed energy in the period of the cyclotron motion is given by

$$\int \mathcal{E}\cdot v\,dt = \mathcal{E}_y^{\circ} v_F \int_0^{2\pi/\omega_0} \exp(iqR\sin\omega_0 t)\sin\omega_0 t\,dt$$

$$= \frac{\mathcal{E}_y^{\circ} v_F}{\omega_0}\int_0^{2\pi} \exp(iqR\sin\phi)\sin\phi\,d\phi = \frac{\mathcal{E}_y^{\circ} v_F}{\omega_0}\,2\pi\,J_1(qR). \qquad (13.130)$$

(13.130) indicates that the resonance absorption appears at the points where $J_1(qR)$ becomes maximum.

Since $\omega_0 \gg \omega$ and $|\omega_0\tau/(1-i\omega\tau)^2| \gg 1$, (13.122) are well approximated by the term $n=0$. By inserting (13.101) and (13.122) into (13.105) we obtain

$$\left\{\begin{aligned}
\sigma_{11}' &= -\frac{3i\omega\tau}{q^2 l^2}\,\frac{(1-i\omega\tau)[1-g_0(X)]}{[1-i\omega\tau-g_0(X)]}, \\
\sigma_{12}' &= -\sigma_{21}' = \frac{-3i\omega\tau\, g_0'(X)}{2ql\,[1-i\omega\tau-g_0(X)]}, \\
\sigma_{22}' &= \frac{3}{1-i\omega\tau}\left\{S_0 + \frac{[g_0'(X)/2]^2}{1-i\omega\tau-g_0(X)}\right\}, \\
\sigma_{33}' &= \frac{3\,r_0(X)}{1-i\omega\tau}.
\end{aligned}\right. \qquad (13.131)$$

The Bessel function in g_0, r_0 and S_0 leads to oscillatory dependence of the components of $\boldsymbol{\sigma}'$ on $\mathbf{H}$. If the condition of $|B_{22}\sigma_0/\sigma_{22}| \ll 1$ is satisfied (it is well satisfied in usual metals, however it does not hold in semimetals for high frequency wave $\omega > 10^7\ \mathrm{sec}^{-1}$), (13.131) leads to

$$S_{11} = \frac{q^2 l^2}{3(1+\omega^2\tau^2)}\left[\frac{1}{1-g_0+(g_0'/2)^2/s_0} - 1\right], \tag{13.132}$$

$$S_{22} = \frac{1}{3\left[s_0 + (g_0'/2)^2/(1-g_0)\right]} - 1. \tag{13.133}$$

$$S_{33} = \frac{1}{3r_0} - 1. \tag{13.134}$$

Calculated curves of S_{ii} are shown in Fig. 13.14.[183]

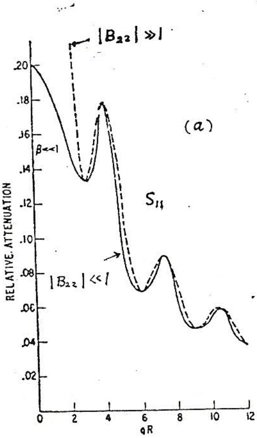


Fig. 13.14 (a). Field dependence of the attenuation coefficient of a longitudinal wave. (Cohen, Harrison and Harrison)

$|B_{22}| \sim (\delta/\lambda)^2$, δ : skin depth.

$q \perp H$.

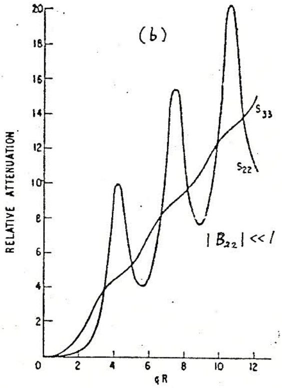


Fig. 13.14 (b) Field dependence of the attenuation coefficient of a transverse wave. (Cohen, Harrison and Harrison) S_{22} corresponds to polarization perpendicular to H, while S_{33} corresponds to polarization parallel to H.

(B) $q \parallel H$:

By putting $X = 0$ in (13.121), we obtain the expression of σ. In the present case relation of the coordinate systems in Fig. 13.12 a is as follows : $1 \leftrightarrow z$, $2 \leftrightarrow y$ and $3 \leftrightarrow -x$.

In the following we shall pay our attention to a longitudinal sound wave. We can readily perform the calculation in the case of a transverse wave. In the case of a longitudinal wave propagating parallel to the magnetic field, the field does not enter and we can obtain the result of Pippard.185)

$$\left\{\begin{aligned} S_{11} &= \mathrm{Re}\left[\,(1/\sigma_{11}') - 1\,\right], \\ \sigma_{11} &= \frac{\sigma_0}{1-i\omega\tau}\,\frac{3}{a^3}\,(a - \arctan a), \quad a = \frac{ql}{1-i\omega\tau}. \end{aligned}\right. \tag{13.135}$$

On making use of (13.101) and (13.105), (13.135) leads to

$$S_{11} = \frac{1}{3}\,\frac{q^2l^2 \arctan ql}{ql - \arctan ql} - 1, \tag{13.136}$$

where $\omega\tau \ll 1$ is assumed. From (13.118) the attenuation coefficient becomes

$$\alpha = \frac{N_0 m}{d\, v_s \tau}\left(\frac{1}{3}\,\frac{q^2l^2 \arctan ql}{ql - \arctan ql} - 1\right), \quad (d = N_0 M). \tag{13.137}$$

This is the result obtained by Pippard.185)

At low frequencies, for which the mean free path is much smaller than the wavelength, that is $ql \ll 1$,

$$\alpha = \frac{4 N_0 m v_F^2 \omega^2 \tau}{15 d v_s^3} \left\{ 1 - \frac{9}{35} (ql)^2 + \frac{23}{175} (ql)^4 - \cdots \right\} . \tag{13.138}$$

As the frequency is raised so that ql exceeds unity, the law of attenuation approaches the limiting form

$$\alpha \approx \frac{\pi N_0 m v_F \omega}{6 d v_s^2} . \tag{13.139}$$

It is worth noticing that this behaviour is reminiscent of the anomalous skin effect (Section 13.3) which also becomes independent of τ when the mean free path is very long.

The physical meaning of the geometric resonance can be simply given by the following argument. From (13.115) and (13.118) the attenuation at low frequencies is given by

$$\alpha = \frac{N_0 m}{d v_s \tau} \mathrm{Re} \left(\frac{\sigma_0}{\sigma_{eff}} - 1 \right), \tag{13.140}$$

where σ_{eff} stands for the appropriate combination of components of the conductivity tensor. It should be noted that the attenuation is not proportional to σ_{eff} but to $1/\sigma_{eff}$. Electrons nearly completely screen the electric field associated with the sound wave. Then, we have a constant current system rather than a constant voltage system, the electron current being forced to equal to $N_0 e u$.

In semiconductors and semimetals we must take into account the deformation potential force acting on carriers (see (13.92)) and the current densities of electrons and holes are given by[183]

$$\begin{aligned} \boldsymbol{j}_e &= \sigma_e^{\circ}\sigma_e' \cdot \left\{ \mathcal{E} + \frac{D_e}{ie\omega} \boldsymbol{q}(\boldsymbol{q}\cdot\boldsymbol{u}) - \frac{m\boldsymbol{u}}{e\tau_e} \right\}, \\ \boldsymbol{j}_h &= \sigma_h^{\circ}\sigma_h' \left\{ \mathcal{E} - \frac{D_h}{ie\omega} \boldsymbol{q}(\boldsymbol{q}\cdot\boldsymbol{u}) - \frac{m\boldsymbol{u}}{e\tau_h} \right\}. \end{aligned} \tag{13.141}$$

In semimetals power dissipation of the sound wave corresponding to (13.106) takes the form

$$\begin{aligned} Q = \frac{1}{2} \mathrm{Re}\, \boldsymbol{u}^{*} \cdot \Big\{ &\left(\frac{i}{e\omega}\right) \boldsymbol{q}\boldsymbol{q} \cdot \left[\boldsymbol{j}\, \tfrac{1}{2}(D_e - D_h) + (\boldsymbol{j}_e - \boldsymbol{j}_p)\, \tfrac{1}{2}(D_e + D_h) \right] \\ &+ \frac{m}{e} \left[\boldsymbol{j}\, \frac{1}{2}\left(\frac{1}{\tau_e} - \frac{1}{\tau_h}\right) + (\boldsymbol{j}_e - \boldsymbol{j}_h)\, \frac{1}{2}\left(\frac{1}{\tau_e} + \frac{1}{\tau_h}\right) \right] + N m \boldsymbol{u} \left(\frac{1}{\tau_e} + \frac{1}{\tau_h}\right) \Big\}, \end{aligned} \tag{13.142}$$

where $\boldsymbol{j} = \boldsymbol{j}_e + \boldsymbol{j}_h$, $n_0 = p_0 = N$ (n_0 (p_0) : electron (hole) density).

13.7 Weinreich Relation

Carriers interacting with the ultrasonic wave beam are dragged along the propagation direction and as a result a voltage is induced under the zero current condition. This is called the acoustoelectric effect (AE-effect). In semiconductors it is easier to measure the AE-voltage than to measure the attenuation.

There is a general relation called "Weinreich relation" between the attenuation coefficient and the AE-voltage.[189] This is readily derived on the analogy of the radiation pressure associated with the electromagnetic wave.

Ultrasonic wave accompanies an energy E_{ac} and also momentum P_{ac}. Denoting the average electron momenterm per particle by P_{el}, we obtain

$$\frac{dE_{ac}}{dt} = v_s \frac{dP_{ac}}{dt} = -Nv_s \frac{dP_{el}}{dt} = -Nev_s \mathcal{E}_{AE} . \qquad (13.143)$$

$\mathcal{E}_{AE}$ is the acoustoelectric field. Since $(d/dt)E_{ac} = -\alpha\gamma$, $\gamma = (1/2)\, d\,|u|^2 v_s$, we obtain the Weinreich relation

$$\mathcal{E}_{AE} = \frac{\alpha\gamma}{Nev_s} . \qquad (13.144)$$

By applying a magnetic field parallel to the z-axis and propagating the sound wave along the x-direction, electrons and holes are oppositely deflected and the acoustomagnetoelectric voltage (AME-voltage) is induced along the y-direction. This was firstly observed in bismuth by Yamada.[190]

13.8 Conduction Electron Spin Resonance (CESR)

Conduction electron spin resonance experiment in alkali metals was extensively performed by Feher and Kip [191]. They observed that the absorption line of CESR is very much different from those of the localized spins. In this connection a beautiful theory was presented by Dyson.[192] The following arguments are mainly due to these two papers.

Since the value of the spin relaxation time T_2 (in metals $T_1 = T_2$) is much longer than the momentum relaxation time τ, the diffusion distance δ_{eff} passed by electrons during T_2 is much larger than the mean free path l. In the case of $\omega_0 \tau \ll 1$ the electron's flight between collisions is, to a good approximation, a straight line. Therefore the displacement of an electron can be described by a random walk motion. Therefore, δ_{eff} is given by

$$\delta_{eff} = \frac{l}{\sqrt{3}} \left(\frac{T_2}{\tau} \right)^{1/2} = (D_0 T_2)^{1/2}, \qquad (13.145)$$

where D is the diffusion coefficient given by $(1/3) v_F^2 \tau$. The g-shift Δg is connected with T_2 by the Elliott relation [193]

$$T_2 / \tau \sim (g/\Delta g)^2. \qquad (13.146)$$

Since $\Delta g \sim 10^{-3}$ in alkali metals, (13.146) leads to $T_2/\tau \sim 10^6$ and accordingly we have $\delta_{eff} \sim 1$ cm from (13.145). As the skin depth δ is several orders smaller than δ_{eff}. (See Sections 13.2 and 13.3), electrons many times go into and go out the skin depth region during the spin reversal time T_2.

The $\omega_o \tau \gg 1$ case differ from that with $\omega_o \tau \ll 1$ because the electron motion perpendicular to the static magnetic field H_o is a circular motion specified by the cyclotron radius

$$R = v_F / \omega_o \equiv l / \omega_o \tau \ll l. \qquad (13.147)$$

After scattering an electron skips to another orbit with a different center. The diffusion distance in the plane normal to the static field in a time T_2 is now given by

$$\delta_{eff\perp} = (D_\perp T_2)^{1/2}, \qquad (13.148)$$

where

$$D_\perp = D_o / [1 + (\omega_o \tau)^2]. \qquad (13.149)$$

When $\omega_o \tau \gg 1$, (13.148) reduces to

$$\delta_{eff\perp} = \frac{R}{\sqrt{3}} \left(\frac{T_2}{\tau} \right)^{1/2}. \qquad (13.150)$$

Since the motion along the field is free electron like, the diffusion constant corresponding to the motion in a direction θ relative to H_o is described by

$$D = D_o \left[\frac{\sin^2\theta}{1 + (\omega_o \tau)^2} + \cos^2\theta \right]. \qquad (13.151)$$

In a time an electron diffuses a distance

$$\delta_{eff}(0) = (D T_2)^{1/2}. \qquad (13.152)$$

Now, we present a qualitative picture on the broadening of a resonance line to be expected.

At low temperatures the mean free path l is very much larger than the skin depth, in this case the time an electron spends in the skin region in metals is roughly

$$t_s \sim \delta / v_F. \quad (\delta : \text{skin depth}) \qquad (13.153)$$

For a $v_F \cong 10^8$ cm/sec and $\delta \cong 10^{-5}$ cm, $t_s \cong 10^{-13}$ sec.

At first glance, the short time spent in the skin depth region might cause the resonance line with large broadening $\Delta\omega \cong 1/t_s$. This large broadening would make it experimentally impossible to observe CESR in metals.

It was Dyson who pointed out the fallacy of this naive argument.[192] CESR line would not be as broad as $1/t_s$, because an electron does not simply traverse the skin depth once. In a time T_2 an electron returns several times to the skin region. Thus, a typical electron senses a set of pulsed rf fields whose intervals are random but phases are coherent. The width of the pulse is approximately t_s, the intervals are random and the Fourier transform of a single pulse is

$$F_{t_0}(\Omega) \sim e^{-i(\Omega-\omega)t_0} \left\{ \frac{\exp[i(\Omega-\omega)t_s] - 1}{\Omega - \omega} \right\}, \qquad (13.154)$$

where ω is the frequency of the rf field and t_0 is the time specifying the onset of a pulse (see Fig. 13.15).

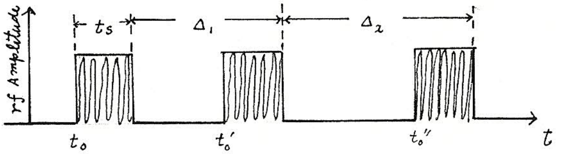


Fig. 13.15 The rf field amplitude sensed by an electron which returns many times to the skin depth region.

(13.54) represents a spectrum centered about ω with width $1/t_s$.

Since the onset times $t_0^{(i)}$ of the rf pulses are distributed at random, the net effect of adding many such pulses is to produce a spectaum which consists of a sharp line superimposed on a broad background of width $1/t_s$. The width of the sharp line of the spectrum is determined by the time T_2.

In order to effectively absorb the microwave energy, it is needed that the electrons spend enough time longer than $1/\omega$ in the skin depth region. An electron repeatedly re-enters the skin layer and spends a total time $T_2(\delta/\delta_{eff}) \sim (\delta/v_F)(T_2/\tau)^{1/2}$ in this layer, where (13.145) is employed. Therefore, it is needed that the condition $(\delta/v_F)(T_2/\tau) \gtrsim 2\pi/\omega$ should be satisfied, or $\omega \gtrsim (2\pi\sigma v_F^2/c^2)(\tau/T_2)$, which is quite easy to realize in the laboratory.

Before going to discuss on the Dyson's theory, it is worthwhile to clarify the physics on the basis of a simple phenomenological equation.

We assume that the space and time dependent macroscopic magnetization in the infinite medium obeys a Bloch-like equation of the form

$$\frac{d\mathbf{M}}{dt} = \gamma_0(\mathbf{H}\times\mathbf{M}) + D\Delta\mathbf{M} - \mathbf{i}\frac{M_x}{T_2} - \mathbf{j}\frac{M_y}{T_2} - \mathbf{k}\frac{M_z - M_0}{T_2}, \qquad (13.155)$$

where $\mathbf{i}$, $\mathbf{j}$ and $\mathbf{k}$ are respectively the unit vectors along x-, y- and z-axis, and $\mathbf{H}$ is composed of the static field $H_0 \parallel z$ and the oscillating rf field H_1 which is perpendicular to $\mathbf{H}_0$. In the conduction electron system the longitudinal spin relaxation time T_1 is equal to the transverse relaxation time T_2.

Decomposing the transverse magnetization and oscillating field into the Fourier components as

$$\left\{\begin{aligned}
\mathbf{M}(\mathbf{r},t) &= \sum_{k,\omega} \mathbf{M}(k,\omega)\, e^{i(\omega t - k\mathbf{r})} \\
\mathbf{H}_1 &= \sum_{k,\omega} \mathbf{H}_1(k,\omega)\, e^{i(\omega t - k r)}, \\
M_+(k,\omega) &= M_x(k,\omega) + i M_y(k,\omega) = \chi_+(k,\omega)\, H_+(k,\omega), \\
H_+(k,\omega) &= H_{1x}(k,\omega) + i H_{1y}(k,\omega).
\end{aligned}\right. \qquad (13.156)$$

and substituting (13.156) into (13.155), we obtain

$$\chi_+(k,\omega) = \frac{-\chi_0 \omega_s}{\omega - \omega_s + i(1/T_2 + Dk^2)}, \tag{13.157}$$

where $\omega_s = \gamma H_0$ and $M_z = \chi_0 H_0$. The expression of $\chi_+(k,\omega)$ in (13.157) includes all of the physics contained in our qualitative discussion of the preceding pages. $\chi_+(0,\omega)$ exhibits a resonance at $\omega=\omega_s$ with a width determined by T_2^{-1}. The diffusion term iDk^2 influences the shape of the line only. In a boundary value problem k will be fixed by the sample dimension, i.e., it will be of the order of L^{-1}, where L is the sample thickness. The fact that k is not determined by δ^{-1} means that the electrons go into and go out the skin depth region several times while diffusing a distance L.[192)]

Now we go on to discuss the Dyson's theory. At the first place we shall consider the microwave absorption due to the localized spins. Let denote the oscillating field by $H' = H_1 e^{-i\omega t}$.

Power absorption of the microwave due to the localized spin system is given by

$$P = \frac{1}{2}\omega H_1^2 \chi'' \Omega, \tag{13.158}$$

where χ'' is the imaginary part of the susceptibility $\chi = \chi' - i\chi''$ and takes the form

$$\chi'' = \frac{\chi_0}{2} \frac{\omega_0 T_2}{1+(\omega-\omega_0)^2 T_2^2}, \tag{13.159}$$

where χ_0 is the static susceptibility and ω_0 is the resonance frequency given by $\hbar\omega_0 = g\mu_B H$. By differentiating P on ω, we have

$$\frac{dP}{d\omega} = -\frac{\omega H_1^2}{2}\Omega\,\omega_0\chi_0 T_2 \frac{2(\omega-\omega_0)T_2^2}{[1+(\omega-\omega_0)^2T_2^2]^2}. \qquad (13.160)$$

$dP/d\omega$ is an odd function of $x \equiv (\omega-\omega_0)T_2$.

As will be shown in the following, the absorption curve of the conduction electrons can not be represented by the simple expression such as (13.158) or (13.160).

Consider an electron whose spin is described by the wave function

$$\psi(t) = a_1(t)e^{-i\omega_0 t/2}\alpha + a_2(t)e^{i\omega_0 t/2}\beta, \qquad (13.161)$$

where α, β are the states with spin + and −. The interaction energy of the electron spin σ with the microwave field is

$$\mu\,\sigma\cdot H_1(r(t))e^{-i\omega t} + \text{c.c.} \quad (\mu = g\mu_B/2). \qquad (13.162)$$

The Schrödinger equation for a_1 is

$$i\hbar\,\dot{a}_1 = \mu\,(H_1\cdot s\,e^{-i(\omega-\omega_0)t} + H_1^*\cdot s\,e^{i(\omega+\omega_0)t})\,a_2, \qquad (13.163)$$

where s is the vector given by $s = (\alpha^*\sigma\beta)$.

Expectation value of the electron spin at t, which was in the α-state at t', is given by

$$\bar{\sigma}(t,t') = k + \frac{i\mu}{\hbar}\int_{t'}^{t} du\,[\,s\cdot H_1(r(u))e^{-i(\omega-\omega_0)u-i\omega_0 t}s^*$$
$$- s^*\cdot H_1(r(u))e^{-i(\omega+\omega_0)u+i\omega_0 t}s\,] + \text{c.c.}, \qquad (13.164)$$

When the electron spin state was β at t', the corresponding value at t is just the opposite sign to (13.164).

In consideration of the spin-flip process, (13.164) should be modified as follows:

$$\bar{\sigma}(t) = (p_1 - p_2)\, T_2^{-1} \int_{-\infty}^{t} \exp[-(t-t')/T_2]\, \bar{\sigma}(t.t')\, dt'$$

$$= (p_1 - p_2)\, \mathbf{k} + \frac{i\mu}{\hbar}(p_1 - p_2) \int_{-\infty}^{t} du \exp[-(t-u)/T_2] [\mathbf{s} \cdot \mathbf{H}_1(r(u))\, e^{-i(\omega-\omega_0)u - i\omega_0 t}\, \mathbf{s}^*$$

$$- \mathbf{s}^* \cdot H_1(r(u))\, e^{-i(\omega+\omega_0)u + i\omega_0 t}\, \mathbf{s}] + \text{c.c.}, \qquad (13.165)$$

where p_1 and p_2 denote, respectively, the probabilities of the states α and β in thermal equilibrium. Let N be the number of electrons per unit volume. $N(p_1 - p_2)$ is directly related to the static susceptibility χ_0 by

$$\chi_0 H = \frac{1}{2} \chi_0 \frac{\hbar\omega_0}{\mu} = -N\mu(p_1 - p_2). \qquad (13\text{-}166)$$

(13.165) is essentially equivalent to the Chambers' formula (13.7).

If $G(\mathbf{r}.t)$ is the probability distribution for the position $\mathbf{r}$ of an electron at time t, G obeys the classical diffusion equation

$$\partial G/\partial t = D \Delta G, \quad D = (1/3)\, v^2 \tau. \qquad (13.167)$$

Averaging (13.165) over the electron trajectories and using (13.166), the magnetization $\mathbf{M}(\mathbf{r}.t)$ becomes

$$M(r.t) = \chi_0 H + \frac{1}{2} i \chi_0 \omega \int_{-\infty}^{t} du \exp[-(t-u)/T_2] \int dr' G(r'.u; r.t) [s \cdot H_1(r')$$

$$\times e^{-i(\omega-\omega_0)u - i\omega_0 t} s^* - s^* \cdot H_1(r') e^{-i(\omega+\omega_0)u + i\omega_0 t} s] + c.c. \qquad (13.168)$$

This is the nonlocal equation between M and H_1 similar to (13.3) or (13.7).

Now it is necessary to solve the Maxwell's equations combining with (13.168). Restricting the following discussions to the normal skin effect region and assuming the field variables varying with time like $\exp(-i\omega t)$, we obtain

$$\begin{cases} \operatorname{curl} H_1 = \dfrac{4\pi}{c} j, \\ \operatorname{curl} \mathcal{E} = -\dfrac{1}{c}\dot{B} = \dfrac{i\omega}{c} B, \\ B = H_1 + 4\pi M, \quad j = \sigma \mathcal{E}, \end{cases} \qquad (13.169)$$

here the displacement current is neglected. The experimentally observed quantity is the power dissipation P of the microwave field per unit area of the metal surface. This is the real part of the normal component of the complex Poynting vector just outside the surface. From (13.22) the surface impedance Z is given by

$$Z = \frac{4\pi}{c} \frac{[n \cdot (\mathcal{E}(0) \times H_1(0)^*)]}{|H_1(0)|^2}, \quad (n \parallel z) \qquad (13.170)$$

and the absorption rate P is related to Z by the relation

$$P = \left(\frac{c}{4\pi}\right)^2 |H_1(0)|^2 \,\mathrm{Re}\, Z. \qquad (13.171)$$

If the sample thickness d is very large compared to the skin depth δ, we may consider the semiinfinite sample ($+\infty > z \geqq 0$) and the solution of (13.167) which satisfies the boundary condition $n \cdot \mathrm{grad}\, G = 0$ at $z=0$ is given by

$$G(z';u;z.t) = \frac{1}{(4\pi D|t-u|)^{1/2}} \left\{ \exp\left[-\frac{(z-z')^2}{4D|t-u|}\right] + \exp\left[-\frac{(z+z')^2}{4D|t-u|}\right]\right\}. \qquad (13.172)$$

(13.172) behaves like as the delta function $\delta(z-z')$ at $t=u$. An average electron will diffuse the skin depth δ in a time of the order of $T_D \simeq \delta^2/D$ and $T_2 \gg T_D$. In (13.168) the space integration ($dr' \to dz'$) extends over values of $z' \sim \delta$, while the time integration du extends over the interval of the order T_2. Hence, we may replace both exponentials in (13.172) by unity. This means that the magnetization induced by the microwave field in the skin region z', goes away in the time T_2 to z which is independent of z'!

The nonresonant term in (13.168) is negligible in comparison with the resonant term and the microwave magnetization $\mathfrak{M}(r.t) = M(r)\, e^{-i\omega t}$ + c.c. is given by

$$M(r) = \frac{1}{2} i \chi_0 \omega_0 \int_0^\infty dw\, [\pi D w]^{-1/2} \exp[-w(T_2^{-1} - i\Delta\omega)] \int_0^\infty dz'\, \mathbf{S} . \mathbf{H}_1(z') \mathbf{S}^*, \qquad (13.173)$$

$(\Delta\omega = \omega - \omega_0)$.

$M(r)$ is independent of r. In the above expression it is permissible to replace H_1 by B, since the error is of the order of $O(\chi_0^{\,2})$.

From (13.169)

$$\frac{i\omega}{c}B = \frac{d}{dz}(n \times \mathcal{E}), \qquad (13.174)$$

and integrating over z', we have

$$\int_0^\infty B(z')\,dz' = \frac{ic}{\omega}(n \times \mathcal{E}(0)). \qquad (13.175)$$

By substituting (13.175) into (13.173), $M(r)$ becomes

$$M(r) = -\frac{\chi_0\,\omega_0\,c}{2\omega}\left(\frac{T_2}{D}\right)^{1/2}(1 - is\omega T_2)^{-1/2}[s\cdot(n \times \mathcal{E}(0))]\,s^*, \qquad (13.176)$$

where

$$(1 - ix)^{-1/2} = 2^{-1/2}(1 + x^2)^{-1/2}(\eta + i\xi), \quad (x \equiv s\omega T_2)$$

$$\eta = [(1+x^2)^{1/2} + 1]^{1/2}, \quad \xi = \operatorname{sgn} x\,[(1+x^2)^{1/2} - 1]. \qquad (13.177)$$

Since $M(r)$ is a constant vector and independent of r, (13.169) are expressed by B and $\mathcal{E}$ and completely independent of M. Thus, B and $\mathcal{E}$ inside the metal are given by the usual theory of skin effect without magnetization. This situation is valid both in the normal and anomalous skin effect regions.

The tangential components of $\mathcal{E}$ and H_1 are continuous on the surface. Accordingly, we have

$$\mathcal{E}(0) = \mathcal{E}(0), \quad H_1(0) = B(0) - 4\pi M_L(0). \qquad (13.178)$$

$\mathcal{E}(0)$ and $B(0)$ are the quantities calculated for $M = 0$ and $M_L(0)$ is the tangential component of (13.176). The surface impedance without magnetization is given by

$$Z_0 = \frac{4\pi}{c}\left[n\cdot(\mathcal{E}(0)\times B(0)^*)\right]/|B(0)|^2, \qquad (13.179)$$

Let introduce the vectors b, b^* defined by

$$b = B(0)/|B(0)|, \quad (b\cdot b^*) = 1. \qquad (13.180)$$

(13.179) and (13.180) lead to

$$n\times\mathcal{E}(0) = \frac{c}{4\pi} Z_0 |B(0)|\, b. \qquad (13.181)$$

By substituting (13.177), (13.178) and (13.181) into (13.170), the surface impedance with magnetization takes the form

$$\begin{aligned} Z &= Z_0\left[1 + Kc(1-ix)^{-1/2} f Z_0\right]^{-1} \\ &\doteqdot Z_0 - Kcf(1-ix)^{-1/2} Z_0^{\,2} + O(\chi_0^{\,2}), \end{aligned} \qquad (13.182)$$

where

$$f = |(s\cdot b)|^2, \quad K = (\chi_0\omega_0 c/2\omega)(T_2/D)^{1/2}. \qquad (13.183)$$

In the normal skin effect region, from (13.23) Z_0 is

$$Z_0 = (1-i)(\sigma\delta)^{-1}. \qquad (13.184)$$

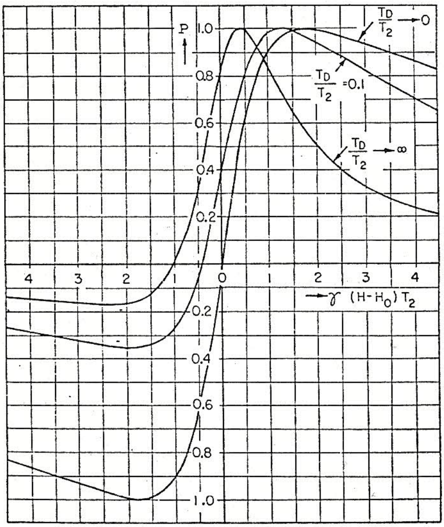
By (13.171), we have

$$P = \frac{\delta\omega\,|H_1(0)|^2}{4}\left[\frac{1}{2\pi} - f\omega_0\chi_0 T_2\left(\frac{T_D}{T_2}\right)^{1/2}\frac{\{(1+x^2)^{1/2}-1\}^{1/2}}{(1+x^2)^{1/2}}\operatorname{sgn} x\right], \qquad (13.185)$$

and

$$\frac{dP}{d\omega} = -\left[\frac{f\delta\omega|H_1(0)|^2}{4}\omega_0\chi_0 T_2\right]\left\{\frac{T_2}{2}\left(\frac{T_D}{T_2}\right)^{1/2}\frac{[2-(1+x^2)^{1/2}[(1+x^2)^{1/2}+1]^{1/2}}{(1+x^2)^{3/2}}\right\}. \qquad (13.186)$$

These expressions correspond to the case of $T_D/T_2 \to 0$, $d \gg l, \delta$. Calculated curves are shown in Figs. 13.16 (a) and 13.16 (b).[191]



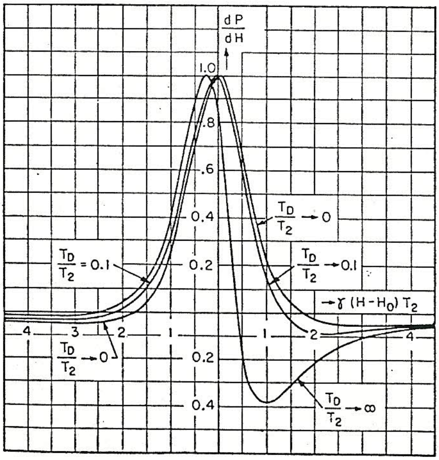


Fig. 13.16 (a) Power absorption due to electron spin resonance in thick metal plates ($d \gg l, \delta$) ($\gamma(H-H_0) = \omega - \omega_0$) (After Feher and Kip).

Fig. 13.16 (b) Derivative of the power absorption due to electron spin resonance in thick metal plates for different values of T_D/T_2. (After Feher and Kip)

General formulae corresponding to the case of finite thickness and $T_D / T_2 \neq 0$ are given in the Dyson's paper.$^{192)}$

It is worthy of note that the behaviors of P and dP/dH represented by Figs. 13.16(a) and 13.16(b) are entirely different from those of (13.158) and (13.160).

Fig. 13.17 shows the experiment for sodium in the region of the completely anomalous skin effect. The theory due to Kittel$^{191)}$ is in good agreement with the observed curve. Fig. 13.18 indicates the experiment for graphite$^{194)}$. As is shown in Fig. 13.16 (b) the effect of the diffusion enhances the ratio A/B.

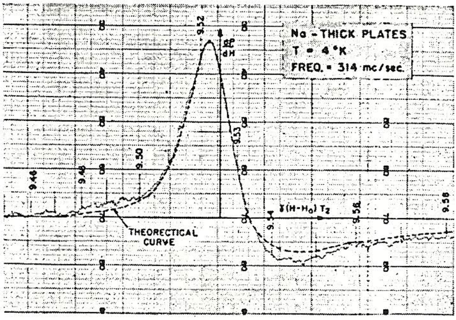


Fig. 13.17 Electron spin resonance absorption for sodium at 4 K and 300 MH/sec in the region of the completely anomalous skin effect (after Feher and Kip).

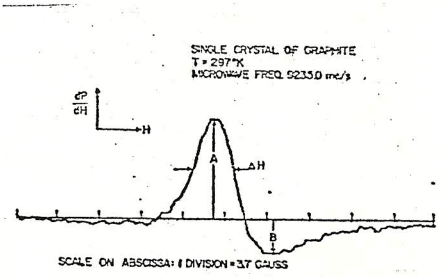


Fig. 13.18 Electron spin resonance absorption for graphite. Magnetic is applied parallel to the c-axis. (after Wagoner)

Chapter 14 Transport Phenomena related to the Nonequilibrium Phonon Distribution

In chapters 9 and 11 the transport coefficients due to the phonon scattering were calculated by assuming the phonon distribution being in thermal equilibrium. The phonon distribution participates in the kinetic equation as a c-number represented by the Planck function and the phonon dynamics is unnecessary. However, as was pointed out in Sections 6.5 and 12.1 the phonon deviation from thermal equilibrium affects the thermoelectric power and/or the electrical conductivity.

In this Chapter we shall treat the phonon drag thermopower, the two-stage drag effect and the mobility change due to the mutual drag effect by solving the electron-phonon coupled kinetic equation.

14.1 Phonon Drag Effect in Semiconductors, Herring Theory

Importance of the non-equilibrium phonons on the thermoelectric power of metals and semiconductors was pointed out by Gurevich[195] and independently by Klemens.[196] The work of Gurevich did not at first attract much attention, perhaps because it was suggested by Pikus[197] that the Gurevich term in the thermoelectric power of a semiconductor would usually be very small. The effect was rediscovered as a result of experiments made by Frederikse 198) and Geballe 199).

They observed that the thermoelectric power of germanium at low temperatures rises to many times the value predicted by the diffusion term only. The interpretation was independently given by Frederikse 198, 200) and by Hering, 201) which accords with the expectation of Gurevich.

Now we shall briefly mention about the erroneous conclusion obtained by Pikus. 197)

The thermal conductivity of a nonmetal is primarily determined by the phonon contribution and is described by the familiar formula

$$\varkappa = \frac{1}{3} C_p v_s l_p = \frac{1}{3} C_p v_s^2 t, \quad (l_p = v_s t) \qquad (14.1)$$

where C_p is the phonon specific heat per unit volume, v_s an average sound velocity and l_p denotes an effective mean free path of the phonons. As already discussed in Section 6.5, the phonon drag thermoelectric power is given by

$$S_p = -\frac{c}{3e} \left\langle \frac{t}{t^{(e)}} \right\rangle, \qquad (14.2)$$

where c is the phonon specific heat per electron, t the phonon relaxation time and $t^{(e)}$ is the phonon relaxation time associated with the electron-phonon scattering. $\langle \cdots \rangle$ means a some average procedure which will be discussed in detail in the present Chapter. Pikus assumed that the phonon relaxation time t in the thermal conductivity formula participates also in the phonon drag effect. This leads to a very small phonon drag thermopower.[197] This conclusion is clearly incorrect in semiconductors, because the phonons contibuting to the thermal conduction are so called the thermal phonons with energy ~ $k_0 T$ and their wave length is much smaller than that of the phonons related to the phonon drag effect.

Let consider a semiconductor specified by an isotropic effective mass m^*. The typical energy of the phonons interacting with electons is

$$\hbar\omega = \hbar v_s q \simeq \hbar v_s \sqrt{\frac{2m^* k_0 T}{\hbar^2}} \equiv m^* v_s v_T, \qquad (14.3)$$

where we employ the relation of $(\hbar^2/2m^*)q^2 \simeq k_0 T$. Assuming $m^* = 0.22 m_0$ which is an average effective of n-Ge $(m^* = (m_\perp^2 m_\perp)^{1/3})$ and putting $T = 77K$, we obtain

$$v_T = 1.03 \times 10^7 \text{ cm/sec} \gg v_s \sim 10^5 \text{ cm/sec}. \qquad (14.4)$$

On the other hand, the wave number of the thermal phonons is given by $q_T \simeq k_0 T/\hbar v_s$ and, consequently we have

$$q/q_T \simeq v_s/v_T \sim 10^{-2} \ll 1. \qquad (14.5)$$

Insensitivity of long wave length phonons to scattering leads to the large phonon drag effect which was firstly predicted by Gurevich.[195] Expressing an electric and heat current by

$$j = \sigma\mathcal{E} - \beta\nabla T, \quad w = \chi\mathcal{E} - \lambda\nabla T. \qquad (14.6)$$

we obtain the thermoelectric power for $H=0$, $\mathcal{E}$, $\nabla T \parallel x$ as

$$S = \frac{\mathcal{E}_x}{dT/dx} = \frac{\beta_{xx}}{\sigma_{xx}} = \frac{\chi_{xx}}{T\sigma_{xx}} . \tag{14.7}$$

In obtaining β it is needed to solve the electron-phonon coupled equations in the presence of $\mathcal{E}$ and ∇T, while in calculating χ it is enough to evaluate w without temperature gradient ∇T. The latter scheme calculating the thermoelectric power is called the Π-approach after Herring.[201) The thermoelectric power is related to the Peltier coefficient Π $(= \chi_{xx}/\sigma_{xx})$ by

$$S = \frac{\Pi}{T} . \tag{14.8}$$

The following argument in this Section is mainly due to Herring.[201)

The procedure calculating the thermoelectric power for $\nabla T \neq 0$ is called the S-approach.

The average energy transfered per electron must be of the order of $k_0 T$, say $\alpha k_0 T$ above the conduction band edge energy E_c.

Then, this energy carried by an electron gives a contribution to the Peltier heat, where

$$-e\Pi_e = E_c - \zeta + \alpha k_0 T. \quad (e>0) \tag{14.9}$$

Accordingly,

$$S = -\frac{1}{eT}\left(E_c - \zeta\right) - \alpha\frac{k_0}{e} . \qquad (14.10)$$

(14.10) is the same expression as (6.100). (In (6.100) E_c is taken to be zero.) α depends on the scattering mechanism. It becomes 2 in the case of longitudinal acoustic phonon scattering and 4 in the ionized impurity scattering regime.

In the intrinsic region carrier concentration n is constant, and then from (6.101) it is shown that $(E_c - \zeta)/T$ is weakly temperature dependent. Let estimate (14.10) for n-Ge. Inserting $n = 10^{14}\ \mathrm{cm}^{-3}$, $T = 100\,\mathrm{K}$, $m^* = 0.220\, m_0$ and $\alpha = 2$ into (6.101) and (14.10),

we have

$$\left\{\begin{aligned} &\frac{1}{eT}\left(E_c - \zeta\right) = -734\,\mu\mathrm{V/deg}, \\ &-\alpha\frac{k_0}{e} = -2\times 86.26\,\mu\mathrm{V/deg}. \end{aligned}\right. \qquad (14.11)$$

and finally $S \doteqdot 0.9\ \mathrm{mV/deg}$. This value corresponds to the dotted lines in Figs. 14.1 and 14.2. However, the steep rise at low temperatures can not be ascribed to the diffusion term S_d given by (14.10). Difference between the observed value and S_d is due to the phonon drag effect. S and Π are composed of the two parts:

$$S = S_d + S_p, \quad \Pi = \Pi_d + \Pi_p. \qquad (14.12)$$

Before carrying out the detailed calculations, we shall make few remarks on the qualitative feature of the phonon drag effect.

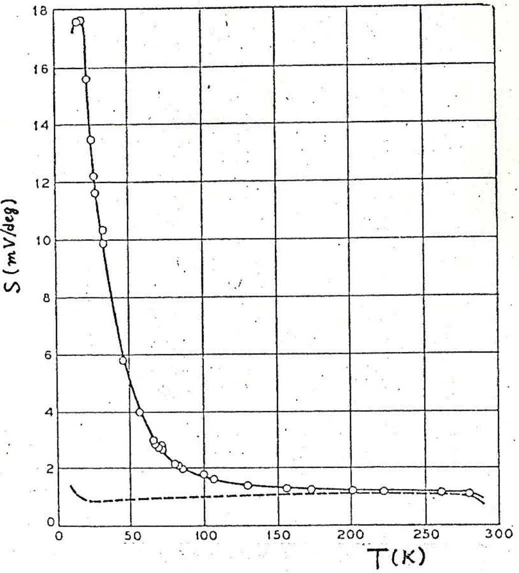


Fig. 14.1 Thermoelectric power of p-Ge. Dotted line indicates (14.10). The room temperature carrier concentration is 5.0×10^{13} cm^{-3}. (Geballe, unpublished work.[201])

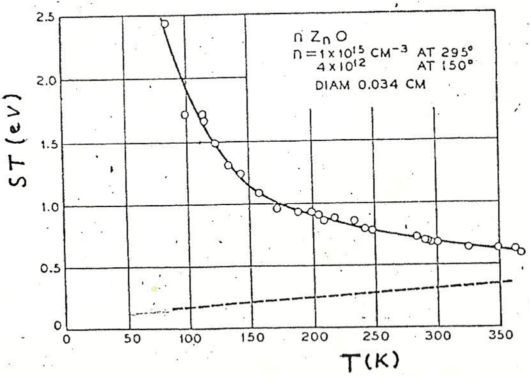


Fig. 14.2 Temperature dependence of ST in n-ZnO. (Hutson (1956) unpublished work.[201])

1) If several kinds of carriers participate in the thermoelectric effect, S_d and S_p are given by the sum of them:

$$\left\{ \begin{aligned} S_d &= \sum_i S_d^{(i)}, \\ S_p &= \sum_i S_p^{(i)}, \end{aligned} \right. \qquad (14.13)$$

and $S_d^{(i)}$ and $S_p^{(i)}$ must always be of the same sign. However, S_d and S_p are not always of the same sign.

2) As shown in Figs. 14.1 and 14.2 the phonon drag effect is remarkable at low temperatures, since the phonon system rapidly restores the equilibrium distribution through strong phonon-phonon interaction at high temperatures.

With further decrease of temperature, the phonon drag effect diminshes since at enough low temperatures the electron-phonon scattering becomes unimportant.

In the following we shall briefly describe the calculation of S- and Π-approach.[201)]

a) Calculation due to S-approach:

Consider the thermal conduction of the phonons interacting with carriers. Let denote the average phonon drift velocity and its energy density by $\bar{v}_{ph}$ and U_{ph}. From (14.1)

$$\bar{v}_{ph} U_{ph} = -\frac{1}{3} C_p v_s l_p \nabla T . \tag{14.14}$$

Since the relevant Phonons are long wave length phonons, U_{ph} is given by $U_{ph} \simeq C_p T$. we have

$$\bar{v}_{ph} \simeq -\frac{1}{3} v_s l_p \frac{\nabla T}{T} . \tag{14.15}$$

If the electrons interact only with the phonons through the electron-phonon interaction, the electron drift velocity $\bar{v}_d$ must be equal to $\bar{v}_{ph}$. In general the electrons are also scattered by impurities, then $\bar{v}_d$ should be expressed by

$$\overline{v_d} = r \, \bar{v}_{ph} , \quad r \equiv \tau / \tau^{(P)} < 1 , \tag{14.16}$$

where τ is the electron relaxation time including all scattering processes and $\tau^{(P)}$ represents the relaxation time associated with the phonon scattering process and clearly r is smaller than unity. Thus, the induced thermoelectric field is

$$\mathcal{E} = \pm \bar{v}_d / \mu \quad (+ : \text{electron}, \; - : \text{hole}) , \tag{14.17}$$

where μ is the mobility and the phonon drag thermoelectric power takes the form

$$S_p = \frac{\mathcal{E}}{\nabla T} \simeq \mp \frac{v_s l_p r}{3 \mu T} = \mp \frac{v_s^2 t r}{3 \mu T} . \tag{14.18}$$

By introducting $\mu = e\tau/m^*$, (14.18) is rewritten as

$$S_p \simeq \mp \frac{m^* v_s^2}{3 e T} \left(\frac{t}{\tau^{(p)}} \right) = \mp \frac{m^* v_s^2}{3 e T} \left(\frac{t^{(e)}}{\tau^{(p)}} \right) \left(\frac{t}{t^{(e)}} \right) , \tag{14.19}$$

where $t^{(e)}$ is the phonon relaxation time related to the electron-phonon scattering and $t/t^{(e)} < 1$. (14.19) is just the same expression as (6.83) apart from a numerial factor with order unity.

b) Calculation due to Π-approach :

The heat current density of the phonon system is

$$w_p = \sum_q N_q \hbar \omega_q v_s (\mathbf{q}/q) = v_s^2 \sum_{\mathbf{q}} N_q \hbar \mathbf{q} , \tag{14.20}$$

where $\sum_q N_q \hbar \mathbf{q}$ denotes the crystal momentum P_{ph} of the phonon system.

The Peltier coefficient is thus given by

$$\Pi_p = \frac{v_s^2 P_{ph}}{j} . \tag{14.21}$$

Electron momentum supplied by an electric field $\mathcal{E}$ per unit time is given by $dP_e/dt = -ne\mathcal{E}$, where n is the electron density and a part of it is transfered to the phonon system by the formula

$$\left(\frac{\partial P_{ph}}{\partial t}\right)_e = \mp rne\mathcal{E}, \quad (r<1) \tag{14.22}$$

where $-$ corresponds to electrons and $+$ to holes. P_{ph} is assumed to obey the following simple relaxation equation

$$\left(\frac{\partial P_{ph}}{\partial t}\right)_c = -\frac{P_{ph}}{t}. \tag{14.23}$$

In the stationary state $(\partial P_{ph}/\partial t)_e + (\partial P_{ph}/\partial t)_c = 0$. Therefore,

$$P_{ph} = \mp rne\mathcal{E}t = \mp rjt/\mu. \tag{14.24}$$

Hence,

$$S_p = \frac{\Pi_p}{T} = \mp\frac{v_s{}^2 t}{\mu T}. \tag{14.25}$$

Apart from a factor 1/3 (14.25) accords with (14.18). By decomposing (14.25) into the sum over the phonon modes q, we have

$$S_p = \mp\sum_q [v_s(q)]^2 t(q) r(q)/\mu T, \tag{14.26}$$

where

$$r = \sum_q r(q) = \tau\sum_q (1/\tau^{(p)}(q)) \tag{14.27}$$

To get an expression of the phonon drag thermoelectric power of the system with several species of carriers, as an example semimetals with electrons and holes, it is convenient to employ the equations similar to (6.79).

Denote the crystal momentums of the three systems by P_e. P_h and P_{ph}.

The kinetic equations for P_e. P_h and P_{ph} are

$$\left\{\begin{aligned} \frac{dP_e}{dt} &= -\frac{P_e}{\tau_e^{(P)}} - \frac{P_e}{\tau_e^{(P)}} + \frac{P_{ph}}{t^{(e)}} - ne\mathcal{E}, \\ \frac{dP_h}{dt} &= -\frac{P_{ph}}{\tau_h^{(P)}} - \frac{P_h}{\tau_h^{(P)}} + \frac{P_{ph}}{t^{(h)}} + pe\mathcal{E}, \\ \frac{dP_{ph}}{dt} &= \frac{P_e}{\tau_e^{(P)}} + \frac{P_h}{\tau_h^{(P)}} - \frac{P_{ph}}{t^{(e)}} - \frac{P_{ph}}{t^{(h)}} - \frac{P_{ph}}{t^{(r)}}. \end{aligned}\right. \qquad (14.28)$$

$\tau_i^{(P)}$ and $\tau_i^{(r)}$ $(i = e, h)$ represent, respectively, the relaxation time due to the phonon scattering and the one due to the scattering processes except the phonon scattering. Relaxation time of the i-th carrier is then given by

$$1/\tau_i = 1/\tau_i^{(P)} + 1/\tau_i^{(r)}. \qquad (14.29)$$

$t^{(i)}$ $(i = e, h)$ denotes the phonon relaxation time related to the scattering by i-th carrier and $t^{(r)}$ is the relaxation time due to the scattering processes except the carrier scattering. From the stationary condition

$dP_e/dt = dP_h/dt = dP_{ph}/dt = 0$, we obtain the phonon drag thermoelectric power as follows:

$$S_p = \frac{e v_s^2 t \, (p r_h \xi_h - n r_e \xi_e)}{\sigma_e^{(0)} \xi_e + \sigma_h^{(0)} \xi_h} , \tag{14.30}$$

where

$$\left\{ \begin{aligned} & 1/t = 1/t^{(e)} + 1/t^{(h)} + 1/t^{(r)} , \quad r_e = \tau_e / \tau_e^{(P)} , \quad r_h = \tau_h / \tau_h^{(P)} , \\ & \xi_e = 1 - \Gamma_h^{(h)} - \frac{p}{n} \Gamma_h^{(e)} , \quad \xi_h = 1 - \Gamma_e^{(e)} - \frac{n}{p} \Gamma_e^{(h)} , \\ & \Gamma_\lambda^{(\beta)} = \frac{\tau_\lambda}{\tau_\lambda^{(P)}} \frac{t}{t^{(\beta)}} , \quad \sigma_e^{(0)} = n e^2 \tau_e / m_e , \quad \sigma_h^{(0)} = p e^2 \tau_h / m_h . \end{aligned} \right. \tag{14.31}$$

In deriving (14.30) and (14.31) the relations of $W_p = v_s^2 P_h = \chi \mathcal{E}$, $S_p = \chi / T \sigma$ and $\sigma = - e P_e / m_e \mathcal{E} + e P_h / m_h \mathcal{E}$ are employed.

If only one type of carriers is present, (14.30) agrees with (6.83). In (6.83) the mutual drag coefficient Γ does not appear, while (14.30) includes Γ in a complicated manner. The electrical conductivity is given by

$$\sigma = (\sigma_e^{(0)} \xi_e + \sigma_h^{(0)} \xi_h) \Delta^{-1}, \quad \Delta = (1 - \Gamma_e^{(e)})(1 - \Gamma_h^{(h)}) - \Gamma_e^{(h)} \Gamma_h^{(e)} . \tag{14.32}$$

By its definition Γ is smaller than unity and mostly it may be negligible. However, in some cases Γ plays an important role in the behaviors of the transport coefficients. An example will be presented in Section 14.3.

To calculate the phonon drag thermopower S_p on the basis of (14.26), it is essentially important to know about the (q, T)-dependence of $t(q)$. Most important process limiting the relaxation rate $1/t(q)$ is the phonon-phonon scattering. On this problem there is an excellent work by Herring.[202] In view of its importance we shall in detail describe the Herring's argument.

The thermal conductivity of the phonon system is given by

$$\varkappa = \frac{1}{3} \sum_q C(q)\, t(q)\, v_s^2(q) \qquad (14.33)$$

and for small values of q $t(q)$ is proportional to q^{-4}. Then, the summation over q in (14.33) becomes $\int dq\, q^2 t(q) \propto \int dq\, q^{-2}$, which tends to infinity. This comes from the assumption of an isotropic elasticity of the crystal. but Herring showed that it does not occur for crystals of the higher symmetry classes, by virtue of the anisotropy of their elasticity.[202] Namely, at low temperatures $(T \ll \Theta_D)$ there is a scaling law for the acoustic wave as

$$t(\lambda q, \lambda T) = \lambda^{-5} t(q, T). \qquad (14.34)$$

For longitudinal waves (14.34) yields

$$t(q) \propto q^{-2} T^{-3} \quad \text{as } q \to 0,\ T \ll \Theta_D \qquad (14.35)$$

for any crystal of the cubic or hexagonal classes. The asymptotic behavior of the relaxation time for transverse modes is not affected by the substitution of anisotropic for isotropic elasticity, and $t(q)$ is given by

$$t(q) \propto q^{-1} T^{-4}. \tag{14.36}$$

In the following we shall verify (14.34) ~ (14.36).

As an effective scattering process, we consider the process illustrated in Fig. 14.3. Energy- and momentum conservation laws are

$$\begin{cases} q_0 + q_1 = q_2 \,, \\ \omega_0 + \omega_1 = \omega_2 \,. \end{cases} \tag{14.37}$$

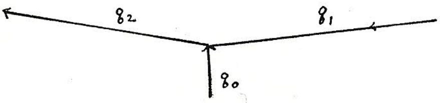


Fig. 14.3 Three-phonon collision process. q_0 is a low frequency phonon interacting with carriers and q_1 and q_2 denote the thermal phonons. ($q_0 \ll q_1, q_2$)

The perturbation which causes the process is the elastic potential energy which is of the third order in the relative displacements of the atoms.

Square of the matrix element for the process corresponding to Fig. 14.3 is

$$|\langle N_0, N_1, N_2 \,|\, U_3 \,|\, N_0 - 1, N_1 - 1, N_2 + 1 \rangle|^2 \propto q_0 q_1 q_2 N_0 N_1 (N_2 + 1) \,, \tag{14.38}$$

and the matrix element for the inverse process is

$$|\langle N_0, N_1, N_2 \,|\, U_3 \,|\, N_0 + 1, N_1 + 1, N_2 - 1 \rangle|^2 \propto q_0 q_1 q_2 (N_0 + 1)(N_1 + 1) N_2 \,. \tag{14.39}$$

With each mode q_0 we may associate a relaxation time defined by

$$1/t(q_0) = -(dN_0/dt)_c/\delta N_0 . \tag{14.40}$$

where $(dN_0/dt)_c$ is the total rate of change of N_0 due to phonon-phonon collisions when N_0 departs from equilibrium but all other modes are in thermal equilibrium. $(dN_0/dt)_c$ is approximately given by the processes (14.38) and (14.39)

$$(dN_0/dt)_c \cong W(2\to 0.1) - W(0.1\to 2), \tag{14.41}$$

since the processes $W(1.2\to 0)$ and $W(0\to 1.2)$ make a minor contribition to $(dN_0/dt)_c$ because of $q_0 \ll q_1, q_2$.

From (14.38) and (14.39), we have

$$dW(2\to 0.1) - dW(0.1\to 2) \propto \delta N_0\, q_0 q_1 q_2 (N_1^{(0)} - N_2^{(0)})\, dS_1 |\partial\Delta\omega/\partial q_{1n}|^{-1}, \tag{14.42}$$

where dS_1 represents the surface element in q_1-space satisfying (14.37) and q_{1n} is the normal component to dS_1. $\Delta\omega$ is given by

$$\Delta\omega = \omega(q_0+q_1) - \omega(q_1) - \omega(q_0). \tag{14.43}$$

Accordingly,

$$-(dN_0/dt)_c/\delta N_0 \propto q_0 \sum q_1 q_2 (N_1^{(0)} - N_2^{(0)})\, dS_1 |\partial\Delta\omega/\partial q_{1n}|^{-1}. \tag{14.44}$$

In the first place we assume an isotropic elasticity and consider the transitions satisfying (14.37). In this case, $\hbar\omega(q_1) \sim \hbar\omega(q_2) \sim k_0 T$ and $\omega(q_1), \omega(q_2) \gg \omega(q_0)$.

Since it is impossible to illustrate (14.37) in the three dimensional space, we shall guess the general case from the curve representing $\omega - q_x$ relation.

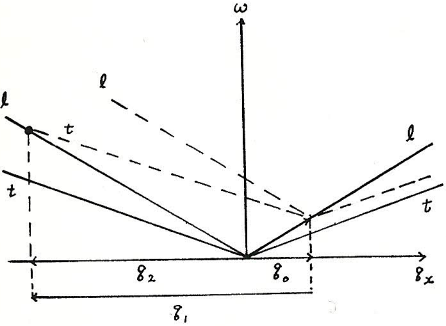


Fig. 14.4(a). Three-phonon collision process : $l_0 + t_1 \rightarrow l_2$. • indicates the point satisfying the conservation law (14.37).[201]

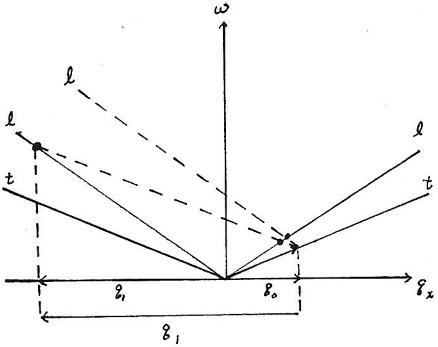


Fig. 14.4(b). Three-phonon collision process : $t_0 + t_1 \rightarrow l_2$. • indicates the point satisfying (14.37).[201]

In an isotropic crystal the two transverse waves are degenerate as shown in Figs 14.4(a) and (b). Only possible collision process for the longitudinal mode q_0 is illustrated by Fig. 14.4(a), and the corresponding process for the transverse phonon q_0 is shown in Fig. 14.4(b). In order to satisfy the condition of $\hbar\omega(q_1) \sim \hbar\omega(q_2) \sim k_0 T \gg \hbar\omega(q_0)$, it is necessary that V_l and V_t have nearly equal values. In the one-dimensional case the process $t_0 + l_1 \rightarrow l_2$ is forbidden but in the three-dimensional case it is possible if q_0 is nearly perpendicular to q_1 (See Fig. 14.3). This process is always possible irrespective of v_l and v_t and then it makes a significant contribution to the relaxation processes of the longwave length phonon q_0.

Factors in the dependence of $1/t(q_0)$ on T and q_0, for small q_0 and $T \ll \Theta_D$, obtained from (14.44) are listed in Table 14.1. Argument on the longitudinal wave in an anisotropic crystal will be given in the following.

Elasticity	any	Isotropic	Anisotropic
Polarization of q_0	Transverse	Longitudinal	Longitudinal
Area of conservation surface ΔS_1	q_1^2	q_0^2	$q_0^{1/2}\, q_1^{3/2}$
$\lvert \partial \Delta\omega / \partial q_{1n} \rvert^{-1}$	$q_0^{-1}\, q_1$	1	$q_0^{-1/2}\, q_1^{1/2}$
$t(q_0)^{-1}$	$q_0\, T^4$	$q_0^4\, T$	$q_0^2\, T^3$

Table 14.1 (q_0, T)-dependence of $1/t(q_0)$ for infinitesimal q_0 and $T \ll \Theta_D$. 201)

The factor $q_0 q_1 q_2 (N_1^{(0)} - N_2^{(0)})$ in (14.44) is proportional to $(q_0^2/T)\, q_1^2\, N_1^{(0)2}$ for $q_0 \to 0$. The dependence of the factors on q_1 is indicated explicitly in Table 14.1, but as the average q_1 of the modes with which q_0 collides is $\sim T$, q_1 is replaced by T in the final product.

By introducing anisotropic elasticity the degeneracy of the two transverse branches of the acoustic phonon spectrum is lifted, except in certain symmetry directions.

In the crystal with cubic symmetry, the sound velocities for $q \parallel [100]$ are

$$v_l = \sqrt{C_{11}/d}\ , \quad v_{t_1} = v_{t_2} = \sqrt{C_{44}/d}\ , \tag{14.45}$$

and for $q \parallel [111]$

$$v_l = \sqrt{\tfrac{1}{3}(C_{11} + 2C_{12} + 4C_{44})/d}\ , \quad v_{t_1} = v_{t_2} = \sqrt{\tfrac{1}{3}(C_{11} - C_{12} + C_{44})/d}\ , \tag{14.46}$$

while the degeneracy of the transverse branches is lifted for $q \parallel [110]$ as

$$v_l = \sqrt{\tfrac{1}{2}(C_{11} + C_{12} + 2C_{44})/d}\ , \quad v_{t_1} = \sqrt{\tfrac{1}{2}(C_{11} - C_{12})/d}\ , \quad v_{t_2} = \sqrt{C_{44}/d}\ . \tag{14.47}$$

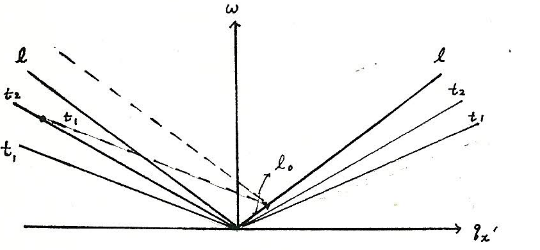


Fig. 14.5 (a). x'-axis is slightly deviated from the symmetry axis x. Collision process $l_0 + t_1 \rightarrow l_2$ with $q_0 \ll q_1, q_2$ is illustrated.[201)]

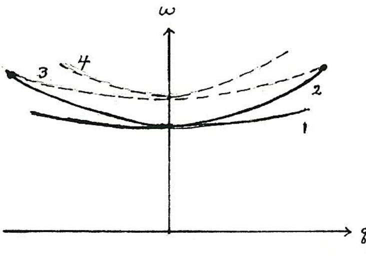


Fig. 14.5 (b). Dispersion relation of the tranverse branch spectrum in the plane normal to the symmetry axis x.[201)]

Fig. 14.5(a) indicates the scattering process $l_0 + t_1 \rightarrow l_2$, and its conservation law, where x'-axis is slightly deviated from the symmetry axis x.

Along x-axis the two transverse waves are degenerate. In Fig. 14.5 (b) dispersion relation of the transverse phonon spectrum with $q_x \neq 0$ is indicated. 1, 2, 3 and 4 represent $\omega_{t_1}(q_x, q_y)$, $\omega_{t_2}(q_x, q_y)$, $\omega_{t_1}(q_x+q_{x0}, q_y)$ and $\omega_{t_2}(q_x+q_{x0}, q_y)$, respectively. As is clearly shown in Fig. 14.5 (b) the intersection points • which satisfy the conservation law converge toward the symmetry line and the area of the conservation surface approaches zero, but the approach is less rapid than for the case of Fig. 14.4 (a). Namely, ΔS_1 is proportional to $q_0^{1/2} q_1^{3/2}$ as $q_0 \to 0$ and $|\partial \Delta\omega / \partial q_{1n}|^{-1}$ to $q_0^{-1/2} q_1^{1/2}$.[202] Consequently, we obtain $1/t(q_0) \propto q_0^2 T^3$. In this stage it is easy to verify the scaling law (14.34). The transformation $(q, T) \to (\lambda q, \lambda T)$ makes $N_1^{(0)} - N_2^{(0)}$ and $|\partial \Delta\omega / \partial q_{1n}|^{-1}$ unchanged, while $q_1 q_2 \to \lambda^2 q_1 q_2$ and $dS_1 \to \lambda^2 dS$, then we have

$$t(\lambda q_0, \lambda T)^{-1} = \lambda^5 t(q_0, T), \qquad T \ll \Theta_D. \qquad (14.48)$$

The above proof does not use any assumption on the magnitude of q_0.

Summarizing the results obtained in the preceding arguments, we have

$$t(q_0)^{-1} \propto A_l\, q_0^2 T^3 \text{ as } q_0 \to 0,\ T \ll \Theta_D \text{ for longitudinal modes,} \qquad (14.49)$$

and

$$t(q_0)^{-1} \propto A_t\, q_0 T^4 \text{ as } q_0 \to 0,\ T \ll \Theta_D \text{ for transverse modes.} \qquad (14.50)$$

The constant A_l may of course depend on the direction of q_0, though for cubic crystals the anisotropy is probably not very pronounced. At high temperatures $T \gg \Theta_0$, $t(q_0)^{-1} \propto T$. In the limited range of T and q_0 where these quantities are not small enough for (14.49) and (14.50) to apply, it is convenient to use the formula

$$1/t(q) = A q^{2+s} T^{3-s-\gamma}. \tag{14.51}$$

This satisfies the scaling law (14.48) for $\gamma = 0$. For longitudinal modes as $q \to 0$, $s \to 0$ and γ goes from 0 at low temperatures to 2 at high temperatures. On the other hand, for transverse modes, as $q \to 0$, $s \to -1$ and γ goes from 0 to 3.

By using (14.25) let estimate the temperature dependence of the phonon drag thermoelectric power. Since q_0 is comparable to the wave number of carriers, (14.49) yields

$$\overline{t(q)^{-1}} \propto \overline{k^2}\, T^3 \propto T^4. \tag{14.52}$$

Accordingly,

$$S_p \propto T^{-4} / T^{-3/2}\, T = T^{-7/2}, \tag{14.53}$$

where we employ the relation $f/\mu \propto 1/\tau_p \propto T^{3/2}$. If we use (14.51) instead of (14.49), S_p becomes as follows;

$$S_p \propto T^{-7/2 + s/2 + \gamma}. \tag{14.54}$$

At enough low temperatures the phonon mean free path is mainly limited by the scattering of the sample boundary and t is given by $\sim L/v_s$, where L denotes the sample dimension. Therefore, we have $S_p \propto T^{1/2}$. With increasing carrier concentration the scattering process by carriers plays an important role in $1/t(8)$. This makes the phonon drag thermoelectric power S_p decrease. This is called the saturation effect. Fig. 14.6 illustrates the effect in p-type silicon observed by Geballe and Hull. 203)

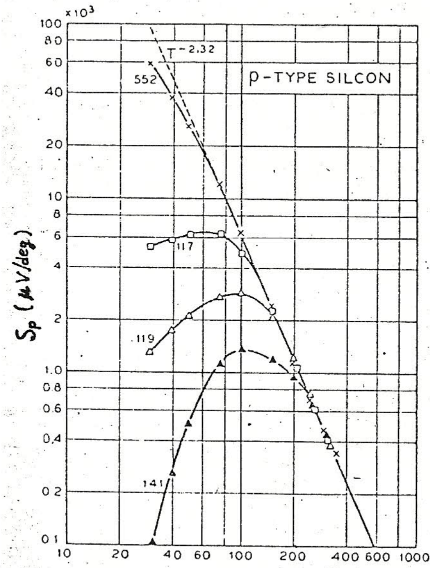


Fig. 14.6 Dependence of the S_p vs T plot on acceptor concentration for p-Si. 552: $N_A - N_D = 8\times10^{14}/\mathrm{cm}^3$, 117: 2.4×10^{16}, 119: 2.0×10^{17}, 141: 1.0×10^{18}. 203)

In this Section an outline of the intuitive theory due to Herring has been presented. This theory clarifies the physics contained in the phonon drag effect.

In the next Section the same problem will be treated by solving the coupled Boltzmann equations.

14.2 Theory of the Phonon Drag Effect based on the Boltzmann Equation

The thermoelectric and thermomagnetic effects in the degenerate semimetal with isotropic effective masses m_e and m_h illustrated in Fig. 14.7, are calculated by solving the two Boltzmann type equations for the electrons and phonons. Energies of electrons and holes are

$$\left\{\begin{aligned} &\varepsilon_e = E_e, \quad \varepsilon_h = \Delta - E_h, \\ &E_e = \frac{\hbar^2}{2m_e}k^2, \quad E_h = \frac{\hbar^2}{2m_h}k^2. \end{aligned}\right. \tag{14.55}$$

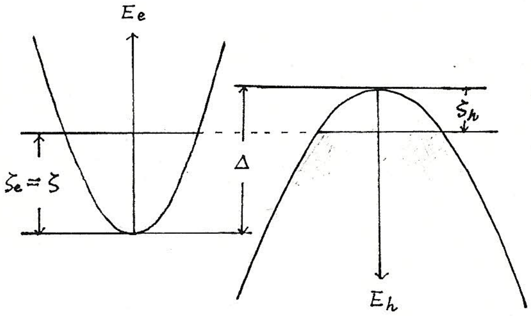


Fig. 14.7. Simple model of the degenerate semimetal.

Electron-phonon interaction is taken to be the deformation potential coupling induced by the longitudinal acoustic waves (cf. (7.4)).

In the presence of an electric and magnetic fields and a temperature gradient, the coupled Boltzmann equations are

$$\left\{\begin{aligned} &-e(\mathcal{E}\cdot v)\frac{\partial f_0^{(\lambda)}}{\partial \varepsilon_\lambda} - s(v\times h)\cdot\nabla_k f^{(\lambda)} + T(v\cdot\nabla T)\frac{\partial}{\partial T}\left(\frac{\varepsilon_\lambda - \zeta}{T}\right)\frac{\partial f_0^{(\lambda)}}{\partial \varepsilon_\lambda} = \left(\frac{\partial f^{(\lambda)}}{\partial t}\right)_{coll.} \\ &\frac{\partial N_q^0}{\partial T}(v_s\cdot\nabla T) = \left(\frac{\partial N_q}{\partial t}\right)_{carrier} - \frac{N_q - N_q^0}{t^{(r)}}, \quad (e>0) \end{aligned}\right. \tag{14.56}$$

where $s = eH/\hbar c$, $\mathbf{h} = \mathbf{H}/H$, $\lambda = (e, h)$, $\mathcal{E}, \nabla T \perp \mathbf{H}$, and $f^{(\lambda)}$ denotes the electron distribution function corresponding to λ-band. Hole distribution is $1 - f^{(h)}$. $\tau^{(r)}$ is defined by (14.28) and (14.31).

Since the coefficients β and $\mathcal{X}$, which are defined by (14.6), are related by $T\beta_{ij}(\mathbf{H}) = \mathcal{X}_{ji}(-\mathbf{H})$, in calculating the thermoelectric and thermomagnetic coefficients it is convenient to calculate $\mathcal{X}$ instead of β. This correponds to Π-approach treated in Section 14.1. The collision term $(\partial f^{(\lambda)}/\partial t)_{coll}$ is assumed to be in the form

$$\left(\frac{\partial f^{(\lambda)}}{\partial t}\right)_{coll.} = \left(\frac{\partial f^{(\lambda)}}{\partial t}\right)_{phonon} - \frac{f^{(\lambda)} - f_0^{(\lambda)}}{\tau_\lambda^{(r)}}, \qquad (14.57)$$

and the distributions for carriers and phonons are assumed as

$$\begin{cases} f^{(\lambda)} = f_0^{(\lambda)} - [\mathbb{V}^{(\lambda)}(\mathcal{E}) \cdot \hbar \mathbf{k}] \dfrac{\partial f_0^{(\lambda)}}{\partial \mathcal{E}_\lambda}, \\ N_q = N_q^\circ - [\mathbb{U}(\omega) \cdot \mathbf{q}] \dfrac{\partial N_q^\circ}{\partial \omega_q}. \end{cases} \qquad (14.58)$$

By use of the electron-phonon interaction (7.4) the rate of change of N_q due to interactions with carriers is given by

$$\left(\frac{\partial N_q}{\partial t}\right)_{carrier} = \frac{2\pi q^2}{\Omega d \omega_q} \sum_\lambda D_\lambda^2 \sum_k \delta(\mathcal{E}_{k'}^{(\lambda)} - \mathcal{E}_k^{(\lambda)} - \hbar\omega_q)\, \delta_{k',k+q} [(1 - f_k^{(\lambda)}) f_{k'}^{(\lambda)} (N_q + 1)$$

$$- f_k^{(\lambda)} (1 - f_{k'}^{(\lambda)}) N_q], \qquad (14.59)$$

where the interband transitions are disregarded. By inserting (14.58) into (14.59) and retaining the first order terms in $\mathbb{V}^{(\lambda)}$ and U, (14.59) becomes

$$\left(\frac{\partial N_q}{\partial t}\right)_{\text{carrier}} = -\frac{N_q - N_q^\circ}{t^{(c)}} + \frac{2\pi q^2}{\Omega\, d\omega_q}\beta N_q^\circ \sum_\lambda D_\lambda^2 \sum_k \left\{ [\mathbb{V}^{(\lambda)}(\mathcal{E}').\hbar k'] - [\mathbb{V}^{(\lambda)}(\mathcal{E}).\hbar k] \right\}$$

$$\times f_{ok}^{(\lambda)}(1 - f_{ok'}^{(\lambda)})\,\delta(\mathcal{E}_{k'}^{(\lambda)} - \mathcal{E}_k^{(\lambda)} - \hbar\omega_q)\,\delta_{k':k+q}\,, \qquad (14.60)$$

where

$$\frac{1}{t^{(c)}} = \frac{2\pi q^2}{\Omega\, d\omega_q}\frac{1}{N_q^\circ + 1}\sum_\lambda D_\lambda^2 \sum_k \delta(\mathcal{E}_{k'}^{(\lambda)} - \mathcal{E}_k^{(\lambda)} - \hbar\omega_q)\,\delta_{k':k+q}\, f_{oK}^{(\lambda)}(1 - f_{oK'}^{(\lambda)}).$$

$$(14.61)$$

(14.61) can be analytically integrated as follows. The summation over k is

$$\sum_k \cdots = \frac{\Omega}{(2\pi)^3}\int dk\, k^2 d\varphi_K \sin\theta_K d\theta_k\, \delta\left[\frac{\hbar^2}{2m_\lambda}(2kq\cos\theta_k + q^2) - \hbar\omega_q\right]$$

$$\times \frac{e^{\beta(\mathcal{E}_K + \hbar\omega_q - \zeta)}}{\left(e^{\beta(\mathcal{E}_K - \zeta)} + 1\right)\left(e^{\beta(\mathcal{E}_K + \hbar\omega_q - \zeta)} + 1\right)} = \frac{\Omega k_0 T e^z}{16\pi^2 q}\left(\frac{2m_\lambda}{\hbar^2}\right)^2 \int_{-\infty}^{\infty} \frac{dx}{(e^{-x} + 1)(e^{x+z} + 1)} \qquad (14.62)'$$

where $z = \beta\hbar\omega_q$. On making use of the relation

$$\int_{-\infty}^{\infty} \frac{dx}{(e^{-x} + 1)(e^{x+z} + 1)} = \frac{z}{e^z - 1}\,, \qquad (14.63)$$

$1/t^{(c)}(q)$ becomes

$$\frac{1}{t^{(c)}(q)} = \sum_\lambda \frac{1}{t^{(\lambda)}(q)} = \frac{\hbar q}{2\pi d}\sum_\lambda \left(\frac{m_\lambda}{\hbar^2}\right)^2 D_\lambda^2 . \qquad (14.64)$$

Ratio of $t^{(\lambda)}(k)$ to the carrier relaxation time $\tau^{(p)}_{\lambda}(k)$ due to the phonon scattering is given by

$$\frac{t^{(\lambda)}(k)}{\tau_{\lambda}^{(P)}(k)} = \frac{k_0 T}{\frac{1}{2} m_{\lambda} v_s^{2}} , \qquad (14.65)$$

where $\tau_{\lambda}^{(P)}$ is given by (7.15). By assuming $m_{\lambda} = 0.1\, m_0$ and $v_s = 4 \times 10^{5}$ cm/s (14.65) becomes 18.9 T. Consequently, $t^{(\lambda)}(k) \gg \tau_{\lambda}^{(P)}(k)$.

By expanding $\mathbb{V}^{(\lambda)}(\mathcal{E})$ in terms of power series in $x = (\mathcal{E}^{(\lambda)} - \zeta)/k_0 T$ as

$$\mathbb{V}^{(\lambda)}(\mathcal{E}) = \mathbb{V}^{(\lambda)}(\zeta) + \sum_{n=1}^{\infty} \mathbb{V}_n^{(\lambda)}(\zeta)\, x^{n} , \qquad (14.66)$$

$\mathbb{V}_n^{(\lambda)}$ can be obtained by iterating procedure. In the present problem the first term $\mathbb{V}^{(\lambda)}(\zeta)$ is enough. In the absence of a magnetic field the variation principle affords us a means of calculating $\mathbb{V}^{(\lambda)}$ and $\mathbb{U}$.204)

By using the approximation

$$\mathbb{V}^{(\lambda)}(\mathcal{E}) = \mathbb{V}^{(\lambda)}(\mathcal{E}') = \mathbb{V}^{(\lambda)}(\zeta) , \qquad (14.66)$$

(14.60) is rewritten as

$$\left(\frac{\partial N_q}{\partial t}\right)_{\text{carrier}} = - \frac{N_q - N_q^{\circ}}{t^{(c)}} + N_q^{\circ}(N_q^{\circ}+1) \sum_{\lambda} \frac{\hbar\, \mathbb{V}^{(\lambda)} \cdot \mathbf{q}}{k_0 T\, t^{(\lambda)}(q)} . \qquad (14.67)$$

Combining (14.67) with the kinetic equation for phonons in (14.56), we obtain the phonon drift velocity $\mathbb{U}(\omega)$ as follows:

$$\mathbb{U}(\omega) = \sum_{\mu} R_{\mu}\, \mathbb{V}^{(\mu)} , \quad (\nabla T = 0) \qquad (14.68)$$

where $$R_\lambda = t/t^{(\lambda)}, \quad 1/t = 1/t^{(c)} + 1/t^{(r)}. \tag{14.69}$$

In the presence of a temperature gradient $\mathbb{U}(\omega)$ is replaced by

$$\mathbb{U}(\omega) = -v_s^2\, t(q)\, \frac{\nabla T}{T} + \sum_\mu R_\mu \mathbb{V}^{(\mu)}. \tag{14.70}$$

The first term in the right hand side is equivalent to (14.15).

By inserting (14.58) into $(\partial f^{(\lambda)}/\partial t)_{phonon}$ in (14.57), $(\partial f_k^{(\lambda)}/\partial t)_{coll.}$ becomes

$$\left(\frac{\partial f_k^{(\lambda)}}{\partial t}\right)_{coll.} = -\frac{f_k^{(\lambda)} - f_{0k}^{(\lambda)}}{\tau_\lambda} + \left(\frac{\partial f_k^{(\lambda)}}{\partial t}\right)_{drag}, \tag{14.71}$$

where

$$1/\tau_\lambda = 1/\tau_\lambda^{(r)} + 1/\tau_\lambda^{(p)}. \quad 1/\tau_\lambda^{(p)} = \frac{D_\lambda^2}{2\pi\hbar}\left(\frac{k_0 T}{d\, v_s^2}\right)\left(\frac{2m_\lambda}{\hbar^2}\right)^{3/2} E_\lambda(k)^{1/2}. \tag{14.72}$$

As mentioned in Section 7.1, (14.72) is applicable to the case $\hbar v_s k/k_0 T \ll 1$. Usually this condition is satisfied in ordinary semiconductors and semimetals except at low temperatures. $(\partial f_k^{(\lambda)}/\partial t)_{drag}$ is the term originating from the deviation of the phonon distribution. Namely, its concrete expression is

$$\left(\frac{\partial f_k^{(\lambda)}}{\partial t}\right)_{drag} = -\frac{\hbar(\tau_\lambda^{(p)})^{-1}}{4k^4}\int_0^{2k} dq\, q^3\, (\mathbb{U}(\omega_q)\cdot k)\, \frac{\partial f_{0k}^{(\lambda)}}{\partial \varepsilon_\lambda}. \tag{14.73}$$

By introducing (14.70) into (14.73) and combining with (14.56), the simultaneous equation for $\mathbb{V}^{(e)}$ and $\mathbb{V}^{(h)}$ is written in the form :

$$\mathbb{V}^{(\lambda)} - \delta_\lambda \theta_\lambda (\mathbf{h} \times \mathbb{V}^{(\lambda)}) - r_\lambda \sum_\mu \langle R_\mu \rangle_\lambda \mathbb{V}^{(\mu)} = -\delta_\lambda \mu_\lambda \mathcal{E} - L_\lambda \frac{\nabla T}{T} , \qquad (14.74)$$

where

$$\left\{ \begin{aligned} & \delta_\lambda = \begin{cases} 1 : \text{electron}, \\ -1 : \text{hole}, \end{cases} \qquad \theta_\lambda = \omega_\lambda \tau_\lambda , \quad \omega_\lambda = \frac{eH}{m_\lambda c} , \quad \mu_\lambda = \frac{e\tau_\lambda}{m_\lambda} , \\ & r_\lambda = \frac{\tau_\lambda}{\tau_\lambda^{(P)}} , \quad \langle R_\mu \rangle_\lambda = \frac{1}{4k_\lambda^4} \int_0^{2k_\lambda} dq\, q^3 R_\mu , \\ & L_\lambda = r_\lambda v_s^2 \langle t \rangle_\lambda + \frac{\delta_\lambda \tau_\lambda}{m_\lambda} (\varepsilon_\lambda - \zeta) , \quad \langle t \rangle_\lambda = \frac{1}{4k_\lambda^4} \int_0^{2k_\lambda} dq\, q^3 t(q) . \end{aligned} \right. \qquad (14.75)$$

In (14.74) $\mathcal{E} + \nabla\zeta/e$ is replaced by $\mathcal{E}$. L_λ in (14.74) and (14.75) includes a term proportional to $(\varepsilon_\lambda - \zeta)$. As mentioned in (14.66) only the terms proportional to the zeroth order of $x \equiv (\varepsilon - \zeta)/k_0 T$ are retained. Therefore, the expression of L_λ is inconsistent with the spirit of the present approximation. In order to perform the calculation consistently, it is needed to develop $\mathbb{V}^{(\lambda)}$ up to the order of $n = 1$. However, as far as we concern the phonon drag effect, this term is immaterial. Clearly, this term is related to the diffusion term of the thermoelectric power.

(14.70) and (14.74) are the basic equations describing the thermoelectric and thermomagnetic effects in the presence of the deviation of the phonon distribution. These equations were firstly derived by L. É. Gurevich and Korenblit.[205] Gurevich is a physicist who predicted the phonon drag effect.[195]

At first we shall consider the case without magnetic field. In the configuration of $\mathcal{E} \parallel \nabla T \parallel x$ (14.74) becomes

$$\begin{cases} V^{(e)}(1-\Gamma_e^{(e)}) - V^{(h)}\Gamma_e^{(h)} = -\mu_e \mathcal{E} - L_e \dfrac{\nabla T}{T}, \\ -V^{(e)}\Gamma_h^{(e)} + V^{(h)}(1-\Gamma_h^{(h)}) = \mu_h \mathcal{E} - L_h \dfrac{\nabla T}{T}, \end{cases} \tag{14.76}$$

where

$$\Gamma_\lambda^{(\mu)} = r_\lambda \langle R_\mu \rangle_\lambda < 1, \tag{14.77}$$

is the mutual drag coefficient which was already introduced in Sections 6.5 and 14.1.

(14.76) provides

$$\begin{cases} V^{(e)} = \Delta^{-1}\left\{\mathcal{E}\left[-\mu_e(1-\Gamma_h^{(h)}) + \mu_h \Gamma_e^{(h)}\right] - \dfrac{\nabla T}{T}\left[L_e(1-\Gamma_h^{(h)}) + L_h \Gamma_e^{(h)}\right]\right\}, \\ V^{(h)} = \Delta^{-1}\left\{\mathcal{E}\left[\mu_h(1-\Gamma_e^{(e)}) - \mu_e \Gamma_h^{(e)}\right] - \dfrac{\nabla T}{T}\left[L_h(1-\Gamma_e^{(e)}) + L_e \Gamma_h^{(e)}\right]\right\}, \end{cases} \tag{14.78}$$

where

$$\Delta = (1-\Gamma_e^{(e)})(1-\Gamma_h^{(h)}) - \Gamma_e^{(h)}\Gamma_h^{(e)}. \tag{14.79}$$

Apart from the term proportional to ∇T (14.78) is equivalent to (14.32). Combining (14.78) and (14.70), one obtains

$$U(\omega) = \frac{\mathcal{E}}{\Delta}\left\{\left[-\mu_e\left(1-\Gamma_h^{(h)}\right) + \mu_h \Gamma_e^{(h)}\right]R_e + \left[\mu_h\left(1-\Gamma_e^{(e)}\right) - \mu_e \Gamma_h^{(e)}\right]R_h\right\}$$

$$-\frac{1}{\Delta}\frac{\nabla T}{T}\left\{t v_s^2 + \left[L_e\left(1-\Gamma_h^{(h)}\right) + L_h \Gamma_e^{(h)}\right]R_e\right.$$

$$\left. + \left[L_h\left(1-\Gamma_e^{(e)}\right) + L_e \Gamma_h^{(e)}\right]R_h\right\}. \tag{14.80}$$

By using (14.78) and (14.80) we can calculate β_{xx} and χ_{xx}. It is readily shown that the Onsager relation $\beta_{xx} = \chi_{xx}/T$ is satisfied for the phonon drag term if the phonon distribution N_q° is approximated by the classical distribution.

By putting $\nabla T = 0$ in (14.80) the phonon drag thermoelectric power is calculated in the following. The thermal current density w_p is

$$w_p = \sum_q \hbar\omega_q v_s\left(\frac{q_x}{q}\right)N_q = \beta\sum_q U(\omega_q)(\hbar v_s q_x)^2 N_q^{\circ}(N_q^{\circ}+1)$$

$$= \frac{k_0 T}{3}\sum_q U(\omega_q)\left(\frac{\hbar\omega_q}{k_0 T}\right)^2 N_q^{\circ}(N_q^{\circ}+1) = \left(\chi_p^{(e)} + \chi_p^{(h)}\right)\mathcal{E}, \tag{14.81}$$

where

$$\left\{\begin{aligned} \chi_p^{(e)} &= -\frac{k_0 T}{3}\,\frac{(1-\xi_e)}{\Delta}\sum_q \mu_e R_e(q)\left(\frac{\hbar\omega_q}{k_0 T}\right)^2 N_q^{\circ}(N_q^{\circ}+1), \\ \chi_p^{(h)} &= \frac{k_0 T}{3}\,\frac{(1-\xi_h)}{\Delta}\sum_q \mu_h R_h(q)\left(\frac{\hbar\omega_q}{k_0 T}\right)^2 N_q^{\circ}(N_q^{\circ}+1), \end{aligned}\right. \tag{14.82}$$

$$1-\xi_e = 1-\Gamma_h^{(h)} - \left(\frac{\mu_h}{\mu_e}\right)\Gamma_e^{(h)}, \quad 1-\xi_h = 1-\Gamma_e^{(e)} - \left(\frac{\mu_e}{\mu_h}\right)\Gamma_h^{(e)}. \qquad (14.83)$$

By using (14.65) and (14.64) $\mu_e R_e$ is written as

$$\mu_e R_e = \frac{e\tau_e}{m_e}\,\frac{t(q)}{t^{(e)}(q)} = \frac{e\tau_e}{m_e\tau_e^{(p)}}\,\frac{\tau_e^{(p)}(k_F^{(e)})}{t^{(e)}(k_F^{(e)})}\,\frac{q}{k_F^{(e)}}\,t(q)$$

$$= \frac{e v_s^2}{2k_0T}\, r_e \left(\frac{q}{k_F^{(e)}}\right) t(q), \quad (k_F^{(e)} : \text{Fermi wave number}) \qquad (14.84)$$

then $\chi_p^{(e)}$ becomes

$$\chi_p^{(e)} = -\frac{e v_s N_e}{2}\left(\frac{1-\xi_e}{\Delta}\right)\langle \mathcal{L}(q)\rangle_e, \qquad (14.85)$$

where

$$\langle \mathcal{L}(q)\rangle_e = \frac{r_e}{4(k_F^{(e)})^4}\int_0^{2k_F^{(e)}} dq\, q^3 \left(\frac{\hbar\omega_q}{k_0T}\right)^2 N_q^0(N_q^0+1)\,\mathcal{L}(q),$$

$$\mathcal{L}(q) = v_s t(q), \quad N_e = \frac{1}{3\pi^2}(k_F^{(e)})^3 : \text{electron density} \qquad (14.86)$$

Similarly,

$$\chi_p^{(h)} = \frac{e v_s N_h}{2}\left(\frac{1-\xi_h}{\Delta}\right)\langle \mathcal{L}(q)\rangle_h. \qquad (14.87)$$

Finally, the phonon drag thermopower becomes

$$S_p = \frac{v_s}{2T}\left\{-N_e\left(\frac{1-\xi_e}{\Delta}\right)\langle \mathcal{L}(q)\rangle_e + N_h\left(\frac{1-\xi_h}{\Delta}\right)\langle \mathcal{L}(q)\rangle_h\right\}(N_e\bar{\mu}_e + N_h\bar{\mu}_h)^{-1}. \qquad (14.88)$$

$\bar{\mu}_e$ and $\bar{\mu}_h$ are

$$\bar{\mu}_e = \mu_e\left(\frac{1-\xi_e}{\Delta}\right), \quad \bar{\mu}_h = \mu_h\left(\frac{1-\xi_h}{\Delta}\right). \tag{14.89}$$

By inserting (14.89) into (14.88) S_p is rewritten as

$$S_p = \frac{v_s}{2T}\left\{-N_e(1-\xi_e)\langle \mathcal{L}(8)\rangle_e + N_h(1-\xi_h)\langle \mathcal{L}(8)\rangle_h\right\}$$

$$\times\left\{N_e(1-\xi_e)\mu_e + N_h(1-\xi_h)\mu_h\right\}^{-1}. \tag{14.90}$$

This is the generalization of the Herring formula (14.18)
In the approximation neglecting $\Gamma_\lambda^{(u)}$, the diffusion contribution to the thermoelectric power is already obtained in Section 6.4.
Namely,

$$S_d = S_d^{(e)} + S_d^{(h)} = \frac{n+3/2}{3}\left(\frac{\pi^2 k_0^2 T}{e}\right)\left(\frac{\sigma_h/\zeta_h - \sigma_e/\zeta_e}{\sigma_e + \sigma_h}\right) \tag{14.91}$$

$$= \frac{S^{(h)}\sigma_h + S^{(e)}\sigma_e}{\sigma_h + \sigma_e},$$

where

$$S^{(\lambda)} = \pm\frac{n+3/2}{3}\left(\frac{\pi^2 k_0^2 T}{e\,\zeta_\lambda}\right). \quad (\lambda = h, e). \tag{14.92}$$

In deriving (14.91) and (14.92) we assume $\tau_\lambda \propto (E_\lambda/\zeta_\lambda)^n$.

When only one type of carriers is present, ratio of S_p to S_d is

$$\frac{S_p}{S_d} = \frac{3}{\pi^2(n+3/2)}\left(\frac{m^* v_s^2}{2k_0T}\right)\left(\frac{\zeta}{k_0T}\right)\frac{\langle t(8)\rangle}{\tau} = \frac{3}{\pi^2(n+3/2)}\left(\frac{\zeta}{k_0T}\right)\frac{\tau^{(p)}(\zeta)}{\tau(\zeta)}\frac{\langle t(8)\rangle}{t^{(c)}(k_F)}. \tag{14.93}$$

If the temperature is high enough and the conditions : i) $\hbar v k_F / k_0 T \ll 1$, ii) $\mathcal{L}(q) \propto q^{-s} T^{-5+s}$, iii) $1/\tau \cong 1/\tau^{(p)} \propto T$, are satisfied; (14.93) leads to $S_p / S_d \propto T^{-6+s}$ and $S_p \propto T^{-5+s}$. At enough low temperatures if the conditions : i) $\hbar v_s k_F / k_0 T \gg 1$, ii) $\mathcal{L}(q) \simeq L$ (sample dimension), iii) $1/\tau \simeq$ constant and $1/\tau^{(p)} \propto T^n$, are fulfilled ; we have $S_p / S_d \propto T^{n+2}$ and $S_p \propto T^{n+3}$ which tends to zero with $T \to 0$.

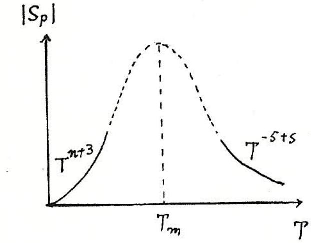


Fig. 14.8 Temperature dependence of the phonon drag thermopower in the degenerate system with one type of carriers.

Therefore, $|S_p|$ exhibits a maximum at a temperature T_m.

(14.93) gives a possibility that the phonon drag thermoelectric power considerably exceeds the diffusion term over a certain temperature range.

As is seen in (14.88) or (14.90), in semimetals electron and hole contributions cancel each other and the situation is more complicated than that of semiconductors. In typical semimetals bismuth, antimony and graphite the anomalous behaviors which are ascribed to the phonon drag effect, have been observed.

An example observed in graphite is illustrated in Fig. 14.9. 206) Kish graphite is a best sample which is nearly close to the single crystal graphite. Negative dip observed around 35 K is considered to be due to the phonon drag effect.[207]

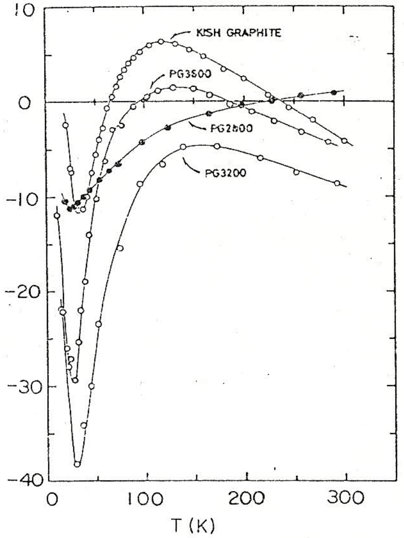


Fig. 14.9 Thermoelectric power of graphite.[206] PG means pyrolytic graphite and number indicates the heat treatment temperature.

Absolute magnitude of the thermopower is small, which is due to the self-cancellation between electron and hole contributions.[207]

In the presence of a magnetic field dramatic change appears in the thermoelectric and thermomagnetic phenomena. Mobile carriers are strongly affected by applying magnetic field and its influence also appears in the phonon drag effect.

In the configuration of $H \parallel z$, $\mathcal{E}$, $\nabla T \perp H$, $V^{(e)}$ and $V^{(h)}$ are given by solving the equation:

$$\mathcal{D} \begin{pmatrix} V_x^{(h)} \\ V_y^{(h)} \\ V_x^{(e)} \\ V_y^{(e)} \end{pmatrix} = \begin{pmatrix} \mu_h \mathcal{E}_x - L_h \dfrac{\nabla_x T}{T} \\ \mu_h \mathcal{E}_y - L_h \dfrac{\nabla_y T}{T} \\ -\mu_e \mathcal{E}_x - L_e \dfrac{\nabla_x T}{T} \\ -\mu_e \mathcal{E}_y - L_e \dfrac{\nabla_y T}{T} \end{pmatrix}, \qquad (14.94)$$

where

$$\mathcal{D} = \begin{bmatrix} 1-\Gamma_h^{(h)} & -\theta_h & -\Gamma_h^{(e)} & 0 \\ \theta_h & 1-\Gamma_h^{(h)} & 0 & -\Gamma_h^{(e)} \\ -\Gamma_e^{(h)} & 0 & 1-\Gamma_e^{(e)} & \theta_e \\ 0 & -\Gamma_e^{(h)} & -\theta_e & 1-\Gamma_e^{(e)} \end{bmatrix}, \qquad (14.95)$$

$$\det \mathcal{D} = (1-\Lambda)^2 + \theta_h^2 (1-\Gamma_e^{(e)})^2 + \theta_e^2 (1-\Gamma_h^{(h)})^2 - 2\theta_e \theta_h \Gamma_e^{(h)} \Gamma_h^{(e)} + \theta_e^2 \theta_h^2$$

$$\Lambda = \Gamma_h^{(h)} + \Gamma_e^{(e)} - \Gamma_h^{(h)} \Gamma_e^{(e)} + \Gamma_e^{(h)} \Gamma_h^{(e)} .$$

By substituting $V_{x,y}^{(e)}$ and $V_{x,y}^{(h)}$ into (14.70), the thermoelectric and thermomagnetic coefficients due to the phonon drag effect are obtained. Most important coefficients are the thermoelectric power (magneto-Seebeck coefficient) and Nernst-Ettingshausen coefficient (cf. (6.139)).

Fig. 14.10 indicates the temperature dependence of the thermoelectric power of bismuth with magnetic field.[208] Negative dip rapidly increases with magnetic field. Fig. 14.11 represents an example of the Nernst-Ettingshausen coefficient of bismuth.[208] Similar experiments were carried out by Korenblit et al[209] and the detailed theory was presented by Korenblit.[210]

In Fig. 14.10 the solid line represents a certain direction of the magnetic field, while the dashed line represents the reversed direction.

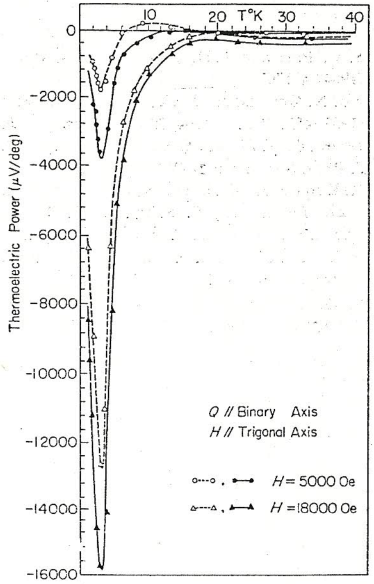


Fig. 14.10 Temperature dependence of the thermoelectric power of bismuth in strong magnetic field. Q indicates the heat current. (After Farag and Tanuma.[208])

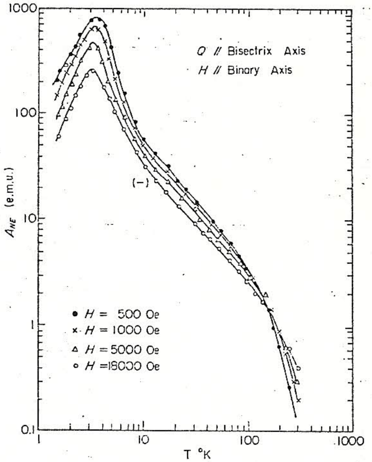


Fig. 14.11 Temperature dependence of the Nernst-Ettingshausen coefficient of bismuth with magnetic field as a parameter. (After Farag and Tanuma[208])

Up to now we have considered mainly the phonon drag effect on the thermoelectric and thermomagnetic effects and paid little attention to the influence on the electrical conductivity. Usually, the effect of the deviated phonon distribution on the electrical conductivity has been considered to be small. In Section 12.1 it is pointed out that in strong magnetic field σ_{xx} becomes very small if the deviation of the phonon distribution from thermal equilibrium is large ($t^{(r)} \gg t^{(c)}$).

This effect was ascertained in the measurement of the magnetoresistivity of antimony at helium temperature.[21] Now, we shall briefly mention about it.

From (14.94) and (14.95) $\mathbf{V}^{(h)}$ and $\mathbf{V}^{(e)}$ can be readily obtained.

In strong magnetic field $\theta_e, \theta_h \gg 1$ ($\nabla T = 0$) $\mathbf{V}^{(h)}$ and $\mathbf{V}^{(e)}$ become as follows:

$$\begin{cases} \mathbf{V}^{(h)} = \mathbf{V}_d + \dfrac{\mathbf{h} \times \mathbf{V}_d}{\theta_h}\left(1 - \Gamma_h^{(h)} - \Gamma_h^{(e)}\right), \quad \mathbf{h} = \dfrac{\mathbf{H}}{H}, \\[2ex] \mathbf{V}^{(e)} = \mathbf{V}_d - \dfrac{\mathbf{h} \times \mathbf{V}_d}{\theta_e}\left(1 - \Gamma_e^{(e)} - \Gamma_e^{(h)}\right), \quad \mathbf{V}_d = \dfrac{c}{H}(\mathcal{E} \times \mathbf{h}). \end{cases} \tag{14.96}$$

Then, we have

$$\begin{cases} \sigma_{xx}^{(h)} = N_h \left(\dfrac{c}{H}\right)^2 \dfrac{m_h}{\tau_h}\left(1 - \Gamma_h^{(h)} - \Gamma_h^{(e)}\right), \\[2ex] \sigma_{xx}^{(e)} = N_e \left(\dfrac{c}{H}\right)^2 \dfrac{m_e}{\tau_e}\left(1 - \Gamma_e^{(e)} - \Gamma_e^{(h)}\right), \end{cases} \tag{14.97}$$

where $1/\tau_\lambda$ ($\lambda = h, e$) is composed of the two contributions; the impurity scattering term and the phonon scattering term:

$$1/\tau_\lambda = 1/\tau_\lambda^{(i)} + 1/\tau_\lambda^{(p)}. \tag{14.98}$$

In consideration of the definition of Γ and (14.98), (14.97) is rewritten in the form

$$\sigma_{xx}^{(\lambda)} = (\sigma_{xx}^{(\lambda)})_{imp.} + (\sigma_{xx}^{(\lambda)})_p (1 - \bar{\gamma}_\lambda), \quad (\lambda = h. e) \tag{14.99}$$

where

$$\begin{cases} (\sigma_{xx}^{(\lambda)})_{imp.} = N_\lambda \left(\dfrac{c}{H}\right)^2 \dfrac{m_\lambda}{\tau_\lambda^{(i)}}, \quad (\sigma_{xx}^{(\lambda)})_p = N_\lambda \left(\dfrac{c}{H}\right)^2 \dfrac{m_\lambda}{\tau_\lambda^{(p)}}, \\ \\ \bar{\gamma}_\lambda = \langle R_\lambda \rangle_\lambda + \langle R_\mu \rangle_\lambda \quad (\mu \neq \lambda). \end{cases} \tag{14.100}$$

Accordingly,

$$\sigma_{xx} = \sigma_{xx}^{(h)} + \sigma_{xx}^{(e)} = (\sigma_{xx})_{imp.} + (\sigma_{xx})_p (1 - \bar{\gamma}), \tag{14.101}$$

where

$$\begin{cases} (\sigma_{xx})_{imp.} = (\sigma_{xx}^{(h)})_{imp.} + (\sigma_{xx}^{(e)})_{imp}, \\ \\ (\sigma_{xx})_p = (\sigma_{xx}^{(h)})_p + (\sigma_{xx}^{(e)})_p, \\ \\ \bar{\gamma} = \dfrac{\sigma_{xx}^{(h)} \bar{\gamma}_p + \sigma_{xx}^{(e)} \bar{\gamma}_e}{\sigma_{xx}^{(h)} + \sigma_{xx}^{(e)}}. \end{cases} \tag{14.102}$$

Tsai et al cleverly estimated $(\sigma_{xx})_p$ by using the difference between the adiabatic conductivity and the isothermal conductivity.211) From this estimation they evaluated $\bar{\gamma} \cong 0.93$ which is close to unity. This means that in antimony phonons are strongly scattered by carriers even at helium temperatures and this fact was confirmed by the measurement of the lattice thermal conduction at low temperatures.212)

14.3 Two-Stage Drag Effect

In the usual theory of the phonon drag effect in semiconductors and semimetals the collision process of a long wave phonon, which can interact with carriers, with the thermal phonons is described by a relaxation time $t(8)$. In this case the thermal phonons do not participate in the kinetic equation. Namely, it is implicitly assumed that the thermal phonons come to an equilibrium state through the active Umklapprocess (U-process). However, with decreasing temperatures the U-process becomes inactive as compared with the Normal process (N-process) and accordingly the thermal phonons deviate from the thermal equilibrium. Then, the thermal phonons drag carriers via the long wave phonons. This is called the two stage drag effect.213, 214) Since the effect is proportional to the relaxation time $t^{(U)}$ of the U-process, at low temperatures it rapidly increases as $\exp(\alpha \Theta_D / T)$, where $\alpha \sim 1$.

With further decrease of temperatures the relaxation process of the phonon system is limited by the scattering with sample boundary and the two-stage drag effect disappears. In the well-crystalline samples with large dimension the boundary scattering does not play an important role even at low temperatures. Then, the two-stage drag effect survives at low temperatures.

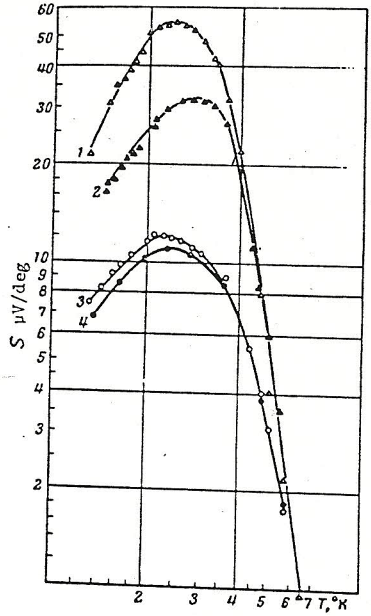


Fig. 14.12 Temperature dependence of the thermoelectric power of Bi. Sample 1 — 6 mm diameter, $b = \rho(300K)/\rho(4.2K) = 450$; 2— 6 mm diameter with deformation, $b = 350$; 3— 2.5 mm diameter, $b = 250$; 4 – 2.5 diameter with deformation, $b = 190$. (After Kopylov and Mezhov-Deglin 213))

In very pure Bi specimens with large dimensions Kopylov and Mezhov-Deglin observed an effect which seems to be the two-stage drag effect. 213) This is shown in Fig. 14.12. They made sure of drastic reduction of the effect after cut or deformation of these samples. The best sample 1 exhibits an exponential dependen of the thermoelectric power on T above 3 K.

Theories on this effect were presented by Kozlov-Nagaev and Kozlov. 214) The Physics of the two-stage drag effect is explainable by using the following simple consideration. This is essentially similar to the procedure employed in Section 6.5.

Denote the crystal momentums of the electron, long wave phonon and thermal phonon systems by P_e, P_L and P_T, respectively, and the kinetic equations govering these quantities are given by the following equations (See Fig. 14.12).

$$\left\{\begin{aligned} \frac{dP_e}{dt} &= -\frac{P_e}{\tau^{(P)}} + \frac{P_L}{t^{(e)}} - ne\mathcal{E}, \\ \frac{dP_L}{dt} &= \frac{P_e}{\tau^{(P)}} - \frac{P_L}{t^{(e)}} - \frac{P_L}{t^{(T)}} + \frac{P_T}{t^{(L)}}, \\ \frac{dP_T}{dt} &= \frac{P_L}{t^{(T)}} - \frac{P_T}{t^{(L)}} - \frac{P_T}{t^{(U)}}. \end{aligned}\right. \qquad (14.103)$$

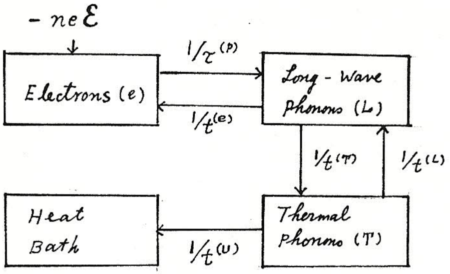


Fig. 14.13 Momentum transfer of the electron, long-wave phonon and thermal phonon systems.

In the stationary state the left hand sides of these equations are zero. Then, we obtain

$$P_L = -ne\mathcal{E}\, t^{(T)}\left(1 + t^{(U)}/t^{(L)}\right). \qquad (14.104)$$

From the heat current of the long-wave phonon system is $W_p = v_s^2 P_L$, the two-stage phonon drag thermopower becomes

$$S_p = S_p^{(0)}\left(1 + t^{(U)}/t^{(L)}\right), \qquad (14.105)$$

where $S_p^{(0)}$ denotes the usual phonon drag thermopower. At low temperatures $t^{(U)}/t^{(L)} \gg 1$ and its main temperature dependence is given by $e^{\alpha\Theta_D/T}$ which increases rapidly with decreasing temperature.

Chapter 15 Theory of the Galvanomagnetic Effects with Magnetic Breakdown

15.1 Application of the Chambers' Theory to the Case with Magnetic Breakdown

In Section 12.6 the probability for magnetic breakdown (MB) was obtained quantum mechanically from a calculation of the transition rate between different magnetic levels, the periodic potential acting as the perturbation. The conclusion obtained there is as follows: the probability for magnetic breakdown is given by

$$P = e^{-H_0/H}, \tag{15.1}$$

where

$$\hbar\omega_0 E_F \simeq E_g{}^2, \quad \omega_0 = eH_0/m^*c, \tag{15.2}$$

E_g denotes the energy gap and E_F is the Fermi energy.[167]~[169]

(15.2) is a remarkable result because it indicates that the threshold field for MB is not given by the condition $\hbar\omega_0 \sim E_g$ but by (15.2).

(15.2) gives a field intensity which is attainable in our laboratories

In Section 12.6 the condition (15.2) was obtained on the basis of a simple model. However, it is a general relation which is applicable to any band models in arbitrary field strength.[168],[169]

In the presence of MB different orbits couple each other and the

the connectivity of the orbits drastically changes with field strength and new types of behavior should be expected.

In this Section we shall formulate the expression of the conductivity tensor which can be applicable to the case with magnetic breakdown.[215]

From the Chambers' theory (Section 13.1, (13.7)) the conductivity tensor σ_{ij} is given by

$$\sigma_{ij} = -\frac{2e^2}{(2\pi)^3}\int d\boldsymbol{k}\, v_i(\boldsymbol{k})\,\frac{df_0}{dE}\int_{-\infty}^{t(\boldsymbol{k})} ds\; v_j(s)\exp\left(-\frac{t(\boldsymbol{k})-s}{\tau}\right), \tag{15.3}$$

where $v_j(s)$ is obtained from the set of equations

$$\hbar\dot{\boldsymbol{k}} = -\frac{e}{c}(\boldsymbol{v}\times\boldsymbol{H}), \quad \boldsymbol{v}(\boldsymbol{k}) = \frac{1}{\hbar}\nabla_{\boldsymbol{k}} E(\boldsymbol{k}). \tag{15.4}$$

In order to include the magnetic breakdown effect, following additional assumption is made. At a finite number of points in the orbit there may exist a finite probability of transition to (and from) another points in other orbits. These are the points where the energy gaps small enough to permit an interband transition. The orbits corresponding to $H\to\infty$ are those closer to the free-electron behavior, i.e., are those which at the transition points show no "Bragg reflection (BR)" due to the lattice potential.

The orbits corresponding to $H\to 0$ are those obtained semiclassically by solving (15.4) for separate, isolated sheets of energy surface with $E(k)$.

Let define the path integral

$$I_j(k) = \exp[-t(k)/\tau] \int_{-\infty}^{t(k)} v_j(s)\, e^{s/\tau}\, ds. \qquad (15.5)$$

(15.4) allows us to introduce a new set of variables (E, t, k_z) instead of $\mathbf{k}$. Then,

$$d\mathbf{k} = \frac{eH}{\hbar^2 c}\, dE\, dt\, dk_z, \qquad (15.6)$$

where $\mathbf{H}$ is parallel to the z-axis, and (15.3) becomes

$$\sigma_{ij} = -\frac{e^2 m^* \omega}{4\pi^3 \hbar^2} \int dE \frac{df_0}{dE} \int dk_z \int_{-\infty}^{t(K)} dt'\, v_i(t')\, I_j(t'), \quad \left(\omega = \frac{eH}{m^* c}\right). \qquad (15.7)$$

Consider the complete network of the orbits for given E, k_z divided into n pieces and each piece is travelled by the electrons in the same length of time t_0. All points at which breakdown is possible should coincide with end-points of the isochronous pieces (See Fig. 14.14).

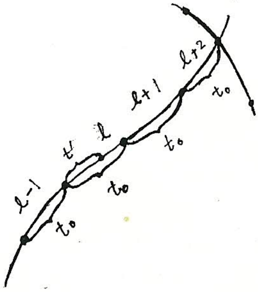


Fig. 14.14 Isochronous division of network of the electron orbits.

Rewriting (15.7), we obtain

$$\sigma_{ij} = -\frac{e^2 m^* \omega}{4\pi^3 \hbar^2} \sum_{\ell=1}^{n} \int dE \frac{df_0}{dE} \int dk_z \int_0^{t_0} v_i(t', \ell)\, I_j(t', \ell)\, dt',$$

$$I_j(t', \ell) = e^{-t'/\tau} \left\{ \int_0^{t'} dt''\, v_j(t'', \ell)\, e^{t''/\tau} + K_j(\ell) \right\},$$

$$K_j(\ell) = \sum_{p=1}^{\infty} \int_0^{t_0} dt''\, v_j(t'', \ell - p)\, e^{(t'' - p t_0)/\tau} \qquad (15.8)$$

where $(\ell - p)$ is determined modulo n. It is now convenient to express $K_j(\ell)$ in a vector form.

Define

$$\mathbb{K}_j = \begin{bmatrix} K_j(1) \\ K_j(2) \\ \vdots \\ K_j(n) \end{bmatrix}, \quad \mathbb{V}_j = \begin{bmatrix} V_j(1) \\ V_j(2) \\ \vdots \\ V_j(n) \end{bmatrix}, \quad V_j(r) = \int_0^{t_0} dt'' \, v_j(t'', r) \, e^{t''/\tau}. \qquad (15.9)$$

and

$$\mathbb{M} = \begin{bmatrix} 0 & 0 & 0 & \cdots & 0 & 0 \\ 1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 1 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & \cdots & 1 & 0 \end{bmatrix}, \quad \begin{array}{l} M_{\ell, r} = \delta_{\ell, r+1} \\ \ell, r : \text{modulo } n. \end{array} \qquad (15.10)$$

$\delta_{\ell-1, r}$

$r \to \ell$ a transition

Then, $\mathbb{K}_j$ is expressed by

$$\mathbb{K}_j = \sum_{p=1}^{\infty} \mathbb{M}^p \cdot \mathbb{V}_j \, e^{-pt_0/\tau} = \mathbb{M} e^{-t_0/\tau} \cdot \mathbb{Y} \cdot \mathbb{V}_j, \qquad (15.11)$$

where

$$\mathbb{Y} = (\mathbb{1} - \mathbb{M} e^{-t_0/\tau})^{-1} \qquad (15.12)$$

$\mathbb{1}$ is the $n \times n$ unit matrix. This rewriting (15.11) adds nothing new but makes the expression unnecessarily complicated. However, by changing the definition of the matrix $\mathbb{M}$ it is readily to generalize the Chambers' formula (15.7) to the case with magnetic breakdown.

In this case $M_{\ell r}$ will be equal to 1, 0, P or $Q = (1 - P)$, depending on the network considered as well as on the pieces l and r.

In the following two Sections we shall calculate the galvanomagnetic coefficients for simple examples.

15.2 Magnetoresistance for the Electron Orbit with a One-dimensional Periodic Potential

Consider the simple case treated in Section 12.6 (See Figs. 14.15 (a), (b)).

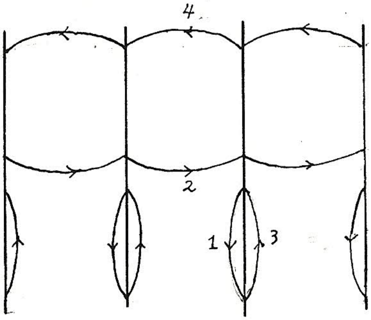


Fig. 14.15 (a) Three Bragg-reflected orbits in coordinate space: $2 \to 2 \to 2 \cdots$, $4 \to 4 \to 4 \cdots$, $1 \to 3 \to 1 \to 3 \cdots$.

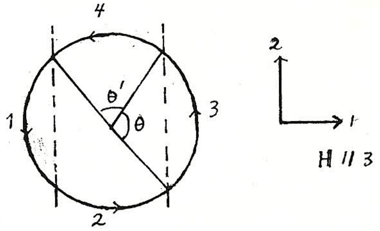


Fig. 14.15 (b) Magnetic breakdown orbit : $1 \to 2 \to 3 \to 4 \to 1$.

Assume that $\theta = \theta' = 90°$.

The transition matrix M takes the form :

$$M = \begin{array}{c} \begin{array}{cccc} 1 & 2 & 3 & 4 \end{array} \\ \left[\begin{array}{cccc} 0 & 0 & Q & P \\ P & Q & 0 & 0 \\ Q & P & 0 & 0 \\ 0 & 0 & P & Q \end{array}\right] \end{array} \begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \end{array}, \quad P + Q = 1. \qquad (15.13)$$

Here, $\omega t_0 = \pi/2$. By substituting (15.13) into (15.12) and (15.11), we can easily calculate the conductivity tensors σ_{ij} and also the resistivity $\rho = \sigma^{-1}$. Fig. 14.16 reprsents the magnetoresistance tensor component ρ_{11} the electron orbits Figs. 14.15(a),(b).[215] When the field intensity is weak, $Q \cong 1$ and $\rho_{11}(H)$ is proportional to H^2. In very strong magnetic field $P \cong 1$ and ρ_{11} saturates. The peak in $\rho_{11}(H)$ in intermediate field strength is the result of the transition from Fig. 14.15(a) to Fig. 14.15(b).

If the threshold field H_0 of MB is very large, ρ_{11} increases as H^2 without saturation. This behavior is due to the open orbits $2 \to 2 \to 2 \cdots$ and $4 \to 4 \to 4 \cdots$.

Fig. 14.16 indicates that the saturation does not appear in the field intensity corresponding to $\omega\tau \simeq 1$ but in the field corresponding to $\omega\tau \cong \omega_0\tau \gg 1$.

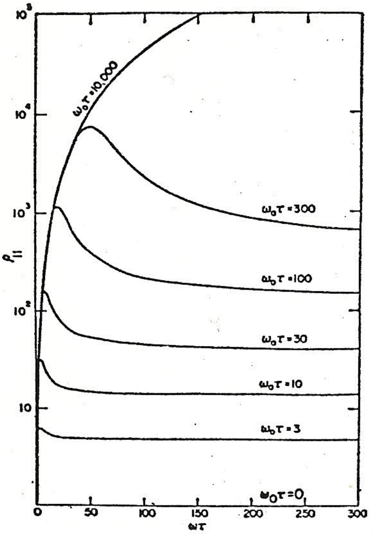


Fig. 14.16 Magnetoresistance for a transition from open orbits (2, 4) plus electron orbit $(1 \to 3 \to 1 \to 3 \cdots)$ to a closed magnetic breakdown orbit $(1 \to 2 \to 3 \to 4 \to 1)$. (After Falicov and Sievert.[215])

15.3 Transition Matrix for the Hexagonal Orbit

Consider the two-dimensional Fermi surface with its center located at hexagon corner, and assume that the lens orbit α formed by the overlapping of neighboring Fermi surfaces is negligibly small (See Fig. 14.17). In this case we assume that the original Fermi surface corresponds to holes. Hence, the orbit β $(1\rightarrow 2\rightarrow 3\rightarrow 4\rightarrow 5\rightarrow 6)$ is an electron-like orbit, while the α-orbit is hole-like.

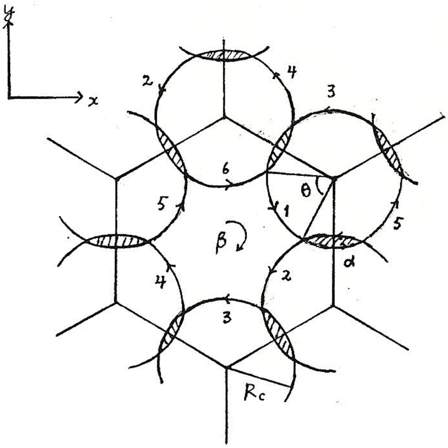


Fig. 14.17 Various orbits formed by the overlapping of the Fermi surfaces. Exach Fermi surface has its center at hexagon corner. Cyclotron radius R_c is equal to v_F/ω.

Since we are considering the case in which the α-orbit is very small, the transition matrix M becomes a 6×6 matrix specified by the effective matrix elements A, B instead of Q, P. A denotes the effective Bragg-reflection probability and B corresponds to the effective magnetic breakdown probability. By including the effect of the lens orbit α, A and B are symbolically described by

(15.14)

From (15.14), A and B are given by

$$\left\{\begin{aligned} A &= Q + QP^2 + Q^3P^2 + Q^5P^2 + \cdots = Q + QP^2/(1-Q^2) = Q + QP/(1+Q), \\ B &= P^2 + P^2Q^2 + P^2Q^4 + \cdots = P^2/(1-Q^2) = P/(1+Q). \end{aligned}\right. \qquad (15.15)$$

Clearly, we have $A + B = 1$, since $P + Q = 1$. In weak field limit $A \to 1$, $B \to 0$, while in strong limit $A \to 0$, $B \to 1$.

The transition matrix M is

$$\mathbf{M} = \begin{pmatrix} 0 & 0 & B & 0 & 0 & A \\ A & 0 & 0 & B & 0 & 0 \\ 0 & A & 0 & 0 & B & 0 \\ 0 & 0 & A & 0 & 0 & B \\ B & 0 & 0 & A & 0 & 0 \\ 0 & B & 0 & 0 & A & 0 \end{pmatrix}. \qquad (15.16)$$

By introducing $\mathbf{M}$ into (15.12), the matrix $\mathbf{Y}$ is obtained as follows:

$$\mathbf{Y} = \begin{array}{cc} \begin{array}{ccc} & r & \end{array} & \\ \left[\begin{array}{ccc} & \vdots & \\ \cdots & Y_{\ell r} & \cdots \\ & \vdots & \end{array}\right] & \ell \end{array}, \quad Y_{ij} = Y_{i+1,j+1} \quad (\text{mod. } 6). \qquad (15.17)$$

and $K_j(\ell)$ is given by

$$\begin{aligned} K_j(\ell) &= e^{-t_0/\tau} \sum_{r,s} M_{r,s} Y_{r,s} V_j(s) \\ &= e^{-t_0/\tau} \sum_{p=1}^{6} (A\, Y_{\ell-1,p} + B\, Y_{\ell+2,p})\, V_j(p), \quad (\omega t_0 = \theta). \end{aligned} \qquad (15.18)$$

We do not enter into the detailed calculation of the conductivity tensor. Results of calculations for several cases based on various models of the Fermi surface topology are given in the paper of Falicov and Sievert. 215)

Saturation of the magnetoresistance is achieved in the field region of $\omega\tau \simeq \omega_0\tau \simeq 1$ (See Fig. 14.16). This is the general feature of the magnetoresistance with magnetic breakdown. 215) Detailed calculations show that the saturation value of the resistivity is given by

$$\rho_{sat} \propto (\tau^{-1} + C\omega_0), \quad C \sim 1. \qquad (15.19)$$

This result can be interpreted that in strong magnetic field.

$$1/\tau_{eff} = 1/\tau + C\omega_0, \qquad (15.20)$$

play a role of an effective relaxation time. 168), 215)

Appendix

Appendix 1.

We shall consider that a stream of electrons moves with velocity v from left to right along the z-axis. This stream of electrons are represented by the plane wave $\exp(ikz)$, where k is equal to $mv/\hbar$. This wave represents a density of electrons of one per unit volume, and therefore a flow of v electrons across unit area per unit time. The wave is scattered by a potential $U(r)$ and the asymptotic form of the scattered wave at (r, θ, ϕ) is represented by

$$\psi = e^{ikz} + \frac{f(\theta)}{r} e^{ikr}, \qquad (A1.1)$$

where $f(\theta)$ is called the scattering amplitude. Our problem is to find the function $f(\theta)$. The number of electrons in the scattered wave crossing an element of area $dS = r^2 d\Omega$ ($d\Omega$: solid angle element) is $v(|f|^2/r^2)\, r^2 d\Omega = v|f|^2 d\Omega$ per unit time; and therefore, the ratio of the scattered electron density to the incident electrons is given by

$$d\sigma = |f(\theta)|^2 d\Omega. \qquad (A1.2)$$

This quantity has a dimension of area and is called the differential cross section. By putting $d\Omega = 2\pi \sin\theta \, d\theta$, (A 1.2) becomes

$$d\sigma = 2\pi \sin\theta \, |f(\theta)|^2 d\theta . \tag{A 1.3}$$

The wave function of Schrödinger equation with a central force potential $U(r)$ can be solved in the form $\psi = F_\ell(r) Y_{\ell m}(\theta . \varphi)$, where F_ℓ satisfies the equation

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2 \frac{dF_\ell}{dr}\right) + \left[k^2 - \frac{\ell(\ell+1)}{r^2} - \frac{2m}{\hbar^2} U(r)\right] F_\ell = 0 , \tag{A 1.4}$$

where $\quad k = \sqrt{2mE/\hbar^2}$.

Defining $F_\ell(r) = R_\ell(r)/r$, we get

$$\left[\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} + k^2\right] R_\ell = \frac{2mU(r)}{\hbar^2} R_\ell . \tag{A 1.5}$$

We are interested in the solution of (A 1.5) which is the superposition of the incident wave and outgoing wave at large distance from the scattered center. To do this, we require an expansion of $e^{ikz} = e^{ikr\cos\theta}$ in Legendre polynomials:

$$\varphi_i(r) = e^{ikz} = \sum_{\ell=0}^{\infty} (2\ell+1) i^\ell j_\ell(kr) P_\ell(\cos\theta) , \tag{A 1.6}$$

where j_ℓ is the Bessel function with half-integral number given by

$$j_\ell(x) = \sqrt{\frac{\pi}{2x}} J_{\ell+1/2}(x) = x^\ell (-1)^\ell \left(\frac{d}{x\,dx}\right)^\ell \frac{\sin x}{x} . \tag{A 1.7}$$

For small and large values of x, $j_l(x)$ takes the form :

$$j_l(x) = \begin{cases} \dfrac{x^l}{1\cdot 3\cdot 5\cdots(2l+1)} & : x \ll l\,, \\[2ex] \dfrac{1}{x}\sin\left(x - \dfrac{\pi}{2}l\right) & : x \gg l\,, \end{cases} \qquad (A1.8)$$

and therefore, the asymptotic form of $\varphi_i(r)$ becomes

$$\varphi_i(r) \approx (kr)^{-1} \sum_{l=0}^{\infty} (2l+1) i^l P_l(\cos\theta) \frac{i}{2} \left\{ e^{-i(kr - l\pi/2)} - e^{i(kr - l\pi/2)} \right\}. \qquad (A1.9)$$

$e^{-i(kr-l\pi/2)}$ represents an incoming wave and $e^{i(kr-l\pi/2)}$ is an outgoing wave.

For large r the two terms $-l(l+1)R_l/r^2$ and $2mU(r)R_l/\hbar^2$ in (A1.5) tend to zero, and we should therefore expect that the asymptotic form of any solution $\psi(r)$ would be

$$\psi(r) \sim A\sin(kr + \varepsilon)\,, \qquad (A1.10)$$

where A and ε are constants. Then, we assume the following asymptotic form

$$\psi(r) = \sum_{l=0}^{\infty} (2l+1) A_l P_l(\cos\theta) \frac{1}{2kr} \left\{ \exp\left[-i\left(kr - \frac{l\pi}{2} + \delta_l\right)\right] - \exp\left[i\left(kr - \frac{l\pi}{2} + \delta_l\right)\right] \right\}. \qquad (A1.11)$$

Phase shift δ_l is induced by the scattering due to the potential $U(r)$.

We have to choose the A_l so that this does actually represent a scattered wave — i.e. so that there are no terms of the type e^{-ikr}/r in the asymptotic expansion of $\psi - e^{ikz}$. Accordingly, we obtain

$$A_l = i^l e^{i\delta_l} . \tag{A 1.12}$$

Then, $\psi(r)$ becomes

$$\psi(r) = \frac{i}{2kr}\sum_{l=0}^{\infty}(2l+1)\,P_l(\cos\theta)\left\{(-1)^l e^{-ikr} - e^{2i\delta_l} e^{ikr}\right\} . \tag{A 1.13}$$

(A 1.13) leads to

$$f(\theta) = \frac{1}{2ik}\sum_{l=0}^{\infty}(2l+1)(e^{2i\delta_l} - 1)\,P_l(\cos\theta) . \tag{A1.14}$$

Total scattering cross section defined by

$$\sigma = \int d\sigma = 2\pi\int_0^{\pi}|f(\theta)|^2 \sin\theta\, d\theta , \tag{A 1.15}$$

is described by

$$\sigma = \frac{4\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)\sin^2\delta_l , \tag{A 1.16}$$

where the orthogonality relation

$$\int_0^{\pi} P_l(\cos\theta)\,P_{l'}(\cos\theta)\sin\theta\, d\theta = \frac{2}{2l+1}\delta_{ll'} . \tag{A 1.17}$$

is employed. (7.172) corresponds to the term $l = 0$ in (A 1.16)

This is called the partial wave method.[2),6)] This method is especially useful in the case where $U(r)$ represents a short range force potential. Let denote the force range by d. For $r>d$ $U(r)$ is effectively zero and the effective potential is the centrifugal force $\hbar^2 l(l+1)/2mr^2$ which represents a repulsive potential.

Then, the closest distance of approach is given by the condition:

$$\frac{\hbar^2 l(l+1)}{2m r_c^2} = \frac{\hbar^2 k^2}{2m} = E, \tag{A1.18}$$

namely $r_c = \sqrt{l(l+1)}/k$. Probability of finding particles in the region of $r<r_c$ exponentially decreases. If $d<r_c$ is satisfied, the relevant partial waves can not penetrate into the force range of $U(r)$ and therefore, these waves do not undergo scattering. Consequently, we arrive at the important conclusion that the partial waves satisfying the condition

$$kd < \sqrt{l(l+1)} \tag{A1.19}$$

do not participate in the scattering process and only the s-wave scattering ($l=0$) is important.

We shall calculate the phase shift δ_l for the case of $kd \ll 1$.

From (A1.5),

$$\frac{d^2 R_\ell}{d r^2} + \left[k^2 - \frac{\ell(\ell+1)}{r^2} - \frac{2m}{\hbar^2} U(r)\right] R_\ell = 0, \quad R_\ell(0) = 0. \qquad (A1.20)$$

The equation for the free particle is

$$\frac{d^2 g_\ell}{d r^2} + \left[k^2 - \frac{\ell(\ell+1)}{r^2}\right] g_\ell = 0, \quad g_\ell(0) = 0. \qquad (A1.21)$$

Multiplying (A1.20) by g_ℓ and (A1.21) by R_ℓ and subtracting each other, we obtain after integration over r

$$\left[g_\ell \frac{d R_\ell}{dr} - R_\ell \frac{d g_\ell}{dr} \right]_r = \frac{2m}{\hbar^2} \int_0^r U(r') R_\ell(r') g_\ell(r') dr'. \qquad (A1.22)$$

Solution of (A1.21) is given by

$$g_\ell(r) = k r j_\ell(kr) \qquad (A1.23)$$

and for large r,

$$g_\ell(r) = \sin(kr - \ell\pi/2), \quad kr \gg \ell. \qquad (A1.24)$$

Assume the asymptotic form of $R_\ell(r)$ as

$$R_\ell(r) = \sin(kr - \ell\pi/2 + \delta_\ell). \qquad (A1.25)$$

Substituting (A1.24) and (A1.25) into (A1.22), we obtain the equation for δ_ℓ :

$$k \sin\delta_\ell = -\frac{2m}{\hbar^2} \int_0^r U(r') R_\ell(r') g_\ell(r') dr'. \qquad (A1.26)$$

Approximating R_l by g_l, then we have

$$k \sin\delta_l \approx -\frac{2mk^2}{\hbar^2}\int_0^r U(r')r'^2 j_l(kr')dr'. \qquad (A1.27)$$

From (A1.8), j_l becomes

$$j_l(kr) \approx \frac{(kr)^l}{1.3.5.\cdots(2l+1)}. \qquad (A1.28)$$

Hence, we have

$$\sin\delta_l \approx -\frac{2m(kd)^{2l+1}}{\hbar^2(1.3.5.\cdots.(2l+1))^2}\int_0^d U(r')\left(\frac{r'}{d}\right)^{2l+1} r'dr'. \qquad (A1.29)$$

Appendix 2.

Our problem here is to obtain an approximate formula for the scattering of a beam of particles by a field $V(r)$. This formula is only valid for fast particles. (Born approximation)

We have to solve the wave equation

$$\Delta\psi + k^2\psi = \frac{2m}{\hbar^2}V(r)\psi \qquad (A2.1)$$

where ψ is a superposition of the incidient wave e^{ikz} and the scattered wave ψ_1:

$$\psi = e^{ikz} + \psi_1, \quad e^{ikz} \gg \psi_1. \qquad (A2.2)$$

First order approximation in ψ_1 gives

$$\Delta\psi_1 + k^2\psi_1 = \frac{2m}{\hbar^2}V(r)e^{ikz}. \qquad (A2.3)$$

The solution of (A 2.3) is given by

$$\psi_1(r) = -\frac{1}{4\pi^2}\frac{2m}{\hbar^2}\int \frac{V(r')\, e^{ik|\mathbf{r}-\mathbf{r}'|}\, e^{ikz'}}{|\mathbf{r}-\mathbf{r}'|}\, d\mathbf{r}' . \qquad (A\,2.4)$$

To obtain $f(\theta)$ we require the asymptotic form of (A 2.4) for large r.

For large r, we have

$$|\mathbf{r}-\mathbf{r}'| \cong r - \cos(\widehat{\mathbf{r}'\cdot\mathbf{r}})\, r', \quad |\mathbf{r}-\mathbf{r}'|^{-1} \cong r^{-1} + r^{-2}\cos(\widehat{\mathbf{r}\cdot\mathbf{r}'})\, r'. \qquad (A\,2.5)$$

Thus, $\psi(r)$ becomes

$$\psi(r) \cong e^{ikz} - \frac{e^{ikr}}{4\pi}\frac{2m}{\hbar^2}\int V(r')\, e^{ik(z'-\cos(\widehat{\mathbf{r}\cdot\mathbf{r}'})r')}\, d\mathbf{r}' . \qquad (A\,2.6)$$

and $f(\theta.\varphi)$ is

$$f(\theta.\varphi) = -\frac{1}{4\pi}\frac{2m}{\hbar^2}\int V(r')\, e^{ik(z'-\cos(\widehat{\mathbf{r}\cdot\mathbf{r}'})r')}\, d\mathbf{r}'$$

$$= -\frac{1}{4\pi}\frac{2m}{\hbar^2}\int V(r')\, e^{i\mathbf{K}\mathbf{r}'}\, d\mathbf{r}' , \qquad (A\,2.7)$$

where $\mathbf{K} = k - k'$.

Appendix 3.

We shall consider the time reversal operator which plays an important role in the quantum mechanics.

Eigenfunctions associated with the Hamiltonian including the spin-orbit interaction (8.34) are doubly degenerate. One of them is expressed by

$$\varphi_{k\uparrow}(r) = \chi_{k\uparrow}\alpha + \eta_{k\uparrow}\beta = e^{ikr}u_{k\uparrow}(r)\,, \qquad (A\,3.1)$$

where α, β are the spin functions. Without spin-orbit interaction $\varphi_{k\uparrow}$ includes only α-state. $\uparrow$ means that $(\varphi_{k\uparrow}\,\sigma_z\,\varphi_{k\uparrow})$ is positive, where σ_z is the z-component of the Pauli spin matrix.

$\varphi_{k\downarrow}$ involves only β.

The time reversal operator K transforms $\mathbb{r}$ into $\mathbb{r}$; $\mathbb{p}$ into $-\mathbb{p}$; $\boldsymbol{\sigma}$ into $-\boldsymbol{\sigma}$. The Hamiltonian (8.34) is invariant under the operation of K.

Thus,

$$K H K^{-1} = H. \qquad (A\,3.2)$$

Operating K on the Schrödinger equation $H\varphi = E\varphi$, we obtain from (A 3.2)

$$H K\varphi = E K\varphi. \qquad (A\,3.3)$$

This means that $K\varphi$ is also an eigenfunction belonging to the same energy E. For a system of a single electron the result of Kramers for the time reversal operator is

$$K = -i\,\sigma_y K_0, \qquad (A\,3.4)$$

where K_0 is the operation of taking the complex conjugate. For a system of n-electron the time reversal operator becomes

$$K_n = (-i)^n \sigma_{1y}\sigma_{2y}\cdots\sigma_{ny} K_0 , \qquad (A\,3.5)$$

where σ_y is the y-component of the Pauli spin matrix, which is given by

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \qquad (A\,3.6)$$

Before proving K being the time reversal operator, we shall enumerate the properties of K.

Since $(\varphi, \psi) = (K_0\psi, K_0\varphi)$, we have

$$(K\psi, K\varphi) = (\varphi, \psi) \qquad (A\,3.7)$$

for any two states φ and ψ, where $\sigma_y^2 = 1$ is employed.

Further, with $\sigma_y^2 = 1$,

$$K^2\varphi = (-i\sigma_y)(-i\sigma_y)\varphi = -\varphi. \qquad (A\,3.8)$$

From (A 3.7) and (A 3.8),

$$(\varphi, K\varphi) = (K^2\varphi, K\varphi) = -(\varphi, K\varphi) = 0. \qquad (A\,3.9)$$

Therefore, φ and $K\varphi$ are independent functions associated with a common energy E.

The state $K\varphi_{k\uparrow}$ is equal to $\varphi_{-k\downarrow}$. It is readily proved.

$$K\varphi_{k\uparrow} = -i\sigma_y K_0 \varphi_{k\uparrow} = e^{-ikr} \times (\text{periodic function of } r)_{\downarrow} .$$

Then, we have

$$K \varphi_{k\uparrow} = \varphi_{-k\downarrow} , \qquad (A\,3.10)$$

where we employ that σ_y reverses the spin direction.

It is easily proved that the sign of the expectation value of σ_z in $\varphi_{k\uparrow}$-state is opposite to that in $\varphi_{-k\downarrow}$-state as follows:

$$\#)\ (\varphi_{k\uparrow} , \sigma_z \varphi_{k\uparrow}) \overset{(A.37)}{\Downarrow}= (K \sigma_z \varphi_{k\uparrow} , K \varphi_{k\uparrow}) = - (\varphi_{-k\downarrow} , \sigma_z \varphi_{-k\downarrow}) , \qquad (A\,3.11)$$

where we recall (A 3.7) and $\sigma_y \sigma_z = - \sigma_z \sigma_y$.

(A 3.10) leads to

$$E_{k\uparrow} = E_{-k\downarrow} \ ; \ E_{k\downarrow} = E_{-k\uparrow} . \qquad (A\,3.12)$$

If the potential field $V(r)$ is invariant under the operation of the space inversion J, then the Hamiltonian including spin-orbit interaction is invariant under J. In this case we can show that

$$\varphi_{k\uparrow}(r) = \varphi_{-k\uparrow}(r) , \quad E_{k\uparrow} = E_{-k} \qquad (A\,3.13)$$

Now let verify that $K = -i \sigma_y K_0$ is the time reversal operator. To do this, we express the Hamiltonian as follows:

$$H(r.p.\sigma) = H_0(r.p)\mathbb{1} + H_x(r.p)\sigma_x + H_y(r.p)\sigma_y + H_z(r.p)\sigma_z . \qquad (A\,3.14)$$

Since $K_0^{-1} = K_0$, we have

$$(K_0 H K_0^{-1})\,\varphi = (K_0 H)\,\varphi^* = (H^*)\,\varphi . \qquad (A\,3.15)$$

Then,

$$K_0 H K_0^{-1} = H_0(\mathbf{r},-\mathbf{p})\mathbb{1} + H_x(\mathbf{r},-\mathbf{p})\sigma_x - H_y(\mathbf{r},-\mathbf{p})\sigma_y + H_z(\mathbf{r},-\mathbf{p})\sigma_z . \quad (A\,3.16)$$

Operating $-i\sigma_y$, one obtains

$$-i\sigma_y K_0 H K_0^{-1}(-i\sigma_y)^{-1} = H_0(\mathbf{r},-\mathbf{p})1 - H_x(\mathbf{r},-\mathbf{p})\sigma_x - H_y(\mathbf{r},-\mathbf{p})\sigma_y$$

$$- H_z(\mathbf{r},-\mathbf{p})\sigma_z = H(\mathbf{r},-\mathbf{p},-\sigma) . \qquad \text{Q. E. D.} \qquad (A\,3.17)$$

Detailed arguments on the time reversal operator are given in the following text books:

A. H. Messiah : Quantum Mechanics. Chapter 15 § 18
(North-Holland, Amsterdam 1961 ~ 1962);

A. S. Davydov : Quantum Mechanics (2nd edition) Chapter 14 § 119
(Translated by D. Ter. Haar, Pergamon Press. 1976).

Arsenic structure shown in Fig. 8.7 contains two atoms in unit cell and its structure has the inversion symmetry. Let prove the relation (A 3.13). The inversion operator J sends $\mathbf{r}$ into $-\mathbf{r}$; $\mathbf{p}$ into $-\mathbf{p}$; and $\boldsymbol{\sigma}$ into $\boldsymbol{\sigma}$. $\boldsymbol{\sigma}$ transforms as the angular momentum does. Therefore, it is invariant under J.

Assume that $J\,V(\mathbf{r})\,J^{-1} = V(\mathbf{r})$. Operation J on $\varphi_{k\uparrow}$ leads to

$$J\varphi_{k\uparrow}(r) = e^{-ikr}\,u_{k\uparrow}(-r). \tag{A 3.18}$$

Hence,

$$T_n J\varphi_{k\uparrow}(r) = e^{-ikt_n}\,J\varphi_{k\uparrow}(r), \tag{A 3.19}$$

where. T_n is the lattice displacement operator. accordingly, we obtain $u_{k\uparrow}(-r) = u_{-k\uparrow}(r)$ apart from a phase factor, and combining with (A 3.13) we get (A 3.13). Here, we introduce the operator

$$C \equiv KJ = -i\,\sigma_y K_0 J = JK, \tag{A 3.20}$$

which is called the conjugation operator. From (A 3.10) and (A 3.13),

$$C\varphi_{k\uparrow} = \varphi_{k\downarrow}. \tag{A 3.21}$$

On making use of these relations, we can verify (8.39) and (8.40).

Arguments mentioned here is due to the following book:

C. Kittel : Quantum Theory of Solids, 9 (John-Wiley & Sons, Inc., New York, London, Sydney (1963)).

Appendix 4.

Consider the relaxation process of the long wave phonons due to the phonon-phonon collision process. At enough low temperatures the U-process is ineffective. The rate of change of the phonon distribution due to the processes indicated by Figs. A 4.1 and A 4.2 is given by

$$\dot{N}_q = \frac{2\pi}{\hbar} \sum_{\mu,\nu} \sum_{q'q''} |U_{\lambda\mu\nu}|^2 q q' q'' \{ [(N_q+1)(N_{q'}+1) N_{q''} - N_q N_{q'} (N_{q''}+1)]$$

$$\times \delta_{q+q', q''} \, \delta(\hbar\omega_{q\lambda} + \hbar\omega_{q'\mu} - \hbar\omega_{q''\nu})$$

$$+ [N_{q'} N_{q''} (N_{q'}+1) - N_q (N_{q'}+1)(N_{q''}+1)] \, \delta_{q, q'+q''} \, \delta(\hbar\omega_{q\lambda} - \hbar\omega_{q'\mu} - \hbar\omega_{q''\mu}) \} , \qquad (A\ 4.1)$$

where suffix λ, μ an ν are omitted in the phonon distributions.

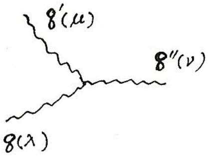


Fig. A 4.1 N-process for the phonon (q, λ).
$q + q' = q''$, $\hbar\omega_{q\lambda} + \hbar\omega_{q'\mu} = \hbar\omega_{q''\nu}$.

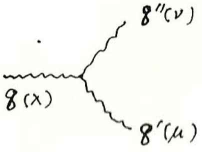


Fig. A 4.2 N-process for the phonon (q, λ). $q = q' + q''$.
$\hbar\omega_{q\lambda} = \hbar\omega_{q'\mu} + \hbar\omega_{q''\nu}$.

Other phonons except the relevant phonon (q, λ) are assumed to be in thermal equilibrium. In (A 4.1) the interaction coefficient $U_{\lambda\mu\nu}$ is considered to be independent of (q, q', q'').

Substituting $N_q = N_q^\circ + \delta N_q$, $N_{q'} = N_{q'}^\circ$ and $N_{q''} = N_{q''}^\circ$ into (A 4.1), we obtain

$$\left\{\begin{aligned} \dot{N}_q &= -\delta N_q / t_{p\text{-}p}, \\ 1/t_{p\text{-}p} &= \frac{2\pi}{\hbar}\sum_{\mu,\nu}\sum_{q'q''} |U_{\lambda\mu\nu}|^2 q q' q'' \Big\{ (N^\circ_{q'} - N^\circ_{q''})\, \delta_{q+q',q''} \\ &\times \delta(\hbar\omega_{q\lambda} + \hbar\omega_{q'\mu} - \hbar\omega_{q''\nu}) + (N^\circ_{q'} + N^\circ_{q''})\, \delta_{q,q'+q''}\, \delta(\hbar\omega_{q\lambda} - \hbar\omega_{q'\mu} - \hbar\omega_{q''\nu}) \Big\}. \end{aligned}\right. \tag{A 4.2}$$

$\sum_{\mu,\nu}\sum_{q'q''}$ can be rewritten in the form

$$q \sum_{\mu,\nu} \int q'^3 dq' d\Omega_{q'}\, q''^3 dq'' d\Omega_{q''} \cdots . \tag{A 4.3}$$

Due to the presence of $\delta_{q\pm q',q''}\, \delta(\hbar\omega_{q\lambda} \pm \hbar\omega_{q'\mu} - \hbar\omega_{q''\nu})$, exponent of q', q'' is $8-4=4$. This leads to $1/t_{p\text{-}p} \propto T^4$.

Appendix 5.

In the first place we shall verify $(c.d) = (d.c)$. On inspection of (9.77) the term which can be directly concluded to be symmetric, is

$$\int_{-\infty}^{\infty} d\eta \int_{-\Theta_D/T}^{\Theta_D/T} dz\; c(\eta)\, d(\eta+z) \left[E + \frac{1}{2} k_0 T z - E_D \left(\frac{T}{\Theta_D}\right)^2 z^2 \right] \frac{z^2}{|1-e^{-z}|} \frac{1}{(e^{\eta+z}+1)(e^{\eta}+1)} . \tag{A 5.1}$$

On making use of the relation

$$\int_{-\infty}^{\infty} \left[\frac{F(\eta+z)}{e^{\eta+z}+1} - \frac{F(\eta)}{e^{\eta}+e^{z}} \right] \frac{d\eta}{e^{-\eta}+1} = 0 , \tag{A 5.2}$$

(A 5.1) is rewritten as

$$\int_{-\infty}^{\infty}\int_{-\Theta_D/T}^{\Theta_D/T} c(\eta - z)\, d(\eta)\left[E - \frac{1}{2}k_0 T z - E_D\left(\frac{T}{\Theta_D}\right)^2 z^2\right]\frac{z^2 dz}{1-e^{-z}}\,\frac{d\eta}{(e^{\eta}+e^{z})(e^{-\eta}+1)}. \qquad (A\,5.3)$$

By changing z into $-z$ in (A 5.3) we can obtain the expression of (A 5.1) in which $c(\eta)d(\eta+z)$ is replaced by $c(\eta+z)d(\eta)$. This proves $(d.c) = (c.d)$.

To prove $(c.c) \geqq 0$ is more difficult. From (9.77) $(c.c)$ becomes

$$(c.c) = -\left(\frac{2}{m^*}\right)^{1/2}\int_{-\infty}^{\infty}\frac{E^2}{l_r}\frac{\partial f_0}{\partial \eta}\{c(E)\}^2 d\eta$$

$$+\frac{1}{A}\left(\frac{T}{\Theta_D}\right)^3\int_{-\infty}^{\infty}\int_{-\Theta_D/T}^{\Theta_D/T}\left[E\,c(\eta)c(\eta) - c(\eta)c(\eta+z)\left\{E+\frac{1}{2}k_0 T z - E_D\left(\frac{T}{\Theta_D}\right)^2 z^2\right\}\right]$$

$$\times\frac{z^2 dz}{|1-e^{-z}|}\,\frac{d\eta}{(e^{\eta+z}+1)(e^{-\eta}+1)}. \qquad (A\,5.4)$$

The first term in the right hand side is clearly positive. By using (A 5.2) and putting $z \to -z$, twice of the square bracket term in (A 5.4)

$$E\,c(\eta)c(\eta) - 2\left\{E+\frac{1}{2}k_0 T z - E_D\left(\frac{T}{\Theta_D}\right)^2 z^2\right\}c(\eta)c(\eta+z) + (E+k_0 T z)\,c(\eta+z)c(\eta+z).$$

$$(A.\,5.5)$$

To prove (A5.5) $\geqq 0$, we must verify that the discriminant of (A5.5)

$$\left\{ E + \frac{1}{2} k_0 T z - E_D \left(\frac{T}{\Theta_D} \right)^2 z^2 \right\}^2 - E (E + k_0 T z) , \qquad (A5.6)$$

is non-positive. By recalling $E_D = (\hbar^2/4m^*)\, q_D^2$, $\hbar v_s q_D = k_0 \Theta_D$ and $E = (\hbar^2/2m^*)\, k^2$. it is shown that (A5.6) $\leqq 0$ is equivalent to the condition:

$$\frac{\hbar k}{2m^* v_s} \geqq \left| \frac{\hbar \omega}{4m^* v_s^2} - \frac{1}{2} \right| . \qquad (A5.7)$$

This condition is just the same as (9.15). Thus, (C.C) $\geqq 0$ is proved.

Appendix 6.

Entropy of the electron system is given by

$$S = - k_0 \sum_k \left\{ f_k \ln f_k + (1 - f_k) \ln (1 - f_k) \right\} . \qquad (A6.1)$$

Suppose that (A6.1) is applicable to the case in which f_k is slightly deviated from the equilibrium state. By assuming f_k in the form (9.3) and retaining the first order terms in Φ, $dS/dt \equiv \dot{S}$ becomes

$$\dot{S} = - \frac{1}{T} \sum_k \Phi_k \dot{f}_k + \frac{1}{T} \sum_k (E_k - \zeta) \dot{f}_k . \qquad (A6.2)$$

The second term is the entropy change corresponding to increase of the average electron energy. In the linear responce theory this term is neglected. $\dot{f}_k$ is composed of the two contributions: $\dot{f}_k = (\dot{f}_k)_{drift} + (\dot{f}_k)_{coll.}$ Entropy change due to $(\dot{f}_k)_{drift}$ is

$$\dot{S}_{drift} = -\frac{1}{T} e \mathcal{E} \sum_k v_k \bar{\Phi}_k \cdot \frac{\partial f_0}{\partial E} = -\frac{1}{T} \mathcal{E} \cdot j \ . \qquad (A\,6.3)$$

In the stationary state $\dot{f}_k = 0$ and $\dot{S} = 0$. Therefore, we have

$$\dot{S}_{drift} + \dot{S}_{coll.} = 0 \qquad (A\,6.4)$$

From (6.7), (6.9) and (6.10), $\dot{S}_{coll.}$ is written in the form

$$\dot{S}_{coll.} = \frac{1}{2 k_0 T^2} \sum_k \sum_{k'} V(k.k') \{\bar{\Phi}(k) - \bar{\Phi}(k')\}^2 > 0 . \qquad (A\,6.5)$$

(A 6.5) is equivalent to the quantity $(\Phi . \Phi) = (1/4\pi^3) \int \Phi \mathcal{L}(\Phi) \, dk$ introduced in Section 9.3, which plays a crucial role in the variation principle. Thus, the variation principle can be replaced by the condition of the maximum entropy production associated with the scattering processes.

Macroscopic entropy production in the presence of an electric current is given by

$$\dot{S}_{macro.} = \frac{1}{T} \mathcal{E} \cdot j = -\dot{S}_{drift} . \qquad (A\,6.6)$$

From (A 6.4), (A 6.5) and (A 6.6) the resistivity defined by $\mathcal{E} = \rho j$ is

$$\begin{aligned} \rho &= (1/2 k_0 T) \sum_k \sum_{k'} V(k.k') \{\bar{\Phi}(k) - \bar{\Phi}(k')\}^2 / j^2 \\ &= (1/2 k_0 T) \sum_k \sum_{k'} V(k.k') \{\Phi(k) - \Phi(k')\}^2 / \Big(\sum_k e v_k \Phi_k \frac{\partial f_0}{\partial E}\Big)^2 . \qquad (A\,6.7) \end{aligned}$$

(A 6.7) indicates that an alternative expression of the variation principle (9.70) has a physical meaning that the solution of the Boltzmann equation makes the resistivity minimum.

Appendix 7

Let assume that the thermodynamic potential Φ (Gibbs Free energy) can be expanded in powers of the order parameter. In the present problem the order parameter is the magnetization $M(r)$.

$$\begin{cases} \Phi = \int dr\, \phi(r), \\ \phi(r) = \phi_0 - B(r)\,M(r) + a(T)\,M(r)^2 + b(T)\,M(r)^4 + c(T)\,(\nabla M(r)\cdot\nabla M(r)). \end{cases} \quad (A7.1)$$

The second term in the right hand side of $\phi(r)$ denotes the interaction term with magnetic field and the third and fourth terms represent the energy and entropy terms, respectively. The last term corresponds to the local fluctuation of the magnetization.

In the absence of a magnetic field $\phi(r)$ should be invariant under the time inversion and therefore, the odd power terms in $M(r)$ do not appear since M changes its sign under the time reversal operation.

We are now interested in the second order phase transition.

Usually, the phase transition from the disordered state ($M(r) = 0$) to the ordered state ($M(r) \neq 0$) occurs with decreasing temperature.

Since this is not a thermodynamical law, there may be several exceptions to this. Behavior of the symmetry of Rochelle salt below and above the low Curie point is an example of the exception.

$M(r)+\delta M(r)$ is inserted into (A 7.1) instead of $M(r)$, and retaining the terms proportional to $\delta M(r)$, we obtain

$$\delta\Phi = \int dr\,\{-B(r)+2a\,M(r)+4b\,M(r)^3-2c\,\Delta M(r)\}\,\delta M(r)\,. \qquad (A\ 7.2)$$

Since δM is arbitrary, $\delta\Phi = 0$ leads to

$$(2a+4b\,M^2-2c\,\Delta)\,M = B. \qquad (A\ 7.3)$$

If M is uniform, (A 7.3) becomes

$$(2a+4b\,M^2)\,M = B. \qquad (A\,7.4)$$

In the absence of a magnetic field, (A 7.4) provides two solutions:

$$M=0\,, \qquad (A\,7.5a)$$

$$M=\pm\left(-\frac{a}{2b}\right)^{1/2}. \qquad (A\,7.5b)$$

The solution (A 7.5a) makes Φ minimum for $a>0$, while (A 7.5b) makes Φ minimum for $a<0$, in both cases b is assumed to be positive. Namely, (A 7.5a) represents the disordered state (symmetric phase) and (A 7.5b) corresponds to the ordered state (non-symmetric phase). Let denote the critical temperature (in the present case

Curie temperature) by T_c. Then, we have

$$\begin{cases} a > 0 : & T > T_c \\ a < 0 : & T < T_c . \end{cases} \qquad (A7.6)$$

Provided that a has no singularity around T_c and assume a in the form ;

$$a(T) = a'(T - T_c) \; , \; (a' > 0) \; , \qquad (A7.7)$$

and further b and C being constants with $T \to T_c$. Accordingly, the system has a non-vanishing magnetization around T_c for $B = 0$.

In the vicinity of T_c a long range fluctuation of the ordered parameter appears.

By using the above considerations it is able to calculate the correlation function of the magnetization :

$$g(r - r') = \langle [M(r) - \langle M(r) \rangle][M(r') - \langle M(r') \rangle] \rangle . \qquad (A7.8)$$

This is carried out as follows. Consider the following Hamiltonian including a parameter h

$$- \int h(r) M(r) \, dr . \qquad (A7.9)$$

Variation of $\langle M(r) \rangle$ accompanied with a small change $h \to h + \delta h$ is expressed by

$$\delta\langle M(r)\rangle = (k_0 T)^{-1}\int dr'\,\delta h(r')\langle [M(r)-\langle M(r)\rangle][M(r')-\langle M(r')\rangle]\rangle . \qquad (A7.10)$$

This is the classical expression of the fluctuation-dissipation theorem in Chapter 11 (Kubo formula). Proof of (A7.10) is very easy.

Statistical average of the magnetization corresponding to the Hamiltonian

$$H = H_0 - \int dr\, h(r) M(r) \qquad (A7.11)$$

is given by

$$\langle M(r)\rangle = \mathrm{Tr}\, M(r)\, e^{-\beta H}/\mathrm{Tr}\, e^{-\beta H}. \qquad (A7.12)$$

Linear response of the magnetization to a small variation δh is readily calculated from (A7.11) and (A7.12) and we obtain (A7.10). In the present problem $h = B$ then, (A7.10) becomes

$$\langle \delta M(r)\rangle = (k_0 T)^{-1}\int dr'\, g(r-r')\,\delta B(r'). \qquad (A7.13)$$

Putting $B \to B+\delta B$, $M \to M+\delta M$ in (A7.3), we get

$$\left\{2a + 12b\langle M(r)\rangle^2 - 2c\Delta\right\}\delta\langle M(r)\rangle = \delta B(r). \qquad (A7.14)$$

Substituting (A7.13) into (A7.14), one obtains

$$\int dr' \left\{[2a + 12b\langle M(r)\rangle^2 - 2c\Delta]\, g(r-r') - k_0 T\,\delta(r-r')\right\}\delta B(r') = 0. \qquad (A7.15)$$

Since δB is arbitrary, (A7.15) leads to

$$[2a + 12b\langle M(r)\rangle^2 - 2c\Delta]\, g(r-r') = k_0 T \delta(r-r'). \qquad (A7.16)$$

In the absence of a magnetic field ($B=0$) the solution of (A7.16) is easily obtained. In this case $\langle M(r)\rangle = 0$ for $T > T_c$, then

$$[2a'(T-T_c) - 2c\Delta]\, g(r-r') = k_0 T \delta(r-r') : T > T_c, \qquad (A7.17)$$

where (A7.7) is employed. By substituting the relation $\langle M(r)\rangle^2 = a'(T-T_c)/2b$ for $T < T_c$ into (A7.16), we have

$$[4a'(T_c-T) - 2c\Delta]\, g(r-r') = k_0 T \delta(r-r') : T < T_c. \qquad (A7.18)$$

From (A7.17) and (A7.18) the correlation function $g(r-r')$ is obtained :

$$g(r-r') = \frac{\exp(-|r-r'|\xi)}{|r-r'|}\left(\frac{k_0 T}{8\pi c}\right), \qquad (A7.19)$$

$$1/\xi = \begin{cases} (c/a')^{1/2}(T-T_c)^{1/2} & : T > T_c \\ (c/2a')^{1/2}(T_c-T)^{-1/2} & : T < T_c. \end{cases} \qquad (A7.20)$$

The expression (A7.1) assumes that c is positive.

See : L. P. Kadanoff et al : Rev. Mod. Phys. 39 (1967) 395 ;

Landau - Lifshitz : Statistical Physics. 3rd edition part. 1 Chapter. 14.

Appendix 8

Consider a system specified by an unperturbed Hamiltonian H_0, subjected to a perturbation $H'(t)$ defined by

$$H'(t) \neq 0 \ : \ 0 \leqq t \leqq \tau \ ; \quad H'(t) = 0 \ : \ t<0, \ t>\tau . \tag{A 8.1}$$

The time-dependent Schrödinger equation is

$$i\hbar \frac{\partial \psi}{\partial t} = [H_0 + H'(t)] \psi . \tag{A8.2}$$

To solve (A8.2), ψ is exapanded by using the eigenfunctions $\{\varphi_n\}$ of H_0 :

$$\psi = \sum_n a_n(t) \varphi_n e^{-iE_n t/\hbar} . \tag{A8.3}$$

Suppose that the system is in the following state for $t \leqq 0$:

$$\psi_{int.} = \varphi_m e^{-iE_m t/\hbar} , \ (a_n(t) = \delta_{m \cdot n}) . \tag{A8.4}$$

For $t > \tau$ the system is described by

$$\psi_{fin} = \sum_n a_{mn}(\tau) \varphi_n e^{-iE_n t/\hbar} . \tag{A8.5}$$

a_{mn} is a function of the time interval τ. The probability of the transition $m \rightarrow n$ in the interval τ is given by

$$W_{nm}(\tau) = | a_{nm}(\tau) |^2 . \tag{A8.6}$$

From (A8.2) and (A 8.3), we obtain

$$i\hbar \frac{d}{dt} a_n(t) = \sum_n \langle n | H'(t) | \ell \rangle e^{i\omega_{n\ell} t} a_\ell(t) , \tag{A8.7}$$

$$\langle n | H'(t) | l \rangle = \int \varphi_n^* H'(t) \varphi_l \, dv, \quad \hbar \omega_{nl} = E_n - E_l . \qquad (A\,8.8)$$

Redefining E_n by $E_n + \langle n | H'(t) | n \rangle$, hereafter we can consider the case $\langle n | H'(t) | n \rangle = 0$ for all n.

To calculate the transition probability it is needed to solve the simultaneous equation (A 8.7) under the initial condition of

$$a_n(0) = \delta_{nm} . \qquad (A\,8.9)$$

If the matrix elements (A 8.8) are not so large and the time interval during which the perturbation is finite, is not so long, the perturbed states must be close to the initial state. In this case we can solve (A 8.7) by iteration procedure.

The first approximation is obtained from (A 8.7) by putting $a_l(t) = \delta_{lm}$;

$$a_{nm}^{(1)}(t) = \frac{1}{i\hbar} \int_0^t \langle n | H' | m \rangle e^{i\omega_{nm} t'} dt', \qquad (A\,8.10)$$

and the second approximation is obtained by combining (A 8.10) and (A 8.7) as

$$i\hbar \frac{d a_{nm}^{(2)}}{dt} = \langle n | H' | m \rangle e^{i\omega_{nm} t} + \frac{1}{i\hbar} \sum_{n'(\neq m)} \langle n | H' | n' \rangle e^{i\omega_{nn'} t} \int_0^t \langle n' | H' | m \rangle e^{i\omega_{n'm} t'} dt',$$

(A 8.11).

By integrating (A8.11),

$$a^{(2)}_{nm}(t) = \frac{1}{i\hbar}\int_0^t \langle n|H'|m\rangle e^{i\omega_{nm}t'}dt' + \frac{1}{(i\hbar)^2}\sum_{n'(\neq m)}\int_0^t \langle n|H(t')|n\rangle e^{i\omega_{nn'}t}$$

$$\times \int_0^{t'} \langle n'|H'(t'')|m\rangle e^{i\omega_{n'm}t''}dt''dt'. \qquad (A8.12)$$

By continuing this procedure $a_{nm}(t)$ can be expressed as follows:

$$a_{nm}(t) = \langle n|\,P\exp\left[-\frac{i}{\hbar}\int_0^t \hat{H}'(t')dt'\right]|m\rangle, \qquad (A8.13)$$

where P is the chronological operator:

$$P\exp\left[-\frac{i}{\hbar}\int_0^t \hat{H}'(t')dt'\right] \equiv 1 + \frac{1}{i\hbar}\int_0^t \hat{H}'(t')dt' + \frac{1}{(i\hbar)^2}\int_0^t \hat{H}'(t')\int_0^{t'} \hat{H}'(t'')dt''dt'$$

$$+\frac{1}{(i\hbar)^3}\int_0^t \hat{H}'(t')\int_0^{t'} \hat{H}'(t'')\int_0^{t''} \hat{H}'(t''')dt'''dt''dt' + \cdots, \qquad (A8.14)$$

and $\hat{H}'(t)$ is the interaction representian of H' defined by

$$\hat{H}'(t) = e^{iH_0t/\hbar}H'(t)e^{-iH_0t/\hbar}. \qquad (A8.15)$$

Suppose that $H'(t)$ is t-independent and switched on at $t=-\infty$. A quantity needed here is $a_{nm}(\infty)$, where m is the initial state at $t=-\infty$. $a_{nm}(\infty) \equiv \langle n|S|m\rangle$ is called the S-matrix.

From (A7.13),

$$\langle n|S|m\rangle = \langle n|\,P\exp\left[-\frac{i}{\hbar}\int_{-\infty}^{+\infty} \hat{H}'(t')dt'\right]|m\rangle, \qquad (A8.16)$$

$$S = P\exp\left[-\frac{i}{\hbar}\int_{-\infty}^{+\infty}\hat{H}'(t')dt'\right] = \sum_{\alpha=0}^{\infty}\frac{1}{(i\hbar)^{\alpha}}\int_{-\infty}^{+\infty}dt_1\int_{-\infty}^{t_1}dt_2\cdots\int_{-\infty}^{t_{\alpha-1}}dt_\alpha\,\hat{H}'(t_1)\hat{H}'(t_2)\cdots\hat{H}'(t_\alpha). \tag{A8.17}$$

Matrix element of each order term in S is calculated as follows:

$$\langle n|S|m\rangle = \sum_{\alpha=0}^{\infty}\langle n|S^{(\alpha)}|m\rangle, \tag{A8.18}$$

$$\langle n|S^{(0)}|m\rangle = \langle n|m\rangle = \delta_{nm} \tag{A8.19}$$

$$\langle n|S^{(1)}|m\rangle = -\frac{i}{\hbar}\langle n|H'|m\rangle\int_{-\infty}e^{i(E_n-E_m)t/\hbar}dt = -2\pi i\,\delta(E_n-E_m)\langle n|H'|m\rangle, \tag{A8.20}$$

$$\langle n|S^{(2)}|m\rangle = \frac{1}{(i\hbar)^2}\sum_f\int_{-\infty}^{+\infty}dt_1\langle n|\hat{H}'(t_1)|f\rangle\int_{-\infty}^{t_1}dt_2\langle f|\hat{H}'(t_2)|m\rangle$$

$$= \frac{1}{(i\hbar)^2}\sum_n\langle n|H'|f\rangle\langle f|H'|m\rangle\int_{-\infty}^{+\infty}e^{i(E_n-E_f)t_1/\hbar}dt_1\int_{-\infty}^{t_1}e^{i(E_f-E_m)t_2/\hbar}dt_2. \tag{A8.21}$$

To make the integral on t_2 converge, $E_f - E_m$ is replaced by $E_f - E_m - i\varepsilon$ ($\varepsilon \to +0$), and then

$$\int_{-\infty}^{t_1}e^{i(E_f-E_m)t'/\hbar}dt' \to \int_{-\infty}^{t_1}e^{i(E_f-E_m-i\varepsilon)t/\hbar}dt = i\hbar\frac{e^{i(E_f-E_m-i\varepsilon)t_1/\hbar}}{E_m-E_f+i\varepsilon}.$$

Accordingly, (A 21) becomes

$$\langle n|S^{(2)}|m\rangle = \frac{1}{i\hbar}\sum_f\frac{\langle n|H'|f\rangle\langle f|H'|m\rangle}{E_m-E_f+i\varepsilon}\int_{-\infty}^{+\infty}e^{i(E_n-E_m+i\varepsilon)t/\hbar}dt$$

$$= -2\pi i\,\delta(E_n-E_m)\sum_f\frac{\langle n|H'|f\rangle\langle f|H'|m\rangle}{E_m-E_f+i\varepsilon}. \tag{A8.22}$$

Higher order terms can be obtained in a similar way. Thus, we may write

$$\langle n | S | m \rangle = -2\pi i\, \delta(E_n - E_m) \langle n | T | m \rangle. \qquad (A8.23)$$

Here, $\langle n | T | m \rangle$ is

$$\langle n | T | m \rangle = \langle n | H' | m \rangle + \sum_{f} \frac{\langle n | H' | f \rangle \langle f | H' | m \rangle}{E_n - E_m + i\varepsilon}$$

$$+ \sum_{f.f'} \frac{\langle n | H' | f \rangle \langle f | H' | f' \rangle \langle f' | H' | m \rangle}{(E_m - E_f + i\varepsilon)(E_m - E_{f'} + i\varepsilon)} + \cdots . \qquad (A8.24)$$

Rewriting

$$\frac{\langle n | H' | f \rangle \langle f | H' | m \rangle}{E_m - E_f + i\varepsilon} = \langle n | H' | f \rangle \langle f | (E_m - H_0 + i\varepsilon)^{-1} | f \rangle \langle f | H' | m \rangle, \qquad (A8.25)$$

we obtain the operator T (T-matrix) as

$$T = H' + H'(E_m - H_0 + i\varepsilon)^{-1} H' + H'(E_m - H_0 + i\varepsilon)^{-1} H'(E_m - H_0 + i\varepsilon)^{-1} H'$$

$$+ \cdots , \qquad (A8.26$$

or

$$T = H' + H'(E_m - H_0 + i\varepsilon)^{-1} T. \qquad (A8.27$$

Since the operator T includes an eigenvalue E_m as a parameter, it is not a general operator which can operate on an arbitrary eigenstate.

Transition probability after elapsing a long time is given by

$$W_{nm}(\infty) = |\langle n | S | m \rangle|^2 = 4\pi^2 \delta^2(E_n - E_m) |\langle n | T | m \rangle|^2 . \qquad (A\,8.28)$$

By transforming $\delta^2(E_n - E_m)$ as follows ;

$$\delta^2(E_n - E_m) = \frac{\delta(E_n - E_m)}{2\pi\hbar} \lim_{T\to\infty} \int_{-T}^{T} e^{i(E_n - E_m)t/\hbar} dt = \frac{\delta(E_n - E_m)}{2\pi\hbar} \lim_{T\to\infty} \int_{-T}^{T} dt .$$

the transition probability per unit time is given by

$$P_{nm} = \frac{W_{nm}(\infty)}{\lim\limits_{T\to\infty} \int_{-T}^{T} dt} = \frac{2\pi}{\hbar} \delta(E_n - E_m) |\langle n | T | m \rangle|^2 . \qquad (A\,8.29)$$

Calculation in this Appendix is due to the following text book :

A. S. Davydov : Quantum Mechanics (2nd edition), translated by

D. Ter. Haar, Pergamon Press, 1976 Chapter XII.

Appendix 9

Consider a system in the mixed state which can not be described by wave functions. The mixed state is represented by mixing the pure states with each statistical weight $W(i)$. Phase of each pure state is random. As an example the state of unpolarized photon beam is considered to be a mixed state and it does not correspond to any wave function.

Average value of a quantity A in the mixed state is given by

$$\overline{\langle A \rangle} = \sum_i W(i) \langle A^{(i)} \rangle, \quad \langle A^{(i)} \rangle = \int \psi^{(i)*} A \psi^{(i)} d\tau, \qquad (A9.1)$$

where $\langle A^{(i)} \rangle$ denotes the quantum mechanical average of A and $-$ in $\overline{\langle A \rangle}$ means the statiscal average. Cleary, $\sum_i W(i) = 1$ should be satisfied.

Expand a pure state $\psi^{(i)}$ by use of a complete orthonormal set $\{ \psi_n \}$.

$$\psi^{(i)} = \sum_n a_n^{(i)} \psi_n, \quad \sum_n a_n^{(i)*} a_n^{(i)} = 1. \qquad (A9.2)$$

By inserting (A9.2) into (A9.1), $\langle \overline{A} \rangle$ becomes

$$\langle \overline{A} \rangle = \sum_i W(i) \sum_{nn'} A_{nn'} a_n^{(i)*} a_{n'}^{(i)}, \quad A_{nn'} = \int \psi_n^* A \psi_{n'} d\tau. \qquad (A9.3)$$

Now, introduce an operator whose matrix element is represented by

$$\rho_{n'n} = \sum_i W(i) a_n^{(i)*} a_{n'}^{(i)}. \qquad (A9.4)$$

From this,

$$\langle \overline{A} \rangle = \sum_{nn'} A_{nn'} \rho_{n'n} = \sum_n (A\rho)_{nn}, \qquad (A9.5)$$

or

$$\langle \overline{A} \rangle = \mathrm{Tr}(A\rho) = \mathrm{Tr}(\rho A). \qquad (A9.6)$$

ρ is called the density matrix which was introduced by

Neumann and Landau. Equation of motion of the density matrix is easily obtained as follows.

$$\frac{\partial}{\partial t}\rho_{n'n}(t)=\sum_i W(i)\left[\frac{\partial a_n^{(i)*}}{\partial t}a_{n'}^{(i)}+a_n^{(i)*}\frac{\partial a_{n'}^{(i)}}{\partial t}\right] \qquad (A9.7)$$

Inserting $\psi^{(i)}=\sum_n a_n^{(i)}(t)\psi_n$ into the Schrödinger equation, we obtain

$$i\hbar\frac{\partial a_n^{(i)}}{\partial t}=\sum_n\langle n|H|m\rangle a_m^{(i)}. \qquad (A9.8)$$

Therefore,

$$i\hbar\frac{\partial}{\partial t}\rho_{n'n}=\sum_l\left[\langle n'|H|l\rangle\rho_{ln}-\rho_{n'l}\langle l|H|n\rangle\right], \qquad (A9.9)$$

or

$$i\hbar\frac{\partial\rho}{\partial t}=[H,\rho]. \qquad (A9.10)$$

(A9.10) is a quantum mechanical analogue to the classical Liouville equation and ρ corresponds to the quantum mechanical distribution function. The density matrix describes the state of a sub-system which contacts with the system with large degrees of freedom (heat bath).

Appendix 10

As already given in (11.210), the thermodynamic potential without spin Zeeman energy is

$$\Phi=-\frac{\Omega k_0T}{2\pi^2}\frac{s}{\hbar}\sum_n\int dp_z\ln\left[1+\exp\left(\frac{\zeta-E_n(p_z)}{k_0T}\right)\right]. \qquad (A10.1)$$

To carry out the summation $\sum_{n} \cdots$, the Euler-Maclaurin's formula is employed.

$$\sum_{l=a}^{b-1} f(l+1/2) \cong \int_a^b f(x)\,dx - \frac{1}{24}\left| f'(x) \right|_a^b . \qquad (A\,10.2)$$

The above formula is valid as long as the following inequality

$$f(x+1/2) - f(x-1/2) - f'(x) \ll f(x) \qquad (A\,10.3)$$

holds. In the present problem (A 10.2) is applicable under the condition $\hbar\omega_0 = 2\bar{\mu}H \ll k_0T$. From (A 10.1) and (A 10.2), non-oscillating term of the thermodynamic potential becomes

$$\Phi_0 \cong - \frac{\Omega k_0 T}{2\pi^2} \frac{S}{\hbar} \int_{-\infty}^{\infty} dp_z \int_0^{\infty} \ln\left[1 + \exp\left(\zeta - 2\mu\bar{H}x - p_z^2/2m^* \right)/k_0T \right] dx$$

$$+ \frac{m^*\Omega}{12\pi^2\hbar^3} (\bar{\mu}H)^2 \int_{-\infty}^{\infty} \frac{dp_z}{1+\exp\left(p_z^2/2m^* - \zeta\right)/k_0T} . \qquad (A\,10.4)$$

By changing variable, (A 10.4) becomes

$$\Phi_0 \cong - \frac{\Omega (2m^*)^{3/2} k_0 T}{2\pi^2\hbar^3} \int_0^{\infty} \ln\left(1 + \exp(\zeta - x)/k_0T \right) x^{1/2}\,dx$$

$$+ \frac{\Omega (2m^*)^{3/2}}{24\pi^2\hbar^3} (\bar{\mu}H)^2 \int_0^{\infty} \frac{x^{-1/2}\,dx}{1+e^{(x-\zeta)/k_0T}} . \qquad (A\,10.5)$$

Developing (A 10.5) in power series of (k_0T/ζ) and retaining the first term, we have

$$\Phi_0 \cong -\frac{\Omega\, 2(2m^*)^{3/2}\zeta^{5/2}}{15\pi^2\hbar^3} + \frac{\Omega\,(2m^*)^{3/2}\zeta^{1/2}}{12\pi^2\hbar^3}(\bar{\mu}H)^2, \qquad (A\ 10.6)$$

and

$$M_0 = -\frac{1}{\Omega}\frac{\partial\Phi_0}{\partial H} = -\frac{(2m^*)^{3/2}\zeta^{1/2}}{6\pi^2\hbar^3}\bar{\mu}^2 H$$

$$= -\frac{\bar{\mu}^2 p_F m^* H}{3\pi^2\hbar^3}, \quad (\zeta = p_F^2/2m^*). \qquad (A\ 10.7)$$

Appendix 11.

In the configuration of $\nabla T = 0$, $\mathcal{E} = (\mathcal{E}_x, \mathcal{E}_y, 0)$ and $H \parallel z$ the thermal current density w_x is expressed by

$$w_x = \chi_{xx}\mathcal{E}_x + \chi_{xy}\mathcal{E}_y . \qquad (A\ 11.1)$$

χ_{xx} is a dissipative term and without scattering processes it vanishes (cf. Section 12.3). Since we are now interested in the collision independent effect, we pay our attention only to $\chi_{xy}\mathcal{E}_y$.

The Hamiltonian takes the form

$$\mathcal{H} = H + e\,\mathcal{E}\cdot\mathbf{r}. \qquad (A\ 11.2)$$

w_x is given by

$$w_x = \mathrm{Tr}\,(\mathcal{H} - \zeta)\,v_x\,\rho(\mathcal{H}), \qquad (A\ 11.3)$$

where $\rho(\mathcal{H})$ denotes the density matrix corresponding (A 11.2).

Picking up a term proportional to $\mathcal{E}_y$ in w_x, we can calculate

χ_{xy}. (A 11.3) is also written in the form

$$w_x = \sum_{\mu,\nu} (E_\mu - \zeta)(v_x)_{\mu\nu}\rho_{\nu\mu} . \tag{A 11.4}$$

Considering $e\mathcal{E}\,\mathbf{r}$ as a perturbation, one obtains the non-diagonal elements of the density matrix:

$$\rho_{\alpha\beta} = f_\alpha \delta_{\alpha\beta} + \frac{f_\alpha - f_\beta}{E_\alpha - E_\beta}\, e\,\mathcal{E}\cdot(\mathbf{r})_{\alpha\beta} + \cdots . \tag{A 11.5}$$

By substituting (A 11.5) into (A 11.4), $\chi_{xy}^{(0)}$ is obtained as follows:

$$\begin{aligned}\chi_{xy}^{(0)} &= \sum_{\mu,\nu} (E_\mu - \zeta)(v_x)_{\mu\nu}\left(\frac{f_\mu - f_\nu}{E_\mu - E_\nu}\right) e\,(y)_{\nu\mu} \\ &= i e\hbar \sum_{\mu,\nu} (E_\mu - \zeta)(v_x)_{\mu\nu}(v_y)_{\nu\mu}\,\frac{f_\mu - f_\nu}{(E_\mu - E_\nu)^2} .\end{aligned} \tag{A 11.6}$$

On utilizing (11.29), (A 11.6) is rewritten as

$$\chi_{xy}^{(0)} = \frac{1}{2}\frac{c}{H}\sum_{n,p_z,X} (2E_{n,p_z} + \hbar\omega_0 - 2\zeta)(n+1)(f_{n+1,p_z} - f_{n,p_z}) . \tag{A 11.7}$$

In consideration of (A 11.7), (12.39), (12.40) and (12.41), we arrive at the expression of (12.26).

Appendix 12.

Consider a system whose Hamiltonian and energy are functions of a paramter λ.

Differentiating $(H-E_n)\psi_n = 0$ on λ and multiplying ψ_n^* on the left hand side, we obtain

$$\psi_n^*(H-E_n)\frac{\partial\psi_n}{\partial\lambda} = \psi_n^*\left(\frac{\partial E_n}{\partial\lambda} - \frac{\partial H}{\partial\lambda}\right)\psi_n . \qquad (A\,12.1)$$

Integration over space coordinate makes the left hand side zero, because

$$\int \psi_n^*(H-E_n)\frac{\partial\psi_n}{\partial\lambda}\,d\boldsymbol{r} = \int \frac{\partial\psi_n}{\partial\lambda}(H-E_n)^*\psi_n^*\,d\boldsymbol{r} = 0. \qquad (A\,12.2)$$

Therefore,

$$\frac{\partial E_x}{\partial\lambda} = \left\langle\frac{\partial H}{\partial\lambda}\right\rangle_n . \qquad (A\,12.3)$$

If we put $\lambda = p_x$, (12.34) is obtained.

Appendix 13

Semiclassical equation of motion of an electron in magnetic field is given by

$$\frac{d\boldsymbol{k}}{dt} = -\frac{e}{\hbar c}(\boldsymbol{v}\times\boldsymbol{H}). \qquad (A\,13.1)$$

(A 13.1) is already given in (4.28). Energy change is zero, because $\partial E/\partial t = (\partial E/\partial\boldsymbol{k})\cdot(d\boldsymbol{k}/dt) = \boldsymbol{v}\{-(e/c)\boldsymbol{v}\times\boldsymbol{H}\} = 0$, and also (A 13.1) leads to the result that the wave vector component k_H along $\boldsymbol{H}$ remains constant.

Namely, (A 13.1) restricts the electron motion along the trajectory :

$$E = \text{constant}, \quad k_H = \text{constant}. \tag{A 13.2}$$

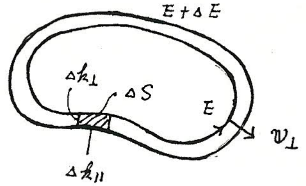


Fig. A 13.1 Cross section of the constant energy surface perpendicular to H. ($\Delta S = \Delta k_\perp \Delta k_\parallel$)

Two trajectories for k_H = constant, E, $E + \Delta E$ are illustrated in Fig. A 13.1. $k_\parallel$ an $k_\perp$ denote, respectively the wave vector component along and normal to the trajectory specified by (A 13.2). In Fig. A 13.1 $v_\perp$ is perpendicular to $k_\parallel$. From (A 13.1) we have

$$\frac{dk_\parallel}{dt} = -\frac{e}{\hbar c} v_\perp H . \tag{A 13.3}$$

If the electron orbit is closed, the period for circulating the orbit is given by

$$T = \frac{\hbar c}{eH} \oint \frac{dk_\parallel}{v_\perp} . \tag{A 13.4}$$

This is already given in (6.164). Cyclotron mass is defined by

$$m^* = \frac{\hbar}{2\pi} \oint \frac{dk_\parallel}{v_\perp} \tag{A 13.5}$$

Since $v_\perp = \partial E / \hbar \, \partial k_\perp$, m^* is rewritten as

$$m^* = \frac{\hbar^2}{2\pi} \oint \frac{dk_\perp}{dE} dk_\parallel = \frac{\hbar^2}{2\pi} \frac{\partial}{\partial E} S(k_H, E) . \tag{A 13.6}$$

After integrating (A 13.1), we get

$$k = -s(\mathbf{r} - \mathbf{r}_0) \times \mathbf{h}, \left(s = \frac{eH}{\hbar c}, \mathbf{h} = \frac{\mathbf{H}}{H} \right). \qquad (A\ 13.7)$$

This shows that the trajectories of the electrons in r-space normal to H are equal to the trajectories in k-space after a rotation by $\pi/2$ and a multiplication by a scale factor s^{-1}.

In the presence of a magnetic field the momentum conjugate to $\mathbf{r}$ is $\hbar k - \frac{e}{c}\mathbf{A}$ (curl $\mathbf{A} = \mathbf{H}$), and therefore the Bohr-Sommerfeld's quantization condition is

$$\oint (\hbar k - \frac{e}{c}\mathbf{A}) \cdot d\mathbf{r} = 2\pi\hbar \left[n + \gamma(n) \right], \quad 0 < \gamma < 1 \qquad (A\ 13.8)$$

In consideration of (A 13.7), left hand side of (A 13.8) becomes

$$\oint \left[\frac{e}{c} \mathbf{H} \cdot (\mathbf{r} \times d\mathbf{r}) - \frac{e}{c} \mathbf{A}\, d\mathbf{r} \right]. \qquad (A\ 13.9)$$

Since $\oint \mathbf{r} \times d\mathbf{r}$ is twice of the area encircled by the orbit, $\oint \mathbf{H} \cdot (\mathbf{r} \times d\mathbf{r})$ is equal to 2Φ, where Φ denotes the magnetic flux. Then, we obtain

$$\frac{e}{c}\Phi = 2\pi\hbar (n + \gamma). \qquad (A\ 13.10)$$

Area in k-space is obtained from the corresponding area in r-space by multiplying a factor s^2. Then, (A 13.10) leads to

$$S(k_H, E) = 2\pi s \left[n + \gamma(n) \right]. \qquad (A\ 13.11)$$

Provided that $n \gg 1$, area between adjacent levels (between n and $n+1$) becomes

$$\Delta S = \frac{2\pi e H}{\hbar c} . \qquad (A\ 13.12)$$

(A 13.11) is called the Onsager - Lifshitz quantization condition. It was derived in Section 11.9.

Appendix 14

In the first place we shall derive (13.121). From Figs. 13.12 (a) and (b) $\mathbf{v}'$ and $\mathbf{r}'$ are obtained as follows :

$$\left\{ \begin{aligned} v_x' &= v_\perp \cos [\, \omega_0 (t' - t) + \phi \,] , \\ v_y' &= v_\perp \sin [\, \omega_0 (t' - t) + \phi \,] , \\ v_z' &= v_z = v \cos\theta \end{aligned} \right. \qquad (A\ 14.1)$$

$$\left\{ \begin{aligned} x' &= x + (v_\perp/\omega_0)\{ \sin [\omega_0 (t' - t) + \phi] - \sin\phi \} , \\ y' &= y - (v_\perp/\omega_0)\{ \cos [\omega_0 (t' - t) + \phi] - \cos\phi \} , \\ z' &= z + v_z (t' - t) , \end{aligned} \right. \qquad (A\ 14.2)$$

where (θ, ϕ) is the polar angle of $\mathbf{v}$. By substituting (A 14.1) and (A 14.2) into (13.97), $J(\mathbf{v})$ and $K(\mathbf{v})$ become

$$J(\mathbf{v}) = \exp(-iX \sin\theta \sin\phi) \begin{pmatrix} (ie\, v/X)\, \partial/\partial\phi \\ ie\, v\, \partial/\partial X \\ -e\, v \cos\theta \end{pmatrix} g(X, \theta, \phi) , \qquad (A\ 14.3)$$

$$K(v) = \exp\left(-iX\sin\theta\sin\phi\right) g(X,\theta,\phi), \tag{A 14.4}$$

where

$$\begin{cases} g(X,\theta,\phi) = \displaystyle\int_0^\infty ds \exp\left\{-i\left[X\sin\theta\sin(\omega_0 s-\phi) + q_z v\cos\theta\, s - \omega s\right] - s/\tau\right\}, & \text{(A 14.5)} \\ X = q_x v/\omega_0 . \end{cases}$$

Integration (A 14.5) is carried out by using the relation

$$e^{iz\sin\psi} = \sum_{n=-\infty}^{\infty} J_n(z)\, e^{in\psi}, \tag{A 14.6}$$

$$g = \tau \sum_{n=-\infty}^{\infty} \frac{J_n(X\sin\theta)\, e^{in\phi}}{1+i(n\omega_0 + q_z v\cos\theta - \omega)\tau} . \tag{A 14.7}$$

On making use of (A 14.7) and (A 14.3) the conductivity (13.99) takes the form

$$\sigma = \frac{3\sigma_0}{4\pi} \sum_n \int d\Omega \begin{pmatrix} \sin\theta\cos\phi \\ \sin\theta\sin\phi \\ \cos\theta \end{pmatrix} e^{-iX\sin\theta\sin\phi} \begin{pmatrix} (-i/X)\,\partial/\partial\phi \\ -i\,\partial/\partial X \\ \cos\theta \end{pmatrix} \frac{J_n(X\sin\theta)\, e^{in\phi}}{1+i(n\omega_0-\omega+q_z v_F\cos\theta)\tau},$$

(A 14.8)

where $X = q_x v_F/\omega_0$.

Integration over ϕ is performed by using the following transformations.

$$\sin\theta\cos\phi\, e^{-iX\sin\theta\sin\phi} = \frac{1}{-iX}\frac{\partial}{\partial\phi} e^{-iX\sin\theta\sin\phi} = \frac{1}{-iX}\frac{\partial}{\partial\phi}\sum_n J_n(-X\sin\theta)e^{in\phi}$$

$$= -\sum_n \frac{n}{X} J_n(-X\sin\theta)e^{in\phi} = -\sum_n \frac{n}{X}(-1)^n J_n(X\sin\theta)\, e^{in\phi} . \tag{A 14.9}$$

Hence,

$$\int_0^{2\pi} d\phi \sin\theta \cos\phi\, e^{-iX\sin\theta\cos\phi}\left(-\frac{i}{X}\frac{\partial}{\partial\phi}\right)J_n(X\sin\theta)e^{in\phi} = 2\pi\left(\frac{n}{X}\right)^2(-1)^n J_{-n}(X\sin\theta)J_n(X\sin\theta)$$

$$= 2\pi\left(\frac{n}{X}\right)^2(-1)^n(-1)^n\{J_n(X\sin\theta)\}^2 = 2\pi\left(\frac{n}{X}\right)^2\{J_n(X\sin\theta)\}^2. \qquad (A\,14.10)$$

Other components σ_{ij} can be calculated by similiar procedure. Finally, we obtain

$$\sigma = \frac{3\sigma_0}{2}\sum_{n=-\infty}^{\infty}\begin{pmatrix} n/X \\ i\partial/\partial X \\ \cos\theta \end{pmatrix} J_n(X\sin\theta)\begin{pmatrix} n/X \\ -i\partial/\partial X \\ \cos\theta \end{pmatrix} J_n(X\sin\theta)\,\frac{\sin\theta\, d\theta}{1+i(n\omega_0-\omega+q_z v_F\cos\theta)\tau}. \qquad (A\,14.11)$$

In the next place we shall give the concrete expressions of $g_n(X)$, $g_n'(X)$, $S_n(X)$ and $r_n(X)$.

From the relation;

$$\int_0^{\pi/2} J_p^2(z\sin\theta)\sin\theta\, d\theta = \frac{1}{z}\sum_{n=0}^{\infty} J_{2p+2n+1}(2z), \qquad (A\,14.12)$$

we obtain

$$g_n(X) = \frac{1}{X}\sum_{m=0}^{\infty} J_{2m+2n+1}(2X), \qquad (A\,14.13)$$

and $2J_p' = J_{p-1} - J_{p+1}$ gives

$$g_n'(X) = \frac{1}{X}\left[J_{2n}(2X) - g_n(X)\right]. \qquad (A\,14.14)$$

Differentiating $r_n(X)$, which is given by (13.123), on X, we get

$$\frac{d\, r_n(X)}{d X} = \frac{1}{X} g_n(X) - \frac{3}{X} r_n(X).$$

Accordingly, $r_n(x)$ becomes

$$X^3 r_n(X) = \int_0^X x^2 g_n(x)\,dx. \qquad (A14.15)$$

By inserting (A14.13) into (A14.15) and using $J_n' = \frac{1}{2}(J_{n-1} - J_{n+1})$, $r_n(X)$ is rewritten as follows:

$$r_n(X) = \frac{g_n(X)}{2} - \frac{1}{2X^3}\int_0^X z^2 J_{2n}(2z)\,dz. \qquad (A14.16)$$

By performing the partial integration of the differential equation satisfied by the Bessel function, (A14.16) is expressed by

$$r_n(X) = \frac{g_n(X)}{2} - \frac{1}{8X^2} J_{2n}(2X) + \frac{1}{8X}\frac{d}{dX} J_{2n}(2X) + \frac{(1-4n^2)}{8X^3}\int_0^X J_{2n}(2x)\,dx.$$

(A14.17)

Since $g_n(X)$ is expressed by

$$g_n(X) = \frac{1}{X}\int_0^X J_{2n}(2x)\,dx. \qquad (A14.18)$$

$r_n(X)$ becomes

$$r_n(X) = \frac{g_n(X)}{2} + \frac{1-4n^2}{8X^2} g_n(X) - \frac{1}{8X^2} J_{2n}(2X) + \frac{1}{8X}\frac{d}{dX} J_{2n}(2X). \qquad (A14.19)$$

By differentiating $g_n(X)$ twice and using the Bessel's differential equation, the following relation is obtained.

$$g_n''(X) = 2S_n(X) - \frac{1}{X} g_n'(X) - 2\left[g_n(X) - r_n(X)\right] + \frac{2n^2}{X^2} g_n(X).$$

In consideration of (A14.14) and the definition of $r_n(X)$ in (13.123), $S_n(X)$ is obtained:

$$S_n(X) = 3r_n(X) - (1 - n^2/X^2)\, g_n(X). \tag{A 14.20}$$

The calculations in this Appendix is due to the following article[183]:

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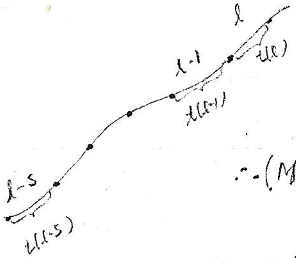
Eq. (15.11) can be easily extended to a case with non-isochronous division of network of the electron orbits.

In this case $K_j(\ell)$ takes the form

$$K_j(\ell) = \sum_{p=1}^{\infty} \int_0^{t(\ell-p)} dt'' v_j(t'', \ell-p) \exp\left[\left\{t'' - \sum_{s=1}^{p} t(\ell-s)\right\}/\tau\right]. \qquad (1)$$



$$\begin{cases} (\mathbb{M}^p)_{\ell,r} = M_{\ell,\ell-1} M_{\ell-1,\ell-2} \cdots M_{\ell-p+1,\ell-p}, \\ M_{\ell r} = \delta_{\ell,r+1} e^{-t(r)} = \delta_{\ell,r+1} e^{-t(\ell-1)}. \end{cases} \qquad (2)$$

$$\therefore (\mathbb{M}^p)_{\ell,r} = \exp\left[-\sum_{s=1}^{p} t(\ell-s)/\tau\right], \quad (\ell = r+p). \qquad (3)$$

$$\mathbb{K}_j = \sum_{p=1}^{\infty} \mathbb{M}^p \cdot \mathbb{V}_j, \quad K_j(\ell) = \sum_{p=1}^{\infty} (\mathbb{M}^p)_{\ell,\ell-p} V_j(\ell-p)$$

$$= \sum_{p=1}^{\infty} \int_0^{t(\ell-p)} dt'' v_j(t'', \ell-p) \exp\left[\left\{t'' - \sum_{s=1}^{p} t(\ell-s)\right\}/\tau\right]. \qquad (4)$$

Eq. (4) is equivalent to Eq. (1). Then, we can get K_j & $\mathbb{M}$ for the case with magnetic breakdown.

$$M_{\ell,r} = W(r \to \ell) e^{-t(r)}, \quad \mathbb{K}_j = \mathbb{M} \cdot (1 - \mathbb{M})^{-1} \cdot \mathbb{V}_j, \qquad (5)$$

where $W(r \to \ell)$ denotes the transition probability from segment r to ℓ.