Boltzmann transport equation (I):
Bloch-Grüneisen law for electrical reesistivity

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We discuss the Boltzmann transport equation which is very useful in understanding the transport properties such as electrical conductivity, thermal conductivity, and thermoelectric power. This equation is used to determine the distribution function of particles (electrons) in the phase space $(\boldsymbol{r}, \boldsymbol{k})$ phase space. Because of the Heisenberg's uncertainty principle, the use of this equation is limited for the transport equation in the quantum mechanics. The number of particles in the range [***r*** and ***r***+d***r***, ***p*** and ***p***+d***p***],

$$dN = f(\boldsymbol{p}, \boldsymbol{r}, t) d\boldsymbol{r} d\boldsymbol{p} .$$

In thermal equilibrium $f(\boldsymbol{p}, \boldsymbol{r}, t)$ is the Fermi-Dirac distribution function. The system is deviated from the thermal equilibrium in the presence of a perturbation such as the electric field and temperature gradient.

((Note))
Here we use the following notation

$$\sum_{\boldsymbol{k}} f(\boldsymbol{k}) \rightarrow \frac{2V}{(2\pi)^3} \int d\boldsymbol{k}$$

instead of using

$$\sum_{\boldsymbol{k}} f(\boldsymbol{k}) \rightarrow \frac{V}{(2\pi)^3} \int d\boldsymbol{k}$$

In other words, the spin weight factor (2) is included in our notation in this section.

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1. Boltzmann transport equation

We assume that the wave functions of the system can be described by on-electron Bloch function (we will discuss later the wave function of Bloch electron)

$$\psi_{\boldsymbol{k}}(\boldsymbol{r}) = |\boldsymbol{k}\rangle = e^{i\boldsymbol{k}\cdot\boldsymbol{r}} u_{\boldsymbol{k}}(\boldsymbol{r}).$$

The number of electrons per unit volume whose wavevectors lie in the interval (***k*** - ***k***+d***k***) is

$$\frac{2}{(2\pi)^3} f(\boldsymbol{k},\boldsymbol{r}) d\boldsymbol{k}, \qquad (1)$$

where the factor 2 is the spin weight. In equilibrium $f(\boldsymbol{k},\boldsymbol{r})$ becomes the Fermi-Dirac distribution function $f_0(E)$, but deviates from $f_0(E)$ in the presence of the electric field, magnetic field, temperature gradient, and so on. We consider the time dependence of the distribution function in the presence of such perturbations. There are two contributions to this time dependence, (i) from the external force (the drift term) and (ii) the collisions (the collision term),

$$\frac{df}{dt} = \left(\frac{\partial f}{\partial t}\right)_{drift} + \left(\frac{\partial f}{\partial t}\right)_{coll}$$

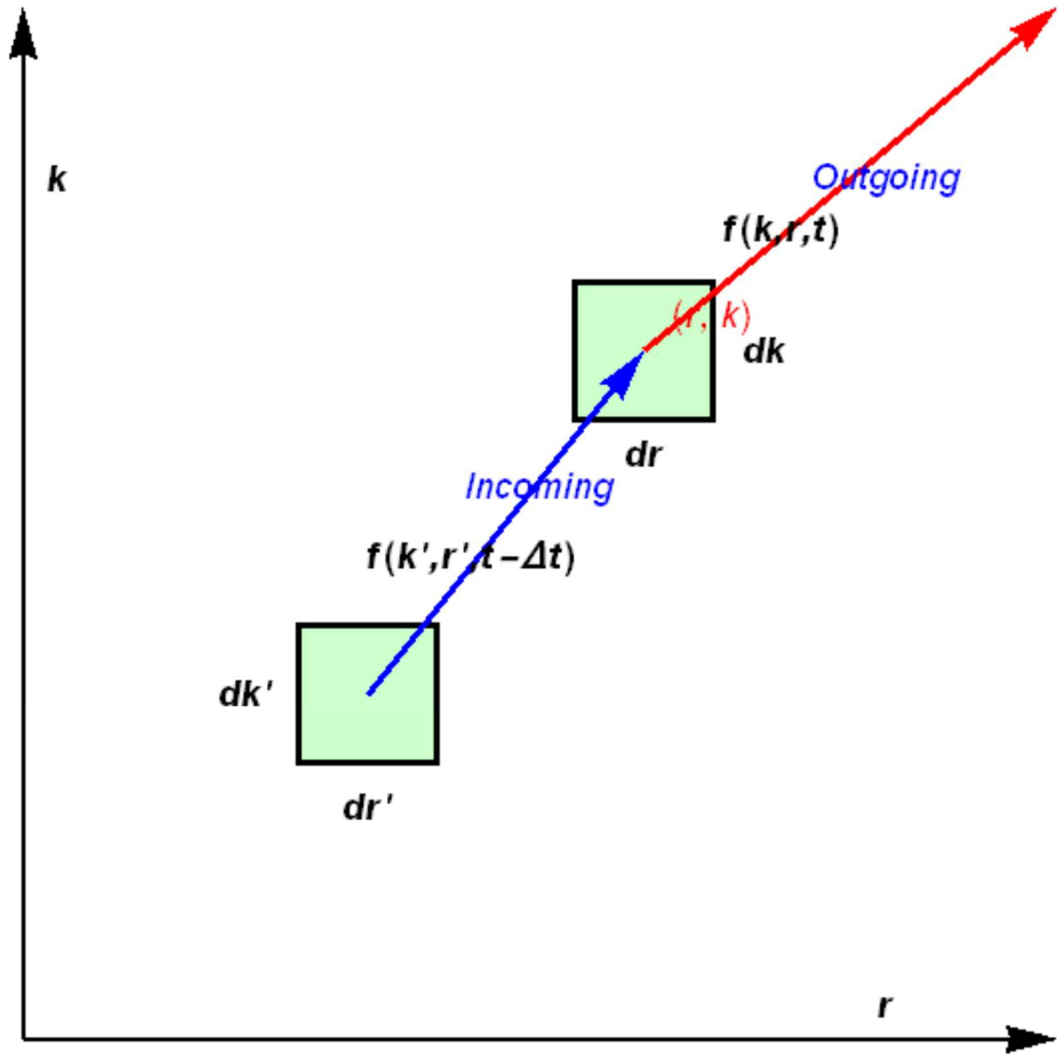


Fig. Phase space trajectory function $f(\boldsymbol{k},\boldsymbol{r},t)$.

In the time interval between t and $t + \Delta t$, the drift term of $f(\boldsymbol{k},\boldsymbol{r})$ corresponds to the difference of the incoming quantity $f(\boldsymbol{k}-\Delta\boldsymbol{k},\boldsymbol{r}-\Delta\boldsymbol{r},)\Delta t$ in the phase space and the outgoing quantity $f(\boldsymbol{k},\boldsymbol{r},)\Delta t$. Then we have

$$
\begin{aligned}
\left(\frac{\partial f}{\partial t}\right)_{drift} &= \frac{f(\boldsymbol{k}-\Delta\boldsymbol{k}, \boldsymbol{r}-\Delta\boldsymbol{r}) - f(\boldsymbol{k}, \boldsymbol{r})}{\Delta t} \\
&= -\frac{d\boldsymbol{r}}{dt}\cdot\nabla_{r} f - \frac{d\boldsymbol{k}}{dt}\cdot\nabla_{k} f \\
&= -\boldsymbol{v}\cdot\nabla_{r} f - \frac{1}{\hbar}\boldsymbol{F}\cdot\nabla_{k} f
\end{aligned} \qquad (2)
$$

where $\boldsymbol{v}$ is the velocity and $\boldsymbol{F}$ is the force due to the presence of the perturbations.

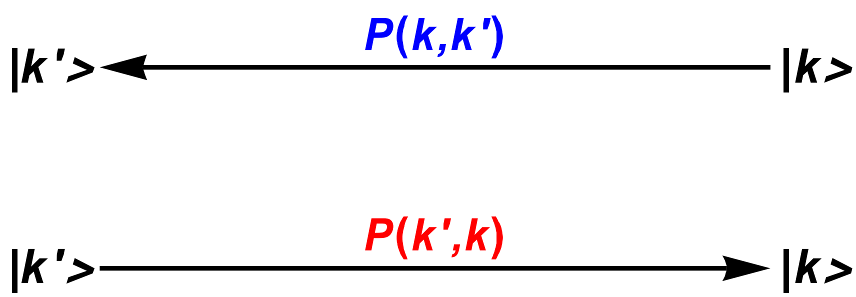


Fig. Probability transition between the states $|\boldsymbol{k}\rangle$ and $|\boldsymbol{k}'\rangle$. $P(\boldsymbol{k}',\boldsymbol{k})f(\boldsymbol{k}')[1-f(\boldsymbol{k})]$. $P(\boldsymbol{k},\boldsymbol{k}')f(\boldsymbol{k})[1-f(\boldsymbol{k}')]$

In consideration of the exclusion principle, the collision term can be expressed

$$
\begin{aligned}
\left(\frac{\partial f}{\partial t}\right)_{coll} &= \sum_{\boldsymbol{k}'}[P(\boldsymbol{k}',\boldsymbol{k})f(\boldsymbol{k}')\{1-f(\boldsymbol{k})\} - P(\boldsymbol{k},\boldsymbol{k}')f(\boldsymbol{k})\{1-f(\boldsymbol{k}')\}] \\
&\approx \sum_{\boldsymbol{k}'}[P(\boldsymbol{k}',\boldsymbol{k})f(\boldsymbol{k}') - P(\boldsymbol{k},\boldsymbol{k}')f(\boldsymbol{k})]
\end{aligned}, \qquad (3)
$$

where we assume that P does not change due to the external fields. In thermal equilibrium, we have the condition of detailed balance,

$$
P(\boldsymbol{k}',\boldsymbol{k})f_0(\boldsymbol{k}') = P(\boldsymbol{k},\boldsymbol{k}')f_0(\boldsymbol{k}).
$$

Then we get

$$
\left(\frac{\partial f}{\partial t}\right)_{coll} = -\sum_{\boldsymbol{k}'} P(\boldsymbol{k},\boldsymbol{k}')[f(\boldsymbol{k}) - \frac{f_0(\boldsymbol{k})}{f_0(\boldsymbol{k}')}f(\boldsymbol{k}')].
$$

As shown below, this can be well described by

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

using a relaxation time $\tau(\boldsymbol{k})$.

We consider the general Boltzmann equation

$$\frac{df}{dt} = \left(\frac{\partial f}{\partial t}\right)_{drift} + \left(\frac{\partial f}{\partial t}\right)_{collt}$$

In the steady state,

$$\frac{df}{dt} = 0$$

or

$$\left(\frac{\partial f}{\partial t}\right)_{drift} + \left(\frac{\partial f}{\partial t}\right)_{collt} = 0$$

This equation is called the Boltzmann equation.

$$f = f_0 - \tau \boldsymbol{v} \cdot \nabla_{\boldsymbol{r}} f - \frac{1}{\hbar} \tau \boldsymbol{F} \cdot \nabla_k f$$

where

$$\boldsymbol{F} = -e[\boldsymbol{E} + \frac{1}{c}(\boldsymbol{v} \times \boldsymbol{B})] \qquad \text{(Lorentz force)}$$

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

$$\left(\frac{\partial f}{\partial t}\right)_{drift} = -\boldsymbol{v}\cdot\nabla_r f - \frac{1}{\hbar}\boldsymbol{F}\cdot\nabla_k f$$

2. Effect of electric field

Here we consider the case when the electric field (sufficiently weak constant field) is applied to the system;

$$\boldsymbol{v}_k = \frac{1}{\hbar}\nabla_{\boldsymbol{k}}\varepsilon(\boldsymbol{k}). \qquad \boldsymbol{F} = -e\boldsymbol{E}$$

where $\boldsymbol{v}_k$ is the group velocity, $\boldsymbol{E}$ is the electric field, and $\boldsymbol{F}$ is the force due to the electric field. We assume that $f(\boldsymbol{k},\boldsymbol{r})$ can be described by

$$f(\boldsymbol{k},\boldsymbol{r}) = f(\boldsymbol{k}) = f_0(\boldsymbol{k}) + f_1(\boldsymbol{k}).$$

which is independent of $\boldsymbol{r}$. We also assume that

$$|f_0(\boldsymbol{k})| >> |f_1(\boldsymbol{k})|,$$

and the energy is conserved (the elastic scattering),

$$\boldsymbol{k}' \approx \boldsymbol{k}, \qquad E(\boldsymbol{k}) \approx E(\boldsymbol{k}'), \qquad f_0(\boldsymbol{k}') \approx f_0(\boldsymbol{k})$$

Then we get

$$\left(\frac{\partial f}{\partial t}\right)_{coll} = -\frac{f(\boldsymbol{k}) - f_0(\boldsymbol{k})}{\tau(\boldsymbol{k})} = -\frac{f_1(\boldsymbol{k})}{\tau(\boldsymbol{k})}$$

where

$$\begin{aligned}\frac{f_1(\boldsymbol{k})}{\tau(\boldsymbol{k})} &= \sum_{\boldsymbol{k}'} P(\boldsymbol{k},\boldsymbol{k}')[f_0(\boldsymbol{k}) + f_1(\boldsymbol{k}) - \frac{f_0(\boldsymbol{k})}{f_0(\boldsymbol{k}')}\{f_0(\boldsymbol{k}') + f_1(\boldsymbol{k}')\}] \\ &= \sum_{\boldsymbol{k}'} P(\boldsymbol{k},\boldsymbol{k}')[1 - \frac{f_1(\boldsymbol{k}')}{f_1(\boldsymbol{k})}]\end{aligned}$$

We also get

$$\left(\frac{\partial f}{\partial t}\right)_{drift} = \frac{e}{\hbar}\boldsymbol{E}\cdot\nabla_{\boldsymbol{k}} f(\boldsymbol{k}) \approx \frac{e}{\hbar}\boldsymbol{E}\cdot\frac{df_0(\varepsilon_k)}{d\varepsilon_k}\nabla_{\boldsymbol{k}}\varepsilon(\boldsymbol{k}) = e\boldsymbol{E}\cdot\boldsymbol{v}_k\frac{df_0(\varepsilon_k)}{d\varepsilon_k}.$$

In the steady state, where

$$\frac{df}{dt} = \left(\frac{\partial f}{\partial t}\right)_{drift} + \left(\frac{\partial f}{\partial t}\right)_{coll} = 0,$$

Then we have

$$f_1(\boldsymbol{k}) = e\boldsymbol{E}\cdot\boldsymbol{v}_k\tau(\boldsymbol{k})\frac{df_0(\varepsilon_k)}{d\varepsilon_k}$$

Since

$$\frac{df_0(\varepsilon_k)}{d\varepsilon_k} \approx -\delta(\varepsilon_k - \varepsilon_F)$$

only the electrons near the Fermi energy contribute to the distribution function $f_1(\boldsymbol{k})$.

3. Relaxation time $\tau(\boldsymbol{k})$

We consider the case when the direction of the electric field is the positive *x* axis. Then we get

$$f_1 = eE_x v_x \tau(\boldsymbol{k})\frac{df_0(\varepsilon_k)}{d\varepsilon_k}$$

We note that

$$\frac{f_1(\boldsymbol{k}')}{f_1(\boldsymbol{k}')} = \frac{eE_x v_x'\tau(\boldsymbol{k})\frac{df_0(\varepsilon_k)}{d\varepsilon_k}}{eE_x v_x\tau(\boldsymbol{k}')\frac{df_0(\varepsilon_{k'})}{d\varepsilon_{k'}}} = \frac{v_x'\tau(\boldsymbol{k})}{v_x\tau(\boldsymbol{k}')} = \frac{v_x'}{v_x} = \frac{k_x'}{k_x}$$

where we assume that

$$\tau(\boldsymbol{k}') = \tau(\boldsymbol{k}).$$

The group velocity $\boldsymbol{v}_k$ is given by

$$v_{\boldsymbol{k}} = \nabla_{\boldsymbol{k}} \varepsilon_k = \frac{\hbar^2}{m^*} \boldsymbol{k} ,$$

where m^* is the effective mass of electrons. Then the relaxation time can be expressed by

$$\frac{1}{\tau(\boldsymbol{k})} = \sum_{\boldsymbol{k}'} P(\boldsymbol{k}, \boldsymbol{k}')(1 - \frac{k_x'}{k_x}) = \frac{2V}{(2\pi)^3} \int d\boldsymbol{k}' P(\boldsymbol{k}, \boldsymbol{k}')(1 - \frac{k_x'}{k_x})$$

4. Expression for the current density and conductivity

From the definition, the current density J_x is given by

$$J_x = \frac{1}{V} \sum_{\boldsymbol{k}} (-e) v_x f_1(\boldsymbol{k}) = -e^2 E_x \sum_{\boldsymbol{k}} v_x^2 \tau(\boldsymbol{k}) \frac{df_0(\varepsilon_k)}{d\varepsilon_k}$$

where

$$f_1(k) = eE_x v_x \tau(\boldsymbol{k}) \frac{df_0(\varepsilon_k)}{d\varepsilon_k}$$

We need to put $1/V$ in the expression of the current density. The unit of [e v] =[Coulomb][cm/s] = [A s]][cm/s]=[A][cm], while the unit of current density is [A/cm^2].

Noting that

$$\frac{df_0(\varepsilon_k)}{d\varepsilon_k} = -\frac{f_0(1 - f_0)}{k_B T},$$

we have

$$J_x = \frac{e^2 E_x}{k_B T V} \sum_{\boldsymbol{k}} v_x^2 \tau(\boldsymbol{k}) f_0 (1 - f_0).$$

5. Born approximation (Quantum mechanics)

We consider the scattering of free electron (plane wave) by a potential $V(\boldsymbol{r})$.

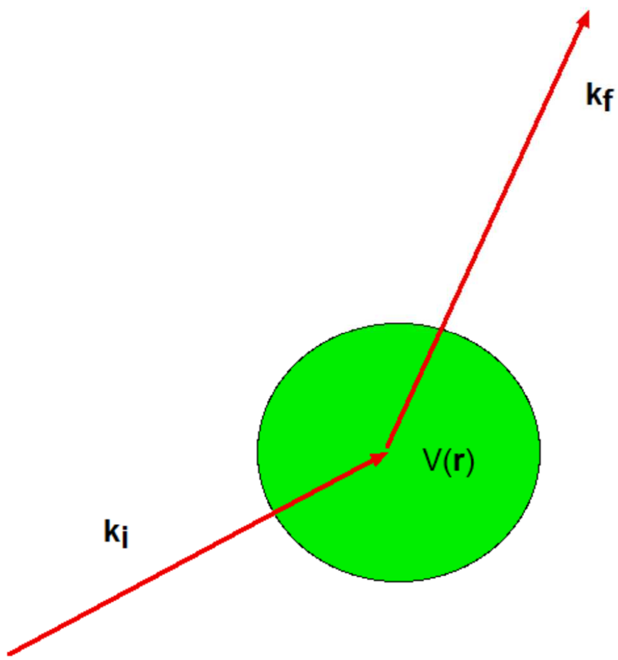


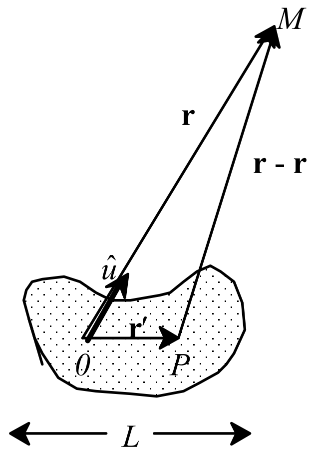
Fig. Scattering of free electron in the presence of potential $V(\boldsymbol{r})$. $\boldsymbol{k}_{\rm i} = \boldsymbol{k}$. $\boldsymbol{k}_{\rm f} = \boldsymbol{k}'$.

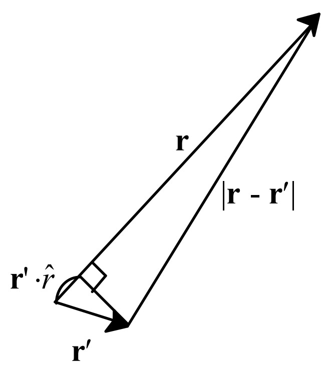
According to the Quantum Mechanics, the wavefunction of the scattered electron can be expressed by

$$\langle \boldsymbol{r} | \psi^{(+)} \rangle = \langle \boldsymbol{r} | \boldsymbol{k} \rangle - \frac{2m}{\hbar^2} \int d\boldsymbol{r}' \frac{e^{ik|\boldsymbol{r}-\boldsymbol{r}'|}}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|} V(\boldsymbol{r}') \langle \boldsymbol{r}' | \psi^{(+)} \rangle$$

where

$$\langle \boldsymbol{r} | \boldsymbol{k} \rangle = \frac{1}{(2\pi)^{3/2}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$$





Here we consider the case of $\langle \boldsymbol{r} | \psi^{(+)} \rangle$.

$$|\boldsymbol{r} - \boldsymbol{r}'| = r - \boldsymbol{r}' \cdot \boldsymbol{e}_r$$

$$\boldsymbol{k}' = k\boldsymbol{e}_r$$

$e^{ik|\boldsymbol{r}-\boldsymbol{r}'|} \approx e^{ik(r-\boldsymbol{r}'\cdot\boldsymbol{e}_r)} = e^{ikr}e^{-i\boldsymbol{k}'\cdot\boldsymbol{r}'}$ for large r.

$$\frac{1}{|\boldsymbol{r} - \boldsymbol{r}'|} \approx \frac{1}{r}$$

Then we have

$$\langle \boldsymbol{r} | \psi^{(+)} \rangle = \langle \boldsymbol{r} | \boldsymbol{k} \rangle - \frac{1}{4\pi} \frac{2m}{\hbar^2} \frac{e^{ikr}}{r} \int d\boldsymbol{r}' e^{-i\boldsymbol{k}'\cdot\boldsymbol{r}'} V(\boldsymbol{r}') \langle \boldsymbol{r}' | \psi^{(+)} \rangle$$

or

$$\langle \boldsymbol{r} | \psi^{(+)} \rangle = \frac{1}{(2\pi)^{3/2}} [e^{i\boldsymbol{k}\cdot\boldsymbol{r}} + -\frac{e^{ikr}}{r} f(\boldsymbol{k}', \boldsymbol{k})]$$

The first term: original plane wave in propagation direction $\boldsymbol{k}$. The second term: outgoing *spherical wave* with amplitude $f(\boldsymbol{k}', \boldsymbol{k})$.

$$\begin{aligned} f(\boldsymbol{k}', \boldsymbol{k}) &= -\frac{1}{4\pi} \frac{2m}{\hbar^2} (2\pi)^3 \int d\boldsymbol{r}' \frac{e^{-i\boldsymbol{k}'\cdot\boldsymbol{r}'}}{(2\pi)^{3/2}} V(\boldsymbol{r}') \langle \boldsymbol{r}' | \psi^{(\pm)} \rangle \\ &= -\frac{1}{4\pi} \frac{2m}{\hbar^2} (2\pi)^3 \langle \boldsymbol{k}' | \hat{V} | \psi^{(+)} \rangle \end{aligned}$$

The differential cross section is defined as

$$\frac{d\sigma}{d\Omega} = |f(\boldsymbol{k}', \boldsymbol{k})|^2$$

with

$$f(\boldsymbol{k}', \boldsymbol{k}) = -\frac{1}{4\pi} \frac{2m}{\hbar^2} (2\pi)^3 \langle \boldsymbol{k}' | \hat{V} | \psi^{(+)} \rangle$$

The first order Born amplitude is

$$f(\boldsymbol{k}', \boldsymbol{k}) = -\frac{1}{4\pi} \frac{2m}{\hbar^2} (2\pi)^3 \langle \boldsymbol{k}' | \hat{V} | \boldsymbol{k} \rangle = -\frac{m}{2\pi\hbar^2} \int d\boldsymbol{r}' e^{i(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{r}} V(\boldsymbol{r}')$$

which is the Fourier transform of the potential with respect to $\boldsymbol{q}$, where

$\boldsymbol{q} = \boldsymbol{k} - \boldsymbol{k}'$: (scattering wave vector).

For the elastic scattering, $\boldsymbol{k}$ and $\boldsymbol{k}'$ lie on the Ewald sphere ($|\boldsymbol{k}| = |\boldsymbol{k}'| = 2\pi/\lambda$).

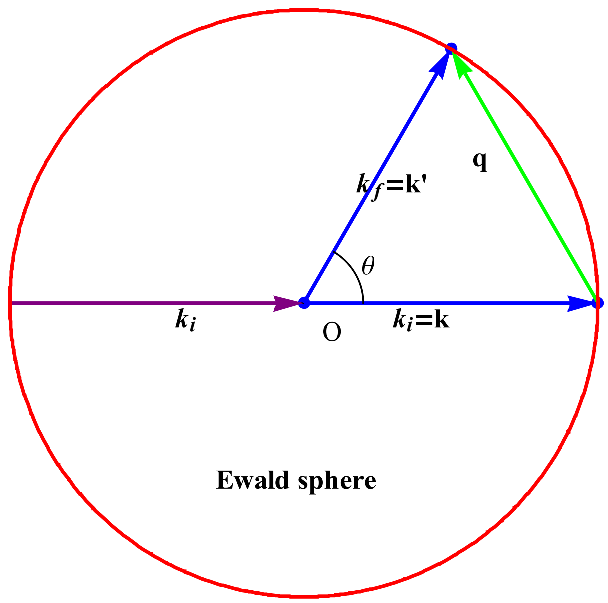


Fig. Ewald sphere. The scattering vector $\boldsymbol{q}$ = k' - $\boldsymbol{k}$. The normal process. In this process, $q = 2k\sin\frac{\theta}{2}$. The elastic scattering is assumed.

5. Expression of 1/τ($\boldsymbol{k}$)

We assume that the transition probability is given by

$$P(\boldsymbol{k},\boldsymbol{k}') = \frac{2\pi}{\hbar}|V(\boldsymbol{k},\boldsymbol{k}')|^2 \delta(\varepsilon_{k'} - \varepsilon_k)$$

for the elastic scattering where the incoming electron with |$\boldsymbol{k}$> is scattered in to an outgoing electron with the state |$\boldsymbol{k}$'>, as a result of the scattering potential (Born approximation). The matrix element is defined by

$$V(\boldsymbol{k},\boldsymbol{k}') = \langle \boldsymbol{k}'|V|\boldsymbol{k}\rangle.$$

Now we calculate the reciprocal relaxation time

$$\frac{1}{\tau(\boldsymbol{k})} = \frac{2V}{(2\pi)^3}\int d\boldsymbol{k}' P(\boldsymbol{k},\boldsymbol{k}')(1-\frac{k_x'}{k_x})$$

$$= \frac{2V}{(2\pi)^3}\frac{2\pi}{\hbar}\int d\boldsymbol{k}'\left|V(\boldsymbol{k},\boldsymbol{k}')\right|^2 \delta(\varepsilon_{k'}-\varepsilon_k)(1-\frac{k_x'}{k_x})$$

Here we note that

$$d\boldsymbol{k}' = k'^2\, dk' \sin\theta_{k'} d\theta_{k'} d\phi_{k'}$$

$$\frac{D(\varepsilon')d\varepsilon'}{4\pi} = \frac{2V}{(2\pi)^3} k'^2\, dk'$$

where θ is the angle between $\boldsymbol{k}$ (the k_x direction) and $\boldsymbol{k}'$, and $D(\varepsilon')$ is the density of states. Then we get

$$\frac{1}{\tau(\mathbf{k})} = \frac{2V}{(2\pi)^3}\frac{2\pi}{\hbar}\int k'^2\, dk' \sin\theta_{k'} d\theta_{k'} d\phi_{k'} \left|V(\theta_{\mathbf{k}'})\right|^2 \delta(\varepsilon_{k'}-\varepsilon_k)(1-\cos\theta_{\mathbf{k}'})$$

$$= \frac{2V}{(2\pi)^3}\frac{2\pi}{\hbar} 2\pi\int \delta(\varepsilon_{k'}-\varepsilon_k) k'^2\, dk'\, d\theta_{k'} \sin\theta_{k'}\left|V(\theta_{\mathbf{k}'})\right|^2 (1-\cos\theta_{\mathbf{k}'})$$

$$= \frac{\pi}{\hbar}\frac{1}{4\pi}\int \delta(\varepsilon_{k'}-\varepsilon_k) D(\varepsilon')d\varepsilon' (d\theta_{k'} \sin\theta_{k'}\left|V(\theta_{\mathbf{k}'})\right|^2 (1-\cos\theta_{\mathbf{k}'})$$

$$= \frac{D(\varepsilon_F)}{4\hbar}\int d\theta_{k'} \sin\theta_{k'}\left|V(\theta_{\mathbf{k}'})\right|^2 (1-\cos\theta_{\mathbf{k}'})$$

The factor (1-cosθ') indicates that the forward scattering does not contribute to the electrical resistivity. It is found that $\frac{1}{\tau(\boldsymbol{k})}$ is proportional to the density of states $D(\varepsilon_F)$.

6. Average velocity along the direction of the electric field

The average velocity of the electron along the direction of the electric field is given by

$$\langle v_x \rangle = \frac{1}{N}\sum_{\boldsymbol{k}} v_x f_1(\boldsymbol{k}) = -\frac{eE_x}{N}\sum_{\boldsymbol{k}} v_x{}^2 \tau(\boldsymbol{k})[-\frac{df_0(\varepsilon_k)}{d\varepsilon_k}]$$

using the relation

$$f_1(k) = eE_x v_x \tau(\boldsymbol{k}) \frac{df_0(\varepsilon_k)}{d\varepsilon_k}.$$

We note that the current along the x direction is given by

$$J_x = -\frac{e^2 E_x}{V} \sum_{\boldsymbol{k}} v_x{}^2 \tau(\boldsymbol{k}) \frac{df_0(\varepsilon_k)}{d\varepsilon_k}.$$

Suppose that the relaxation time $\tau(\boldsymbol{k})$ is independent of $\boldsymbol{k}$. Then we get

$$J_x = -\frac{e^2 E_x \tau}{V} \sum_{\boldsymbol{k}} v_x{}^2 \frac{df_0(\varepsilon_k)}{d\varepsilon_k},$$

and

$$\langle v_x \rangle = \frac{eE_x \tau}{N} \sum_{\boldsymbol{k}} v_x{}^2 \frac{df_0(\varepsilon_k)}{d\varepsilon_k}.$$

This leads to the classical expression

$$\frac{J_x}{\langle v_x \rangle} = -\frac{\frac{e^2 E_x \tau}{V}}{\frac{eE_x \tau}{N}} = -\frac{N}{V} e = -ne,$$

or

$$\langle J_x \rangle = n(-e) \langle v_x \rangle,$$

where $\tau(\mathbf{k}) = \tau$ is assumed.

7. Scattering by phonon

In previous section, we have discussed the scattering of neutron by phonon. From the analogy we may write similar expression of the scattering of electron by phonon.

The first term corresponds to the absorption of phonon and the second term corresponds to the emission of phonon. For simplicity, b_j is independent of j. Then we get the scattering amplitude as

$$S_{inelastic}(\boldsymbol{Q},\omega_0) = U_0\{u_{\boldsymbol{q}}(\boldsymbol{Q}\cdot\boldsymbol{e}_q)\delta(\omega_0-\omega_q)\delta(\boldsymbol{Q}-\boldsymbol{q}-\boldsymbol{G})$$
$$+u_{\boldsymbol{q}}^{*}(\boldsymbol{Q}\cdot\boldsymbol{e}_q)\delta(\omega_0+\omega_q)\delta(\boldsymbol{Q}+\boldsymbol{q}-\boldsymbol{G})\}$$

where U_0 is constant, $\boldsymbol{Q} = \boldsymbol{k}' - \boldsymbol{k}$ (scattering vector), $\boldsymbol{e}_q$ is the polarization vector, $\boldsymbol{G}$ is the reciprocal lattice vector. Note that

$$|u_{\boldsymbol{q}}|^2 = \frac{\hbar\left(\langle n_{\boldsymbol{q}}\rangle + \frac{1}{2}\right)}{NM\omega_{\boldsymbol{q}}} \approx \frac{\hbar\langle n_{\boldsymbol{q}}\rangle}{NM\omega_{\boldsymbol{q}}},$$

where $\langle n_{\mathbf{q}}\rangle$ is the phonon distribution function. The reciprocal relaxation time for the normal process ($\boldsymbol{G} = 0$),

$$\frac{1}{\tau(\boldsymbol{k})} = \frac{D(\varepsilon_F)}{4\hbar}\int d\theta_{k'}\sin\theta_{k'}|V(\theta_{\boldsymbol{k}'})|^2(1-\cos\theta_{\boldsymbol{k}'})$$

for

$$|V(\theta_{\boldsymbol{k}'})|^2 \to U_0{}^2|u_{\boldsymbol{q}}|^2|\boldsymbol{Q}\cdot\boldsymbol{e}_q|^2 \approx U_0{}^2\frac{\hbar\langle n_{\boldsymbol{q}}\rangle}{NM\omega_{\boldsymbol{q}}}|\boldsymbol{q}\cdot\boldsymbol{e}_q|^2 \approx U_0{}^2\frac{\hbar\langle n_{\boldsymbol{q}}\rangle}{NM\omega_{\boldsymbol{q}}}\frac{1}{3}q^2$$

where we use the approximation

$$|\boldsymbol{q}\cdot\boldsymbol{e}_q|^2 \approx \frac{1}{3}q^2$$

Suppose that phonons are acoustic phonons, we get

$$|V(\theta_{\boldsymbol{k}'})|^2 \to U_0{}^2\frac{\hbar q\langle n_{\boldsymbol{q}}\rangle}{3cNM}.$$

Then we have

$$\frac{1}{\tau(\boldsymbol{k})} = \frac{1}{\tau} = \frac{D(\varepsilon_F)}{4\hbar}\frac{\hbar U_0{}^2}{3cNM}\int d\theta q\langle n_{\boldsymbol{q}}\rangle \sin\theta(1-\cos\theta)\,,$$

where

$$q = 2k_F \sin\frac{\theta}{2}\,,$$

and the upper limit of θ is determined from the upper limit of q;

$$q_D = 2k_F \sin\frac{\theta_0}{2}\,.$$

8. Temperature dependence of resistivity

We discuss the temperature dependence of the electrical resistivity of metal using the expression

$$\rho = \frac{1}{\sigma} = \frac{m}{ne^2}\frac{1}{\tau}\,.$$

(a) High temperature limit (T>>Θ).

We use the approximation

$$q\langle n_{\boldsymbol{q}}\rangle = \frac{q}{e^{\hbar\omega_q/k_BT}-1} = \frac{qk_BT}{\hbar\omega_q} = \frac{k_BT}{\hbar c} = \frac{k_BT}{k_B\Theta}\frac{k_B\Theta}{\hbar c} = \frac{T}{\Theta}\frac{\hbar c q_D}{\hbar c} = \frac{q_D T}{\Theta}$$

Then

$$\frac{1}{\tau} = \frac{D(\varepsilon_F)}{4}\frac{U_0{}^2}{3cNM}\frac{q_D T}{\Theta}\int_0^{\pi} d\theta \sin\theta(1-\cos\theta) = \frac{U_0{}^2 q_D D(\varepsilon_F)}{6cNM}\frac{T}{\Theta}$$

with

$$\int_0^{\pi} d\theta \sin\theta (1-\cos\theta) = 2$$

The electrical resistivity at low temperatures is proportional to *T* at high temperatures (*T*>>*Θ*),

$$\rho = \frac{m}{ne^2} \frac{U_0^{\ 2} q_D D(\varepsilon_F)}{6cNM} \frac{T}{\Theta}.$$

(b) The low temperature limits (*T*<<*Θ*).

$$\frac{1}{\tau} = \frac{D(\varepsilon_F)}{4\hbar} \frac{\hbar U_0^{\ 2}}{3cNM} \int d\theta \frac{q}{e^{\beta\hbar\omega_q} - 1} \sin\theta (1-\cos\theta).$$

We use the relation for the calculation.

$$q = 2k_F \sin\frac{\theta}{2} = q_D \frac{T}{\Theta} x,$$

$$x = \frac{\hbar\omega_q}{k_B T} = \frac{\hbar c q}{k_B T} = \frac{2k_F}{q_D} \frac{\Theta}{T} \sin\left(\frac{\theta}{2}\right)$$

$$dx = \frac{k_F}{q_D} \frac{\Theta}{T} \cos\left(\frac{\theta}{2}\right) d\theta$$

$$\begin{aligned} \sin\theta (1-\cos\theta) d\theta &= 4\sin^3\left(\frac{\theta}{2}\right) \cos\left(\frac{\theta}{2}\right) d\theta \\ &= \frac{1}{2} \left(\frac{q_D}{k_F}\right)^4 \left(\frac{T}{\Theta}\right)^4 x^3 dx \end{aligned}$$

Then

$$\frac{1}{\tau} = \frac{D(\varepsilon_F)}{24\hbar} \frac{\hbar k_F U_0^{\ 2}}{cNM} \left(\frac{q_D}{k_F}\right)^5 \left(\frac{T}{\Theta}\right)^5 \int_0^{\Theta/T} \frac{x^4}{e^x - 1} dx$$

where

$$x_0 = \frac{\hbar c q_D}{k_B T} = \frac{\Theta}{T}$$

becomes infinity at low temperatures. Noting that

$$\int_0^\infty \frac{x^4}{e^x - 1} dx = 24\varsigma(5) = 24.8863,$$

we have

$$\frac{1}{\tau} = \frac{D(\varepsilon_F)}{24\hbar} \frac{\hbar k_F U_0^2}{cNM} \left(\frac{T}{\Theta}\right)^5 \left(\frac{q_D}{k_F}\right)^5 24\varsigma(5) = \frac{k_F U_0^2}{c\hbar NM} D(\varepsilon_F) \left(\frac{q_D}{k_F}\right)^5 \left(\frac{T}{\Theta}\right)^5 \varsigma(5)$$

The electrical resistivity at low temperatures is proportional to T^5 at high temperatures ($T<<\Theta$),

$$\rho = \frac{m}{ne^2} \frac{k_F U_0^2}{c\hbar NM} D(\varepsilon_F) \left(\frac{q_D}{k_F}\right)^5 \left(\frac{T}{\Theta}\right)^5 \varsigma(5).$$

9. Bloch T^5 law; Grűneisen law

We do not take into account the effect of the Umklapp process on the electrical resistivity. The Umklapp scattering of electron by phonons is a scattering process in which a reciprocal lattice vector G is involved,

$$\boldsymbol{k}' - \boldsymbol{k} = \boldsymbol{q} + \boldsymbol{G}$$

This process significantly contributes to the electrical conductivity or electrical resistivity. In this process the scattering is inelastic. The scattering amplitude can be described as

$$S_{inelastic}(\boldsymbol{Q}, \omega_0) = U_0\{u_{\boldsymbol{q}}(\boldsymbol{Q}\cdot\boldsymbol{e}_q)\delta(\omega_0 - \omega_q)\delta(\boldsymbol{Q} - \boldsymbol{q} - \boldsymbol{G}) \\ + u_{\boldsymbol{q}}^*(\boldsymbol{Q}\cdot\boldsymbol{e}_q)\delta(\omega_0 + \omega_q)\delta(\boldsymbol{Q} + \boldsymbol{q} - \boldsymbol{G})\}$$

where

$$\hbar\omega_{q} = \omega_{k'} - \omega_{k}$$

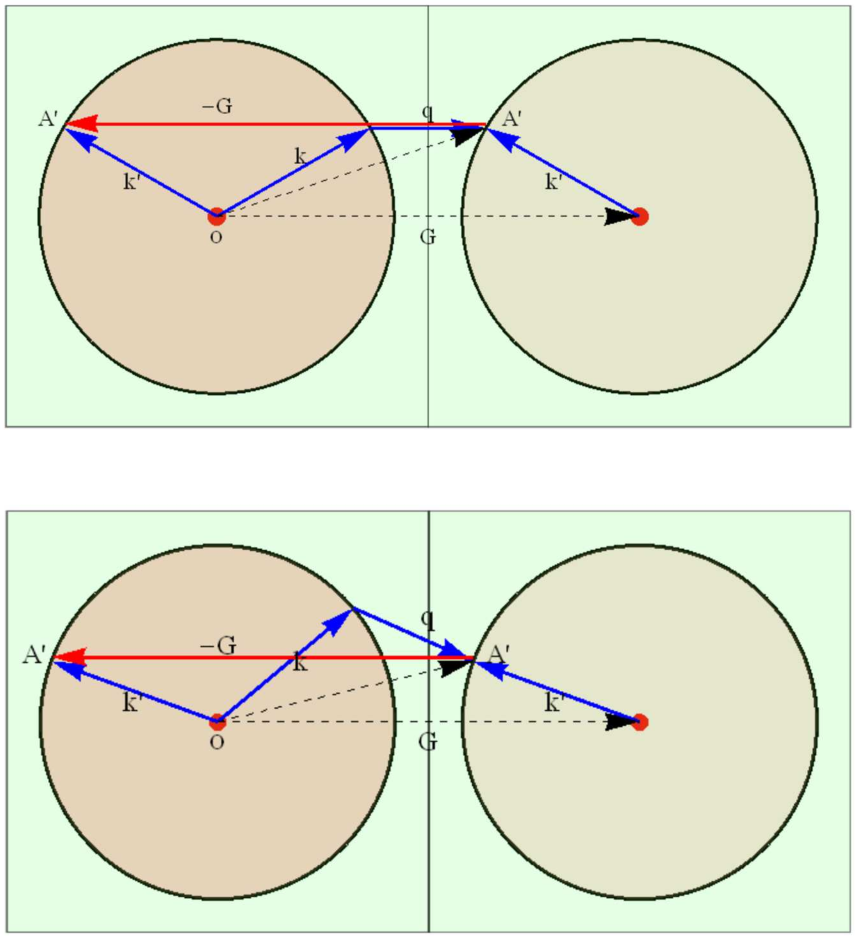


Fig. The center of the Fermi sphere is at the reciprocal lattice vector ***G***. The green zone is the Brillouin zone (Bz). ***k*** and ***k***' are located on the Fermi surface. The wavevector ***k***+***q*** is at the Point A; on the Fermi sphere in the adjacent Bz. The point A is equivalent to the point A' inside the original zone. ***k***' and ***k*** are almost antiparallel in this figure.

When the umklapp process is included in the model, the electrical resistivity can be expressed by a scaling function of T/Θ,

$$\rho = 4\rho_0 (\frac{T}{\Theta})^5 \int_0^{\Theta/T} \frac{z^5 dz}{(e^z - 1)(1 - e^{-z})}$$

(Grűneisen, Bloch T^5 law)

At high temperatures ($T >> \Theta$),

$$\int_0^{\Theta/T} \frac{z^5 dz}{(e^z - 1)(1 - e^{-z})} \approx \int_0^{\Theta/T} \frac{z^5 dz}{z^2} = \frac{1}{4}\left(\frac{\Theta}{T}\right)^4 .$$

Then we get

$$\rho = \rho_0 (\frac{T}{\Theta})$$

At low temperatures ($T << \Theta$),

$$\rho = 4\rho_0 (\frac{T}{\Theta})^5 \int_0^{\infty} \frac{z^5 dz}{(e^z - 1)(1 - e^{-z})} = 497.725 \rho_0 (\frac{T}{\Theta})^5$$

where

$$\int_0^{\infty} \frac{z^5 dz}{(e^z - 1)(1 - e^{-z})} = 5! \varsigma(5) = 124.431$$

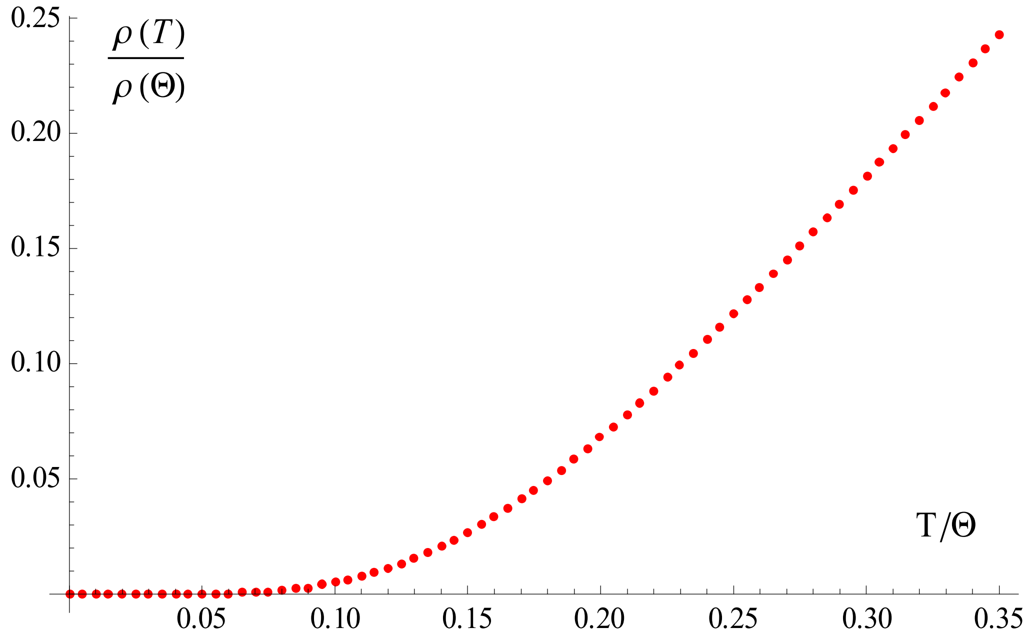


Fig. The normalized resistivity $\rho(T)/\rho(\Theta)$ vs T/Θ. Bloch T^5 law.

APPENDIX

Current density:

$$\boldsymbol{J} = \frac{1}{V}\sum_{\boldsymbol{k}}(-e)\boldsymbol{v}_{\boldsymbol{k}} f_1(\boldsymbol{k})$$
$$= \frac{1}{V}\frac{2V}{(2\pi)^3}\int d\boldsymbol{k}(-e)\boldsymbol{v}_{\boldsymbol{k}} f_1(\boldsymbol{k})$$
$$= (-e)\frac{2}{4\pi^3}\int d\boldsymbol{k}\boldsymbol{v}_{\boldsymbol{k}} f_1(\boldsymbol{k})$$

Note that

$$d\boldsymbol{k} = dk_{\perp} dS$$

The group velocity is given by

$$v_{\boldsymbol{k}} = \frac{1}{\hbar}\nabla_{\boldsymbol{k}}\varepsilon, \qquad \frac{\partial\varepsilon}{\partial k_\perp} = \left|\nabla_{\boldsymbol{k}}\varepsilon\right| = \hbar v_{\boldsymbol{k}}, \qquad dk_\perp = \frac{d\varepsilon}{\hbar v_{\boldsymbol{k}}}$$

$\nabla_{\boldsymbol{k}}\varepsilon$ is normal to the surface with constant energy (Fermi surface).

$$f_1 = e(\boldsymbol{E}\cdot v_{\boldsymbol{k}})\tau(\boldsymbol{k})\frac{\partial f_0}{\partial \varepsilon_{\boldsymbol{k}}}$$

where -*e* is the charge of electron, and *e*>0.

$$\begin{aligned} J &= \frac{e^2}{4\pi^3}\int d\boldsymbol{k}\boldsymbol{v}_{\boldsymbol{k}}(\boldsymbol{E}\cdot\boldsymbol{v}_{\boldsymbol{k}})\tau(\boldsymbol{k})(-\frac{\partial f_0}{\partial\varepsilon_{\boldsymbol{k}}}) \\ &= \frac{e^2}{4\pi^3}\int dS\int\frac{d\varepsilon}{\hbar v_{\boldsymbol{k}}}\tau(\boldsymbol{k})\boldsymbol{v}_{\boldsymbol{k}}(\boldsymbol{E}\cdot\boldsymbol{v}_{\boldsymbol{k}})(-\frac{\partial f_0}{\partial\varepsilon_{\boldsymbol{k}}}) \\ &= \frac{e^2}{4\pi^3\hbar}\int dS\int\frac{d\varepsilon}{v_{\boldsymbol{k}}}\tau(\boldsymbol{k})\boldsymbol{v}_{\boldsymbol{k}}(\boldsymbol{E}\cdot\boldsymbol{v}_{\boldsymbol{k}})(-\frac{\partial f_0}{\partial\varepsilon_{\boldsymbol{k}}}) \end{aligned}$$

since

$$d\boldsymbol{k} = dSdk_\perp = dS\frac{d\varepsilon}{\hbar v_{\boldsymbol{k}}}$$

Noting that

$$-\frac{\partial f_0}{\partial\varepsilon} = \delta(\varepsilon - \varepsilon_F)$$

the current density can be expressed by

$$\boldsymbol{J} = \frac{e^2\tau}{4\pi^3\hbar}\int\frac{\boldsymbol{v}_{\boldsymbol{k}}(\boldsymbol{E}\cdot\boldsymbol{v}_{\boldsymbol{k}})}{v_{\boldsymbol{k}}}dS$$

The density of states is

$$D(\varepsilon)d\varepsilon = \frac{V}{4\pi^3} d\varepsilon \int \frac{dS}{\hbar v_{\boldsymbol{k}}}$$

or

$$D(\varepsilon) = \frac{V}{4\pi^3} \int \frac{dS}{\hbar v_{\boldsymbol{k}}}$$

The conductivity is obtained as

$$J_x = \sigma_{xx} E_x$$

$$\sigma_{xx} = \frac{e^2\tau}{4\pi^3} \int d\boldsymbol{k} \boldsymbol{v}_x{}^2 \left(-\frac{\partial f_0}{\partial \varepsilon_{\boldsymbol{k}}}\right)$$

We now consider the conductivity for the free electron fermi gas model,

$$v_x = \frac{\hbar}{m} k_x = \frac{\hbar}{m} k \sin\theta \cos\phi$$

$$\begin{aligned}
\int d\boldsymbol{k} \boldsymbol{v}_x{}^2 \left(-\frac{\partial f_0}{\partial \varepsilon_{\boldsymbol{k}}}\right) &= \iiint dk k^2 \sin\theta d\theta d\phi \frac{\hbar^2}{m^2} k^2 \sin^2\theta \cos^2\phi \left(-\frac{\partial f_0}{\partial \varepsilon_{\boldsymbol{k}}}\right) \\
&= \frac{\hbar^2}{m^2} \iiint dk k^4 \sin^3\theta d\theta \cos^2\phi d\phi \left(-\frac{\partial f_0}{\partial \varepsilon_{\boldsymbol{k}}}\right) \\
&= \frac{\hbar^2}{m^2} \int_0^\infty dk k^4 \left(-\frac{\partial f_0}{\partial \varepsilon_{\boldsymbol{k}}}\right) \int_0^\pi \sin^3\theta d\theta \int_0^{2\pi} \cos^2\phi d\phi
\end{aligned}$$

Note that

$$\int_0^\pi \sin^3\theta d\theta = \frac{4}{3}, \qquad \int_0^{2\pi} \cos^2\phi d\phi = \pi$$

Then we get

$$\int d\boldsymbol{k}\boldsymbol{v}_x^{\ 2}(-\frac{\partial f_0}{\partial \varepsilon_{\boldsymbol{k}}}) = \frac{4\pi}{3}\frac{\hbar^2}{m^2}\int_0^\infty dkk^4(-\frac{\partial f_0}{\partial \varepsilon_{\boldsymbol{k}}})$$

The energy dispersion of free electron is given by

$$\varepsilon = \frac{\hbar^2}{2m}k^2, \qquad k = \left(\frac{2m}{\hbar^2}\right)^{1/2}\sqrt{\varepsilon}$$

$$dk = \left(\frac{2m}{\hbar^2}\right)^{1/2}\frac{d\varepsilon}{2\sqrt{\varepsilon}}$$

$$\int d\boldsymbol{k}\boldsymbol{v}_x^{\ 2}(-\frac{\partial f_0}{\partial \varepsilon_{\boldsymbol{k}}}) = \frac{2\pi\hbar^2}{3m^2}\int_0^\infty \left(\frac{2m}{\hbar^2}\right)^{5/2} d\varepsilon\varepsilon^{3/2}(-\frac{\partial f_0}{\partial \varepsilon_{\boldsymbol{k}}})$$

The conductivity is

$$\begin{aligned}\sigma_{xx} &= \frac{e^2\tau}{4\pi^3}\frac{2\pi\hbar^2}{3m^2}\left(\frac{2m}{\hbar^2}\right)^{5/2}\int_0^\infty d\varepsilon\varepsilon^{3/2}(-\frac{\partial f_0}{\partial \varepsilon_{\boldsymbol{k}}}) \\ &= \frac{e^2\tau}{4\pi^3}\frac{2\pi\hbar^2}{3m^2}\frac{2m}{\hbar^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\int_0^\infty d\varepsilon\varepsilon^{3/2}(-\frac{\partial f_0}{\partial \varepsilon_{\boldsymbol{k}}}) \\ &= \frac{e^2\tau}{3\pi^2 m}\left(\frac{2m}{\hbar^2}\right)^{3/2}\int_0^\infty d\varepsilon\varepsilon^{3/2}(-\frac{\partial f_0}{\partial \varepsilon_{\boldsymbol{k}}})\end{aligned}$$

Noting that

$$\int_0^\infty d\varepsilon\varepsilon^{3/2}(-\frac{\partial f_0}{\partial \varepsilon_{\boldsymbol{k}}}) = \frac{3}{2}\int_0^\infty d\varepsilon\varepsilon^{1/2}f_0$$

we have the conductivity

$$\sigma_{xx} = \frac{e^2\tau}{2\pi^2 m}\left(\frac{2m}{\hbar^2}\right)^{3/2}\int_0^\infty d\varepsilon\varepsilon^{1/2}f_0$$

Using the number density given by

$$n = \frac{N}{V} = \frac{1}{2\pi^2}(\frac{2m}{\hbar^2})^{3/2}\int_0^\infty d\varepsilon\varepsilon^{1/2} f_0$$

$$\sigma_{xx} = \frac{ne^2\tau}{m}.$$

APPENDIX

General result for $D(\varepsilon)$

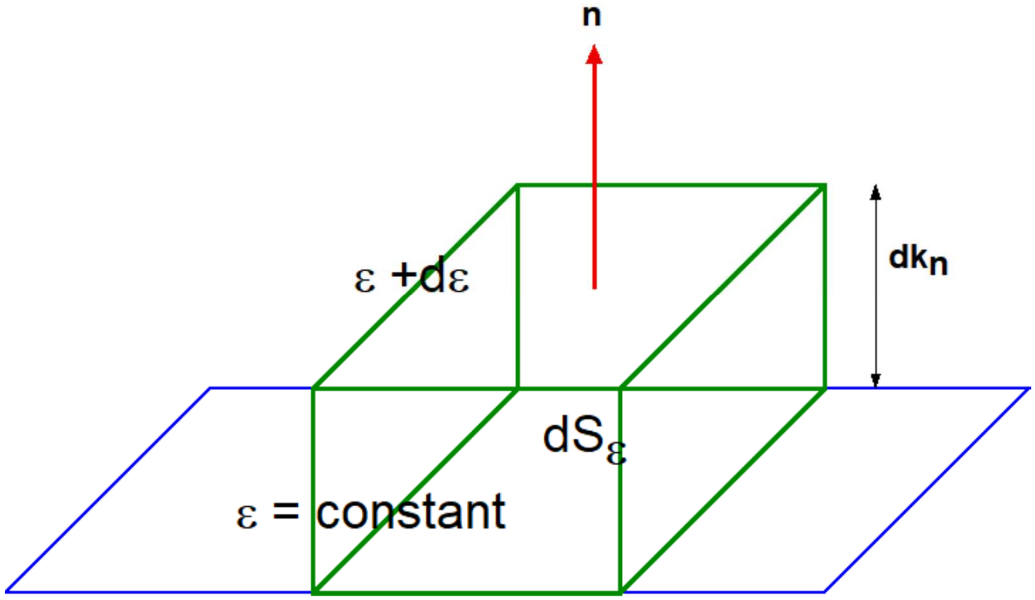


Fig. The volume element in the k space. $dk_n = dk_\perp$. $d^3k = dS_\varepsilon dk_n = dS_\varepsilon dk_\perp$

The group velocity is defined by

$$\boldsymbol{v}_k = \frac{1}{\hbar}\nabla_k\varepsilon,$$

which is normal to the surface of e = constant. We note that from the definition, we have

$$d\varepsilon = \nabla_{\boldsymbol{k}}\varepsilon \cdot d\boldsymbol{k} = \hbar \boldsymbol{v}_{\boldsymbol{k}} \cdot d\boldsymbol{k} .$$

When $d\varepsilon = 0$ (ε = constant surface), $\nabla_{\boldsymbol{k}}\varepsilon\cdot$ is perpendicular to any vector on the surface (ε = constant). In other words, the group velocity $\boldsymbol{v}_k = \frac{1}{\hbar}\nabla_k\varepsilon$ is normal to the surface with ε = constant.

$$v_g = |\boldsymbol{v}_k| = \frac{1}{\hbar}\frac{\partial\varepsilon}{\partial k_\perp} ,$$

or

$$d\varepsilon = |\boldsymbol{v}_k| dk_\perp ,$$

we have the k-space volume element as

$$dS_\varepsilon dk_\perp = dS_\varepsilon \frac{d\varepsilon}{\hbar|\boldsymbol{v}_k|} = dS_\varepsilon \frac{d\varepsilon}{\hbar v_{\boldsymbol{k}}} .$$

Then we get

$$D(\varepsilon)d\varepsilon = \frac{2V}{(2\pi)^3}\frac{dS_\varepsilon d\varepsilon}{\hbar v_{\boldsymbol{k}}} ,$$