Understanding of physics on electrical conductivity in metals; Drude – Sommerfeld - Kubo

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1. Overview

Around 1900, Drude (Paul Karl Ludwig Drude) improved the theory of classical conduction given by Lorentz. He reasoned that since metals conduct electricity so well, they must contain free electrons that move through a lattice of positive ions (the discovery of electron by J.J. Thomson in 1897). This motion of electrons led to the formation of Ohm's law. The free-moving electrons act just as atomic gas; moving in every direction throughout the lattice. These electrons collide with the lattice ions as they move about, which is key in understanding thermal equilibrium. The average velocity due to the thermal energy is zero since the electrons are going in every direction. There is a way of affecting this free motion of electrons, which is by use of an electric field. This process is known as electrical conduction and theory is called Drude-Lorentz theory; Conventionally we call the Drude model here.

In Modern Physics (Phy.323 in Binghamton University)) and Solid State Physics (Phys.472/572 in BU) of the undergraduate physics courses in U.S.A., it is taught that the electrical resistivity of metal can be explained in terms of the quantum mechanical model (Sommerfeld model) that the electrons are fermions and obeys the Fermi-Dirac statistics. In this model, only the conduction electrons near the Fermi surface contribute to the electrical resistivity. These electrons have the Fermi velocity v_F ($\approx 10^6$ m/s) for copper (Cu) metal. The mean free path is evaluated as $\Lambda_{qm} = v_F\tau = 10^6 \times 10^{-14} = 10^{-8}$ m = 100 Å, which is much larger than the lattice constant (3.61 Å in Cu). This means that electrons behave like wave. In quantum mechanics, only electrons at the Fermi surface (having the Fermi velocity) contributes to the electrical conductivity of metals; $\tau = \tau(\varepsilon_F)$ is the relaxation time of electrons at the Fermi energy. For Cu metal, the relaxation time of conduction electrons is 10^{-14} sec from the electrical resistivity measured at room temperature. The electrical conductivity of metals can be clearly explained by using the concept of quantum mechanics, in particular, solid-state physics. If there are *n* particles per unit volume, the electrical conductivity of metals is given by the formula

$$\sigma_{qm} = \frac{ne^2}{m}\tau(\varepsilon_F), \qquad \text{(Sommerfeld model)}$$

where q (=-e) is the charge of electron. This conductivity depends only on the properties of the electron at the Fermi energy ε_F, not on the total number of electrons in the metal. The high conductivity of metals is to be ascribed to the high velocity of the few electrons at the top of the Fermi distribution, rather than to a high total density of free electrons which can be set slowly drifting.

In spite of our understanding of physics, unfortunately the conductivity of metals is conventionally explained in terms of the classical Drude model in the General Physics Course of the universities in U.S.A., including our Binghamton University (Phys.132, Calculus based, General Physics). According to Drude model, the electrical conductivity is given by

$$\sigma_{cl} = \frac{ne^2}{m}\tau , \qquad \text{(classical Drude model)}$$

where τ is the relaxation time (classical model) and is also the same as the relaxation time in quantum mechanical model; relaxation time of electrons at the Fermi energy. In a classical gas of particles of mass *m* at temperature *T*, the root-mean square velocity v_{rms} of the particle is given by

$$\frac{1}{2}m{v_{rms}}^2 = \frac{3}{2}k_B T .$$

where k_B is the Boltzmann constant. For electrons at room temperature, this root-mean square velocity is about 10^5 m/s; $v_{rms} = 1.168 \times 10^5$ m/s using the mass *m* of free electron. If we use this value as the velocity, the mean free path can be evaluated as $\Lambda_{cl} = v_{rms}\tau = 10^5 \times 10^{-14} = 10^{-9}$ m = 10 Å, which is on the same order as the lattice constant of Cu atoms ($a = 3.61$ Å). It means that electrons behave like a particle, colliding with positive ions at the lattice sites.

It seems to us that undergraduate physics students in this country (U.S.A.) may be very confused about the different explanations, depending on the classes (for classical model in general physics and for quantum mechanical model in modern physics and solid-state physics). Here we try to present a proper understanding of the electrical resistivity of metals in terms of the Boltzmann transport equation of conduction electrons obeying Fermi-Dirac statistics (Sommerfeld). The Kubo formula for the electrical conductivity will be also discussed. With the use of this formula, the expression of the electrical conductivity can be derived for both Drude model and Sommerfeld model without the use of Boltzmann equation.

2. Four probes method of electrical resistivity: validity of Ohm's law

How can we measure the electrical resistivity of metals such as copper experimentally? We use the four probes method for the measurement of electrical resistivity of metals; two probes for the current and two probes for the voltage measurement. We use the constant current source. The constant current (*I*) flows through two current probes. The voltage (*V*) between two voltage probes is measured by using the digital voltmeter (such as nanovolt meter). The resistance *R* is evaluated as

$$R = \frac{V}{I} . \qquad (\Omega)$$

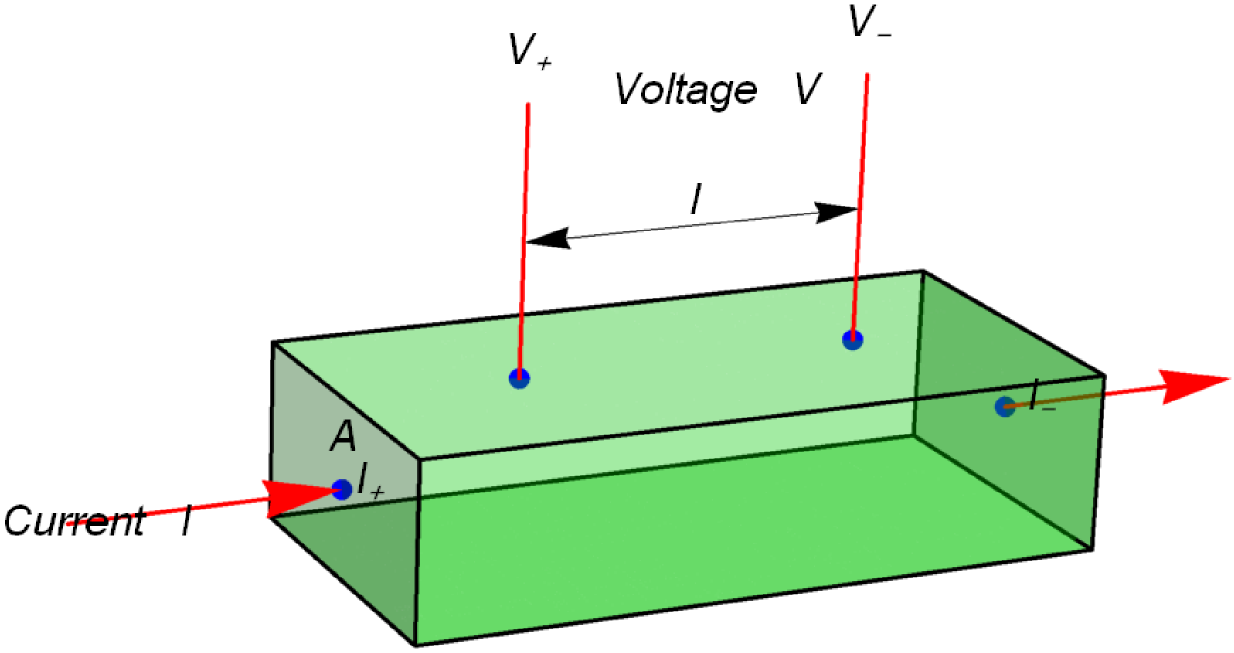


Fig.1 Four probes measurement of electrical resistivity of metal. The cross-sectional area is A. Two current probes (I_+, I_-). Two voltage probes (V_+, V_-). l is the distance between two voltage probes. The current is fed to one of the current probe (I_+) using constant current source. The voltage between the voltage probes can be measured using a digital nano-voltmeter.

The electrical resistivity ρ (Ω m) is related to the resistance by

$$R = \rho \frac{l}{A},$$

or

$$\rho = R\frac{A}{l} = \frac{V}{I}\frac{A}{l}, \qquad (\Omega \mathrm{m})$$

where A (m^2) is the cross-sectional area of sample and l (m) is the distance between two voltage probes. We consider the case of copper (Cu) with the electrical resistivity at room temperature,

$$\rho = 1.72 \times 10^{-8} \ \Omega\mathrm{m} \qquad \text{at } T = 300 \text{ K (room temperature)}$$

Experimentally we use the sample of copper having typical dimensions such as $A = 1\ \mathrm{mm}^2 = 10^{-6}\,\mathrm{m}^3$ and l =1 cm = 10^{-2} m. Thus, the resistance R can be evaluated as

$$R = \rho \frac{l}{A} = 0.172\ \mathrm{m}\Omega,$$

When the constant current I = 1 A flows through the current probes, we obtain the voltage across the voltage probes by

$$V = IR = 0.172\ \mathrm{mV} = 172\ \mu\mathrm{V}.$$

Although this voltage is very small, we can measure it by using a digital nano-voltmeter. The magnitude of the electric field E is evaluated as

$$E = \frac{V}{l} = I\frac{R}{l} = 1.72 \text{ x } 10^{-2}\ \mathrm{V/m},$$

which is sufficiently small. So that the Ohm's law ($J = \sigma E$) is valid. No quadratic term (proportional E^2) is significant. Thus, there is no Joule heating.

4. Electrical resistivity of Cu metal at low temperatures

We find the data for the temperature dependence of electrical resistivity copper at low temperatures in the book of G.K. White. The electrical resistivity is proportional to T^5 at low temperatures (Bloch-Grüneisen T^5 law). The resistivity at the lowest temperature around 4 K is called a residual resistivity, It depnds on impurituries.

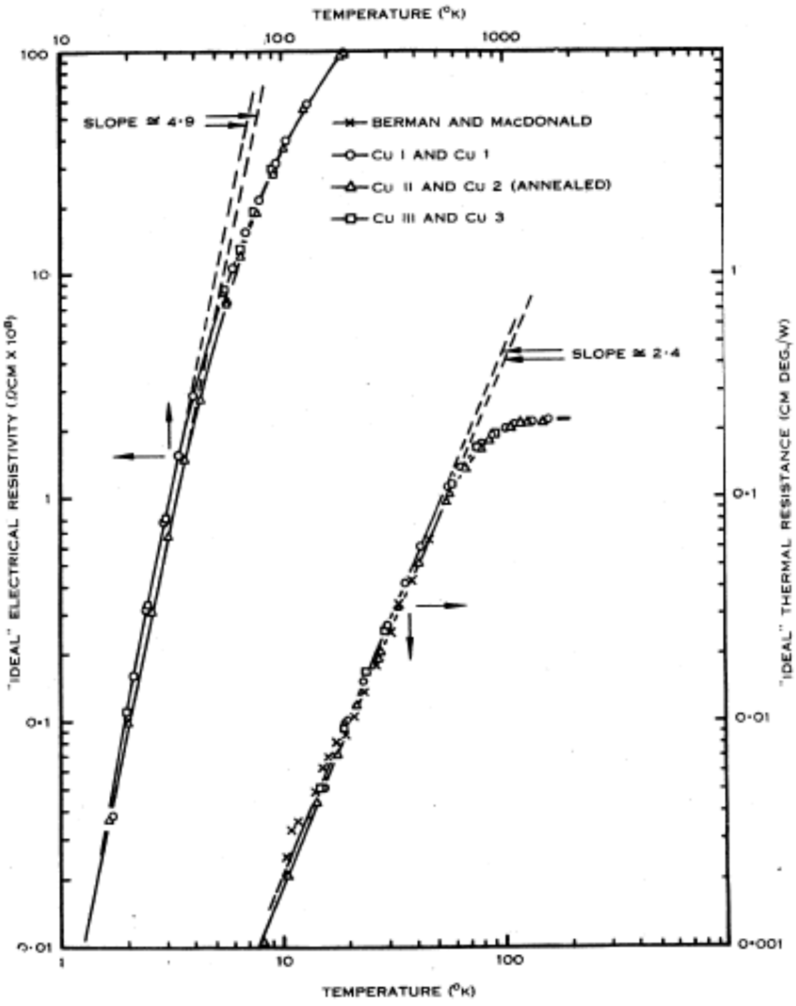


Fig.2 Temperature dependence of electrical resistivity (left) and thermal resistance (right) for copper at low temperatures.[G.K. White, Experimental Techniques in Low-Temperature, 3rd edition (Oxford, 1979)]. For Cu sample (used in this Fig),

$\rho = (0.00458 \ + 2.75\times10^{-4} T^5) \ \mu\Omega \ cm$ at liquid ^{4}He temperature (T = 4.2 K).

$\rho = 0.00458036 \ \ \mu\Omega cm$ at T = 4.2 K.

((**Kittel, 1996**))

It is possible to obtain crystals of copper so pure that their conductivity at liquid helium temperature (4 K) is nearly 10^5 times that at room temperature; for these conditions $\tau = 2\times10^{-9}$ s at 4 K. The mean free path Λ of conduction electron at 4 K is defined as $\Lambda(4K) = 0.3$ cm.

$l(4K) = 0.3$ cm.

4. Conversion of cgs units and SI units for resistivity using the Klitzing constant

In general physics, we mainly use the S.I. units for the resistivity (Ωm), while in solid state physics, we often use the cgs units for the resistivity (s). Here we discuss how to change of the units of resistivity or conductivity between the cgs units and SI units.

Suppose that we have the following two expressions

$$qV = \hbar\omega \qquad \text{(energy)}$$

and

$$I = \frac{q}{t_p} = \frac{q\omega}{2\pi} \qquad \text{(current)}$$

where $q\ (= -e)$ is the charge of electron, V is the voltage, ω is the angular frequency, $\hbar$ is the Dirac constant, I is the current, and t_p is the period; $t_p = \frac{2\pi}{\omega}$. The resistance is evaluated as

$$R = \frac{V}{I} = \frac{\hbar\omega}{q}\frac{2\pi}{q\omega} = \frac{2\pi\hbar}{e^2}.$$

We calculate this value of R in the SI units;

$$R = R_K = 25812.80755718\,\Omega \qquad \text{(von Klitzing constant)}$$

where we use the values of $\hbar$ and e in the SI units. We also calculate this value of R in the units of cgs;

$$R = 2.87206\times 10^{-8}\ \text{(s/cm)}$$

where we use the values of $\hbar$ and e in the cgs units. Thus we get the relation as

$$\text{(s/cm)} = \frac{25812.80755718}{2.87206\times 10^{-8}} = 8.98756\times 10^{11}\ (\Omega)$$

or

(s) = 8.98756 × 10^{11} (Ω cm) = 8.98756 × 10^{9} (Ω m)

The resistivity of Cu at room temperature is $\rho = 1.72$ (μΩcm). This value of ρ in the cgs unit is evaluated as

$$\rho = \frac{1.72\times 10^{-6}}{8.98756\times 10^{11}} = 0.19138\times 10^{-11}\ (\mathrm{s}).$$

Correspondingly the conductivity of Cu at room temperature is

$$\sigma = \frac{1}{\rho} = 5.2250\times 10^{17}\ \ (1/\mathrm{s})\,.$$

(see **Kittel, ISSP 2nd edition,1956**).

5. Historical perspective: Drue -Sommerfeld - Kubo

In 1900, Paul Drude derived his famous formula for the electrical conductivity of metals. His theory assumes that electrons are formed of a classical gas. Such a classical model survives even after the quantum mechanics appears in 1920's. The propagation of conduction electrons inside the metal is a quantum mechanical behavior. Electrons are fermions, and obey the Fermi-Dirac statistics. According to the Pauli's exclusion principle, two electrons cannot occupy the same state. In other words, the state of electron is clearly specified by $\left|\boldsymbol{k}, s\right\rangle$, where $\boldsymbol{k}$ is the wave number and s is the spin state ($s = \pm 1$), depending on the up state or down state. The electrical resistivity can be explained only using the quantum mechanical model, but not in terms of classical model.

The characteristic properties of metals are due to their conduction electrons: the electrons in the outermost atomic shells, which in the solid state are no longer bound to individual atoms, but are free to wander through the solid. A proper understanding of metallic behavior could not begin, obviously, until the electron had been discovered by J.J. Thomson in 1897, but once this had happened, the significance of the discovery was at once recognized. By 1900 Drude had already produced an electron theory of electrical and thermal conduction in metals, which (with refinements by Lorentz a few years later) survived until 1928.

Not surprisingly, this very early theory did not manage to explain everything – after all, the structure of the atom itself was quite unknown until Rutherford and his co-workers discovered the nucleus in 1911 – but it did have one or two striking success, and it is worth starting with a brief look at this classical model, because it already contained many of the right ideas.

Historically, the Drude formula was first derived in a limited way, namely by assuming that the charge carriers form a classical ideal gas. Arnold Sommerfeld considered quantum theory and extended the theory to the free electron model, where the carriers follow Fermi–Dirac distribution. Amazingly, the conductivity predicted turns out to be the same as in the Drude model, as it does not depend on the form of the electronic speed distribution.

In the Drude model, each atom is assumed to contribute one electron (or possibly more than one) to the gas of mobile conduction electrons. The remaining positive ions form a crystal lattice, through which the conduction electrons can move more-or-less freely. This gas of conduction electrons differs from an ordinary gas (e.g. O_2) in three ways. First, the gas particles – the electrons – are far lighter than an ordinary gas molecule. Secondly, they carry an electric charge. Thirdly, they are travelling through the lattice of positive ions, rather than through empty space, and presumably are colliding constantly with these positive ions. They may also collide with each other, as ordinary gas molecules do, but we can expect these electron-electron collisions to be less frequent, and less important, than the electron-ion collisions.

We can work out the properties of this model very easily, using the kinetic theory of gases. If m and v are the mass velocity of an electron, then according to classical physics the average kinetic energy at temperature T is given by

$$\frac{1}{2}m{v_{rms}}^2 = \frac{3}{2}k_B T ,$$

where k_B is the Boltzmann constant and ${v_{rms}}^2$ denotes the average value of $|\boldsymbol{v}|^2$ over all the conduction electrons, so that v_{th} is their rms speed. Note that this equation is in fact wrong for electrons. Quantum mechanics gives a different answer (**Sommerfeld**, **Bloch**). Every so often the electrons will collide with the ions of the crystal lattice. We assume that between collisions an electron travels with constant velocity v, and that the effect of a collision is to randomize the direction of v, but to leave its magnitude v practically unchanged, because the ions are far heavier than the electrons. For any one electron, the collisions occur at more or less random intervals, and the average time interval between collisions is called the relaxation time, τ. The corresponding average distance between collisions, $\Lambda = v\tau$, is called the mean free path.

More general expression of the electrical conductivity of metals is given by the **Kubo** formula. Using this formula, one can derive the form of the electrical resistivity.

6. Contribution of Niels Bohr to the Lorentz-Drude theory (1911)

L.Hoddeson, E. Braun, J. Teichmann, and S. Weart, Out of the Crystal Maze; Chapters from the History of Solid State Physics (Oxford, 1992).

Niels Bohr began his epoch-making study of the structure of matter with his master's thesis on the electron theory of metals - a topic that he further elaborated in his Ph.D. dissertation completed in 1911. The theory on which Bohr based his study was the Lorentz-Drude model, according to which metals were depicted as gases of electrons moving almost freely in a potential generated by positive charged ions fixed in a crystal structure. The Lorentz-Drude theory explained some of the electrical and thermal properties of metals, but several experiments disagreed with the values predicted by the theory. By generalizing the assumptions of the Lorentz-Drude theory, Bohr deduced that it was not possible to derive the diamagnetic and paramagnetic properties of metals from the accepted laws of electromagnetism. This conclusion was fundamental in giving Bohr the conviction that a revision of classic electromagnetism was necessary, in order to deal with atomic phenomena. The problem Bohr underlined in his dissertation was, indeed, resolved only after fundamental developments of quantum theory, such as the formulation of the exclusion principle by Wolfgang Pauli in 1925 and the independent development by Enrico Fermi and Paul Dirac of the statistics of the particles obeying said principle in 1926.

The following steps of Bohr's intellectual life concerned his research in England with two of the most authoritative experimental physicists of the period: J. J. Thomson, who had received the Nobel Prize in Physics in 1906 for his discovery of the electron; and E. Rutherford, who had been awarded the Nobel Prize in Chemistry in 1908 for his studies on radioactivity. Both Thomson and Rutherford had established two flourishing schools of experimental physics housed in two different laboratories. The former succeeded Lord Rayleigh as the third director of the Cavendish Laboratory in Cambridge in 1884, while the latter had instituted his laboratory in Manchester in 1907. They had also formulated two different models of the atom. Thomson had been building the first well-known dynamical model of the atom since 1903. At that time, electrons were the only subatomic particles whose existence was widely accepted because of various experimental observations, culminating in Thomson's verification of the constancy of the electron charge-mass ratio in 1897. In the Thomson model, the negatively charged electrons were the only corpuscular constituents of the atom, while the electrical neutrality was obtained by hypothesizing a substance that surrounded the electrons and whose positive charge perfectly balanced that of the atomic electrons.

Rutherford proposed a different model in 1911 after the result of the Geiger-Marsden experiments performed at the Manchester laboratory had convinced him that all the positive charge was concentrated in the point-like center of the atom, which he later called the nucleus. Rutherford hypothesized a planetary model of the atom in which a sphere of negative electrification of charge $-Ne$ (where e is the charge of the electron) surrounded the nucleus of total charge $+Ne$ due to the attraction generated by the Coulomb potential of the nucleus. In his proposal of the nuclear atom, however, Rutherford did not attempt to resolve the theoretical issues concerning the mechanical and electromagnetic stability of the atom. The major outcomes of Rutherford's proposal were the clarification of the role of the nucleus in the scattering of alpha particles as well as of its contribution to the total atomic mass. In spite of its success in explaining some specific experimental results, the Rutherford atom lacked the mathematical refinements of the Thomson model and was rarely cited by the scientific community in the period 1911-1913.

7. The advantage and disadvantage of the Drude theory

In the textbook of Modern Physics, **Taylor et al.** discussed why the Drude formula is still used to explain the conductivity of metal, in spite of wrong concept. In about 1900, long before an exact theory of the solid state physics was available, Drude described metallic conductivity using the assumption of an ideal electron gas in the solid. In this model, all the electrons contribute to the current. This view is in contradiction with the Pauli exclusion principle. For the Fermi gas, this forbids electrons well below the Fermi level from acquiring small amounts of energy, since all neighboring higher energy states are occupied.

1. Only the electrons with the Fermi velocity contribute to the electrical conductivity.
2. Electrons are fermions, and obey the Fermi-Dirac statistics.
3. The number density of electrons is tremendously large.
4. The relaxation time of electrons at the Fermi energy is significant.
5. The Drude theory is not correct, even though the expression of conductivity is similar.
6. Newton's cradle model. The scattering occurs only at the Fermi energy.

In the Drude model, all electrons contribute to the conductivity, with the scattering with the same relaxation time. Using this expression, we get an unrealistically small drift velocity. The drift velocity is completely different from the Fermi velocity.

Here is the discussion given Taylors et al of the textbook of Modern Physics. We have mentioned before, Drude's work was done well before the advent of quantum mechanics, so there was no way for Drude to evaluate the Fermi velocity or the mean free path. Why then was Drude's model immediately successful? It was because Drude's calculations contained two large mistakes that canceled! From the known values of the conductivity of metals, Drude used his formula, $\sigma_{cl} = ne^2\tau / m$, to correctly evaluate the relaxation time τ. As a check on the theory, he also evaluated the relaxation time using $\tau = \Lambda_{cl} / v$, where Λ_{cl} is the mean free path and v is the mean electron velocity. But his values for l and v were both too small by an order of magnitude. He assumed, incorrectly, that the electrons scattered from individual ions, so his estimate of the mean free path l was a few nanometers (order of 10Å) – smaller by a factor of at least 10 than the correct value for metals at room temperature (order of 100 Å). He also incorrectly assumed that the velocity of the electrons is given by the thermal velocity of about 10^5 m/s, which is about 10 times smaller than the correct Fermi velocity. Because both numbers were wrong appeared to be nicely self-consistent and it was immediately accepted by physicists. More than 30 years passed before enough quantum mechanics was known for the correct picture to emerge. Today we remember Drude because his simple but wrong model leads to the correct formula, $\sigma_{qm} = ne^2\tau(\varepsilon_F) / m$.

The Drude theory and his formula of the electrical conductivity are still used in standard textbook of general physics and modern physics. One of the reasons is that the form of conductivity derived by Drude is very similar to that derived from the quantum mechanical model,

$$\sigma_i = \frac{ne^2\tau_i}{m}. \qquad \text{[i = cl (classical) or qm (quantum)]}$$

8. What is the Drude model?

Here we discuss the Drude model which is a simple but powerful model of electrical conductivity of metals. This model is a typical example of a semi-classical model, which means the combination of classical and quantum ideas. In the Drude model we think of conduction electrons as classical particles with a definite position and velocity, but to understand the interaction of these electrons with their surroundings, we use the results of quantum calculations. The classical view of electrons that are point particles can be made roughly consistent with the quantum view of electrons as de-localized wave function through the notion of wave packets. In a periodic lattice, the wave function of electron is well described by the Bloch theorem. These electrons move about as a cloud through the spaces separating the ion cores. Their motion is random, bearing some similarities to gas molecules, especially scattering, but the nature of the scattering is different. Electrons do not obey classical gas laws; their motion in detail must be analyzed quantum-mechanically. However, much information about conductivity can be understood classically.

We can now work out the electrical conductivity σ of a metal on the Drude model; that is, we can work out the current density

$$\boldsymbol{J} = \sigma \boldsymbol{E},$$

produced by an electric field ***E***. Macroscopically, ***J*** is given by

$$J = \rho_c \boldsymbol{v}_d,$$

where $\boldsymbol{v}_d$ is the velocity at which the charge density ρ_c is moving. If our metal contains *n* conduction electrons per unit volume, each carrying charge $q = -e$, we have

$$\rho_c = qn = -en, \qquad \boldsymbol{J} = -ne\boldsymbol{v}_d,$$

if all the electrons have the same velocity. More generally, if the i-th electron has velocity $\boldsymbol{v}_i$, we have

$$J = q\sum_i^n \boldsymbol{v}_i \quad .$$

If $\boldsymbol{E} = 0$, the electron gas as a whole, is in thermal equilibrium, with as many electrons moving to the right as to the left, so that

$$\sum_i^n \boldsymbol{v}_i = 0$$

and there is no net current. But in a field ***E***, each electron experiences a force $-e\boldsymbol{E}$, and an acceleration $-e\boldsymbol{E}/m$. If, at any instant, the average electron has travelled for a time τ since its last collision, it will therefore have acquired a drift velocity

$$\boldsymbol{v}_d = -\frac{e\tau}{m}\boldsymbol{E},$$

which is different form thermal velocity $\boldsymbol{v}_{rms}$ discussed above. Thus we have the current density as

$$\boldsymbol{J} = -ne\boldsymbol{v}_d = \frac{ne^2\tau}{m}\boldsymbol{E},$$

so that we have

$$\sigma_{cl} = \frac{ne^2\tau}{m}, \qquad \text{(Drude model; classical model)}$$

which is called the Drude model, if we assume that the relaxation time τ is the same for all electrons. If instead, we assume that the mean free path Λ is the same for all electrons (and this would be more plausible on the Drude model) we have

$$v_d = -\frac{ev\tau}{mv}\boldsymbol{E} = -\frac{e\Lambda}{mv}\boldsymbol{E}\ .$$

where $\Lambda = v\tau$ is the mean-free path. Here we discuss the magnitude of the drift velocity for typical values of E and τ. When we use $E = 1.72$ x 10^{-2} V/m (which is obtained above) and $\tau = 10^{-14}$ s, we get

$$|v_d| = \frac{e\tau}{m}E = 3.025\times 10^{-5}\,\text{m/s}$$

which is too small compared to the Fermi velocity; $v_F = 1.57\times 10^6$ m/s for Cu; $v_d / v_F \simeq 1.93\times 10^{-11}$.

In quantum mechanics, the electrical conductivity is given by

$$\sigma_{qm} = \frac{ne^2\tau(\varepsilon_F)}{m}. \qquad \text{(Sommerfeld model, quantum mechanical model)}$$

Using the mean free path $\Lambda(\varepsilon_F) = \tau(\varepsilon_F)v_F$ at the Fermi energy, σ can be rewritten as

$$\sigma_{qm} = \frac{ne^2\tau(\varepsilon_F)v_F}{mv_F} = \frac{ne^2\Lambda(\varepsilon_F)}{mv_F}, \qquad (6)$$

where v_F is the Fermi velocity and ε_F is the Fermi energy. This formula is based on the quantum mechanics with the duality of wave and particle, gives a proper evaluation of real electrical resistivity of metals.

9. Role of the relaxation time: first order differential equation

In order to understand the role of the relaxation time in the Drude theory, we discuss the solution of the first order differential equation,

$$m(\frac{dv}{dt} + \frac{v}{\tau}) = qE\ ,$$

or

$$\frac{dv}{dt} + \frac{v}{\tau} = \frac{qE}{m},$$

where $q = -e$, and τ is the relaxation time. For simplicity, we introduce the terminal velocity v_0 which is defined by

$$v_\infty = \frac{qE}{m}\tau \qquad \text{(the terminal velocity)}$$

In the steady state ($dv/dt = 0$), the above equation becomes

$$v_\infty = \frac{qE}{m}\tau \; .$$

Using the terminal velocity v_∞, the differential equation can be rewritten as

$$\frac{d}{dt}(v - v_\infty) + \frac{1}{\tau}(v - v_\infty) = 0 \, ,$$

The solution of this equation is given by

$$v = v_\infty[1 - \exp(-\frac{t}{\tau})] \, ,$$

When $E = 0$ (E-off), we have the differential equation

$$\frac{dv}{dt} = -\frac{v}{\tau} \, , \qquad v = v_\infty e^{-\frac{t}{\tau}} \, ,$$

or

$$p = mv = p_\infty e^{-t/\tau} \, ,$$

where $p_\infty = m v_\infty$. The time used for the terminal velocity is the same as the relaxation time. After the cut-off of the electric field ***E***, the momentum obtained by the electric field decays with the same relaxation time. The electrons are scattered by phonons as well as impurities.

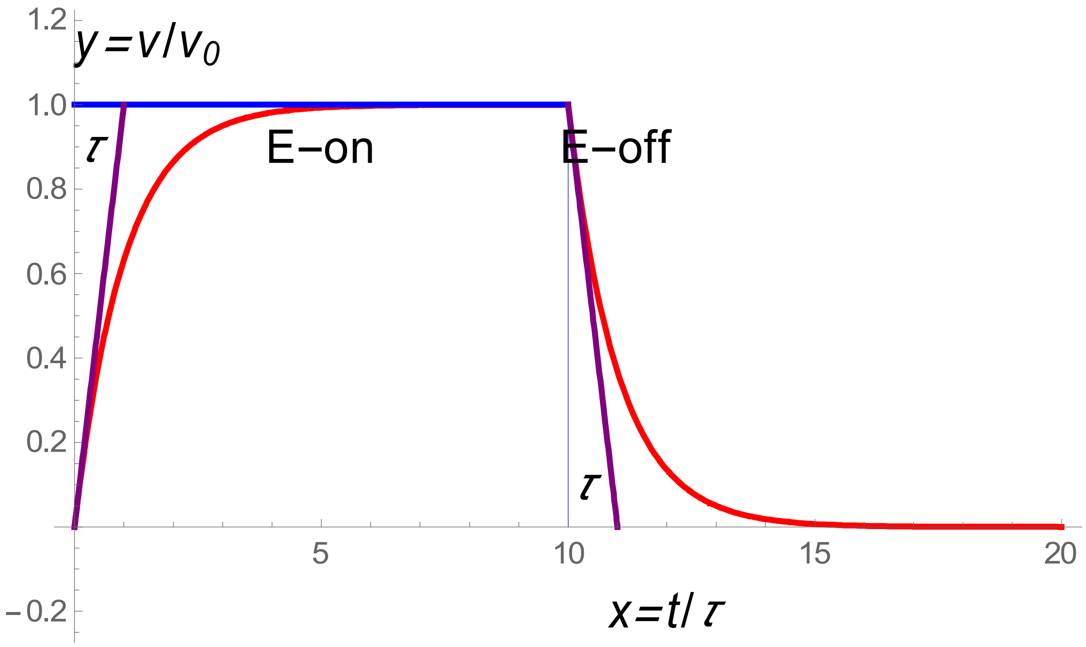


Fig.3 At $t = 0$ the electri field E is turned on. After sufficiently long times, the velocity v reaches the terminal velocity. $v_0 = qE\tau / m$. After that, the electric field E is turned off. The velocity is reduced to zero with the relaxation time τ. $v_0 = qE\tau / m$. Note that the relaxation time for the terminal velocity is the same as the decay time due to the relaxation.

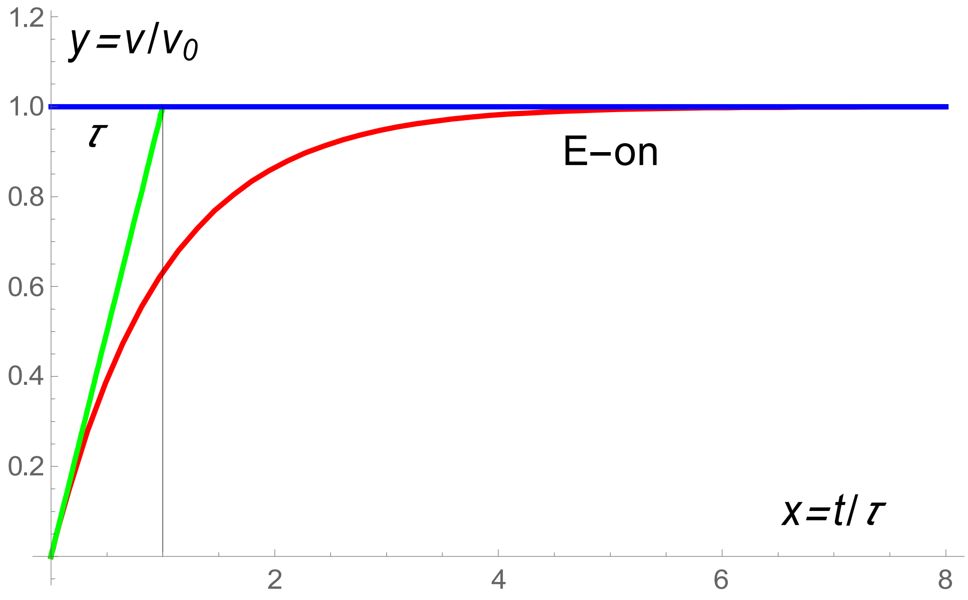


Fig.4 The electric field E is turned on at $t = 0$. The velocity increases with increasing time and reaches a terminal velocity $v_0 = qE\tau / m$, where τ is the relaxation time τ.

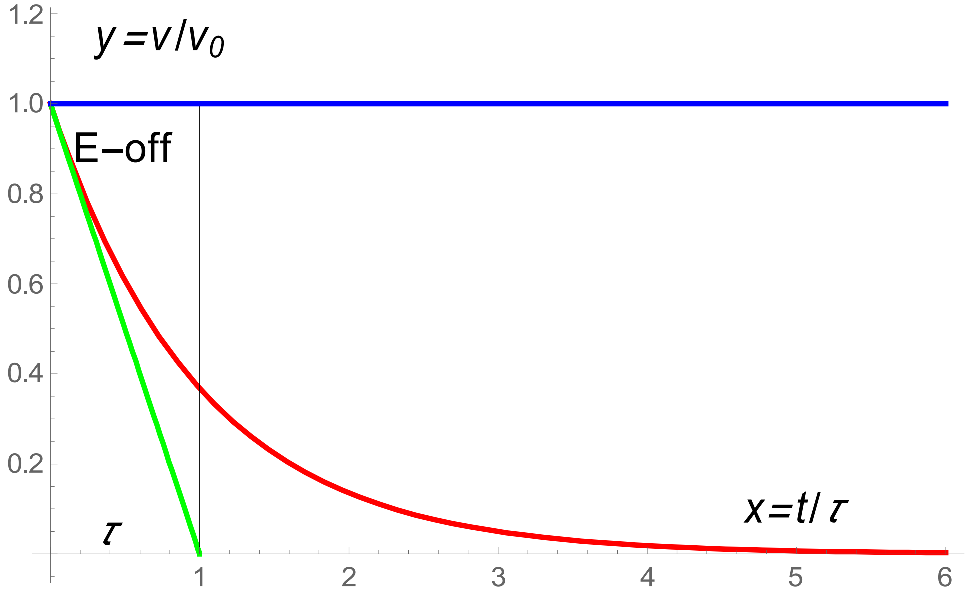


Fig.5 At t = 0, the velocity v is equal to the terminal velocity v_0. The electric field is turned off at t = 0. The velocity is reduced to zero with the relaxation time τ. $v_0 = qE\tau / m$

10. Physical properties of Copper

Here we discuss the electrical properties of copper (Cu), which is one of typical metals. Copper has a fcc (face-centered cubic) structure. There are four Cu atoms per conventional cubic unit cell with the lattice constant $a = 3.61$ Å. Here is a list of the electrical resistivity of copper at 295 K (ISSP, 8-th edition, **C. Kittel, 2005**).

$n = 8.45 \times 10^{28} m^{-3}$	(number density)
$v_F = 1.57 \times 10^6$ m/s	(Fermi velocity)
$k_F = 1.36 \times 10^{10} / m$	(Fermi wave number)
ε_F = 7.00 eV	(Fermi energy)
T_F =8.12 x 10^4 K	(Fermi temperature)
$\rho = 1.72 \times 10^{-8}$ Ωm	(electrical resistivity at 300 K)
a = 3.61 Å	(conventional cubic unit cell, fcc structure)

From the value of electrical resistivity, the relaxation time can be calculated as

$$\tau = \frac{m}{\rho n e^2} = 2.44165 \times 10^{-14} \text{ s}.$$

where $n = 8.45 \times 10^{28} m^{-3}$ and $\rho = 1.72 \times 10^{-8}$ Ω m. Correspondingly we have the mean free path as

$$\Lambda(\varepsilon_F) = v_F \tau = 3.8334 \times 10^{-8} \text{m} = 383.34 \text{ Å}$$

This value of $\Lambda(\varepsilon_F)$ is much larger than the lattice constant of copper, suggesting the wave-like nature of the conduction electrons in copper. Note that $\Lambda(\varepsilon_F)/a \approx 106$.

((**Note-1**)) **Calculation of Fermi energy and Fermi velocity from the number density in Cu**

There are four Cu atoms in the conventional cubic unit cell with the lattice constant $a = 3.61$ Å. From this we can derive the physical properties of Cu.

The number density:

$$n = \frac{4}{a^3} = 8.50234 \times 10^{28} \text{ (/m}^3\text{)}.$$

The Fermi wave number:

$$k_F = (3\pi^2 n)^{1/3} = 1.36036 \times 10^{10} \text{(1/m)}.$$

The Fermi energy:

$$\varepsilon_F = \frac{\hbar^2 k_F^{\ 2}}{2m} = 7.5065 \text{eV}.$$

The Fermi velocity:

$$v_F = \frac{\hbar k_F}{m} = 1.57485 \times 10^6 \text{ m/s}.$$

((**Note-2**)) **The ground state of electron in the hydrogen atom (see Appendix-III)**

For comparison, we show the velocity of electron and the period of orbit in the ground state of electron in the hydrogen atom;

$$v_{orbit} = 2.18679 \times 10^6 \text{ m/s.} \qquad t_{orbit} = 1.51983 \times 10^{-16} \text{ s.}$$

11. 1D-energy dispersion of electrons in the presence of periodic potential

(a) Electron in a quantum box

The energy dispersion is essentially the same as that of free electron. However, the energy level is quantized, since the wave number becomes discrete.

$$k = \frac{2\pi}{L_0}\nu_0,$$

where k has a discrete value, L_0 is the size of the system, and ν_0 is an integer. The separation of states in the k-space is

$$\Delta k = \frac{2\pi}{L_0}.$$

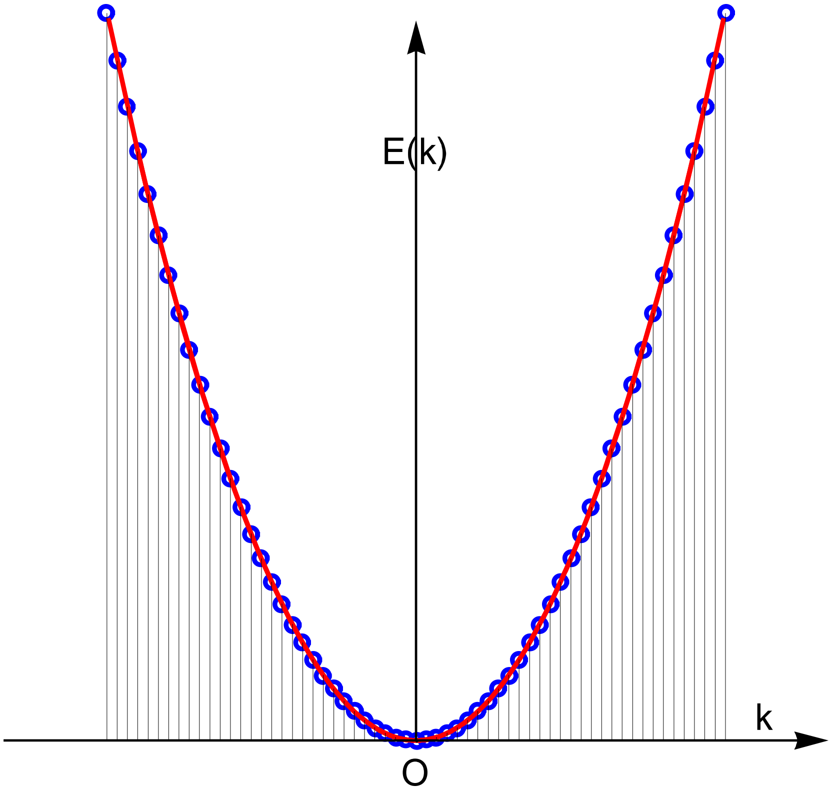


Fig.6 1D-energy dispersion curve for electrons in a quantum box. $\Delta k = \frac{2\pi}{L_0}$. L_0 is the size of the system.

(b) Energy of electron in a periodic potential (Bloch theorem)

The occupied states below Fermi energy is shown below.

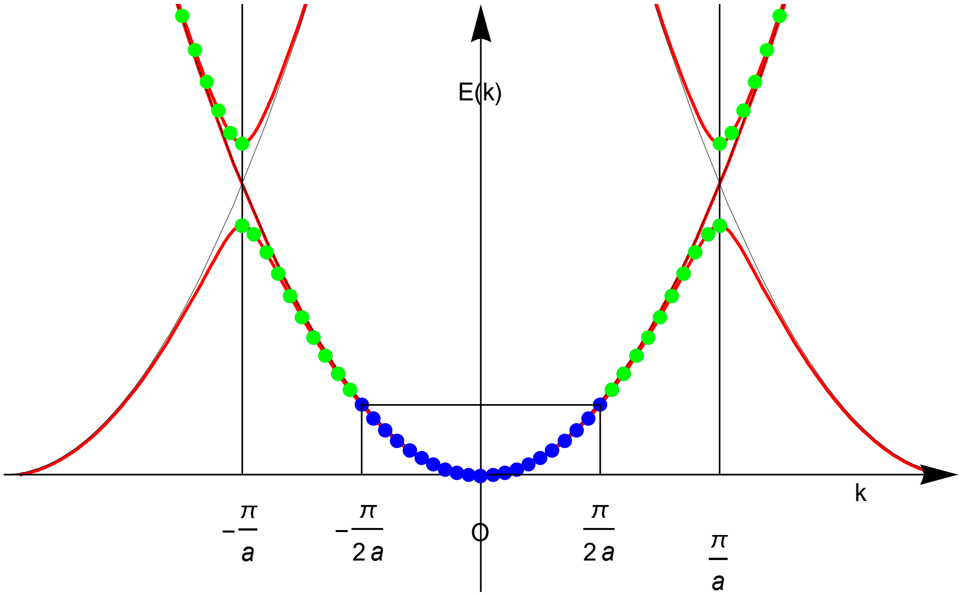


Fig.7 Half-filled energy band (first Brillouin zone). Band-1 (in the first Brillouin zone) and band-2. The total number of states is $2N$ states for the first Brillouin zone when the system consists of N unit cells. The Brillouin-zone boundary is $k = \pm\frac{\pi}{a}$.

12. 1D-energy vs *k* diagram with and without the electric field

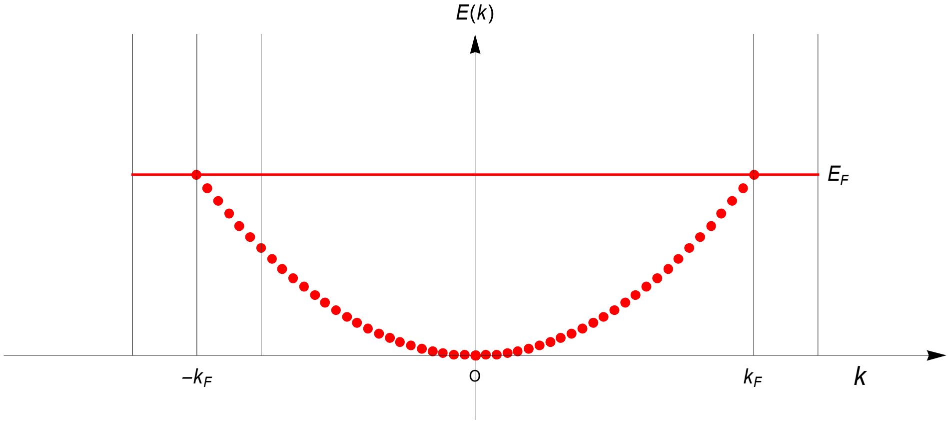


Fig.8(a) The energy vs wave number of the 1D system. The states below the Fermi energy ($|k| \le k_F$) are fully occupied in thermal equilibrium. No electric field is applied.

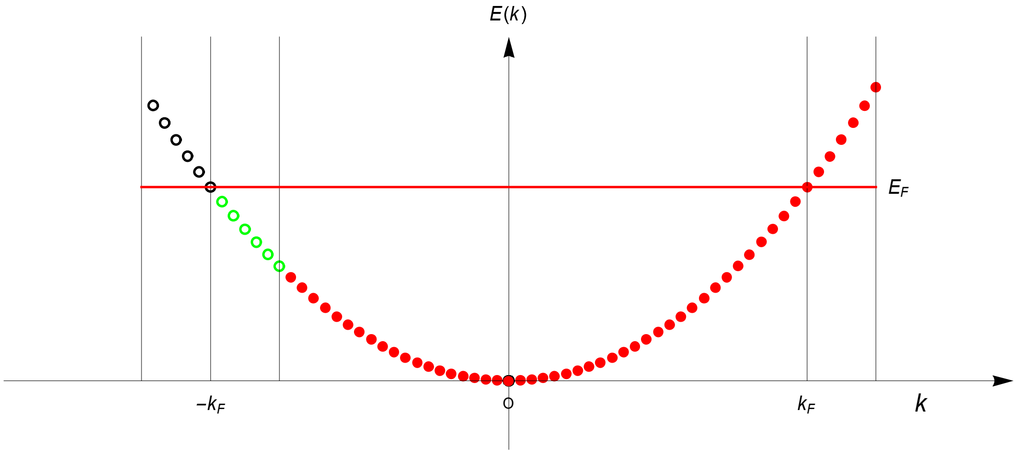


Fig.8(b) The 1D energy vs *k* diagram after the electric field *E* is applied along the negative *k*-axis. In other words, the force is applied along the positive axis, because of negative charge of electrons. The occupied states below the Fermi energy at $E = 0$ shfts to the positive *k*-axis. A part of states (denoted by red dots) is outside the Fermi surface with $k > k_F$, accompanied with the appearance of the the empty states (denoted by the green dots) in the vicinity of $k = -k_F$ below the Fermi energy. Such an asymmetric distribution becomes stable well after the relaxation time τ.

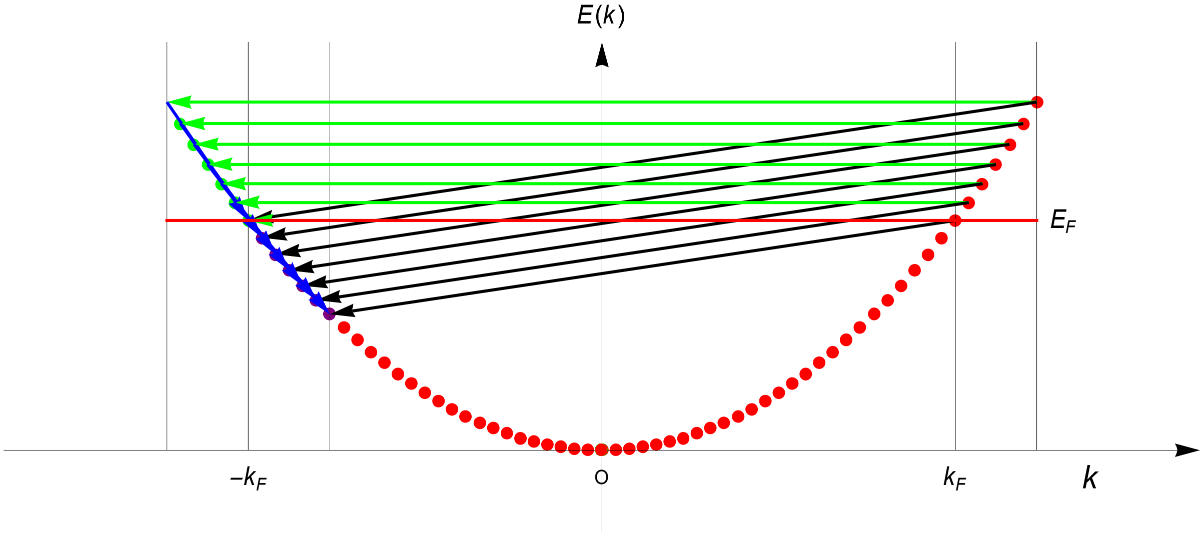


Fig.8(c) The energy vs *k* of the 1D system, after the electric field *E* is turned off. The occupied states above the Fermi energy (with $k > k_F$) are shifted to unoccupied states (near $k = -k_F$) below the Fermi energy by both elastic and inelastic scattering. After the sufficiently large times, the distribution becomes into the original one at $E = 0$. Such a redestribution after the switch-off of E is characterized by the relaxation time τ. Note that this value of τ is the same as that for the shit $\Delta k = \tau qE / \hbar$ in the presence of the electric field E.

13. 2D energy vs k diagram with and without the electric field

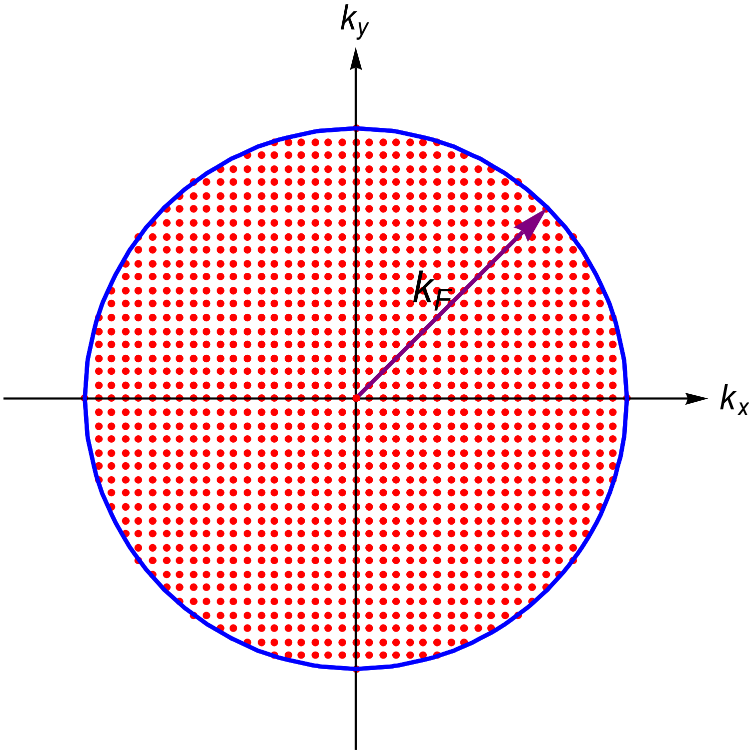


Fig.9(a) Ground state of electrons in the two-dimensional (2D) $\boldsymbol{k}$ – space in thermal equilibrium. All the states are occupied inside the Fermi surface $(k < k_F)$ .The Fermi surface of a hypothetical solid containing N free electrons. The occupied electron energy levels fill a sphere of radius k_F , which is known as the Fermi wave number.

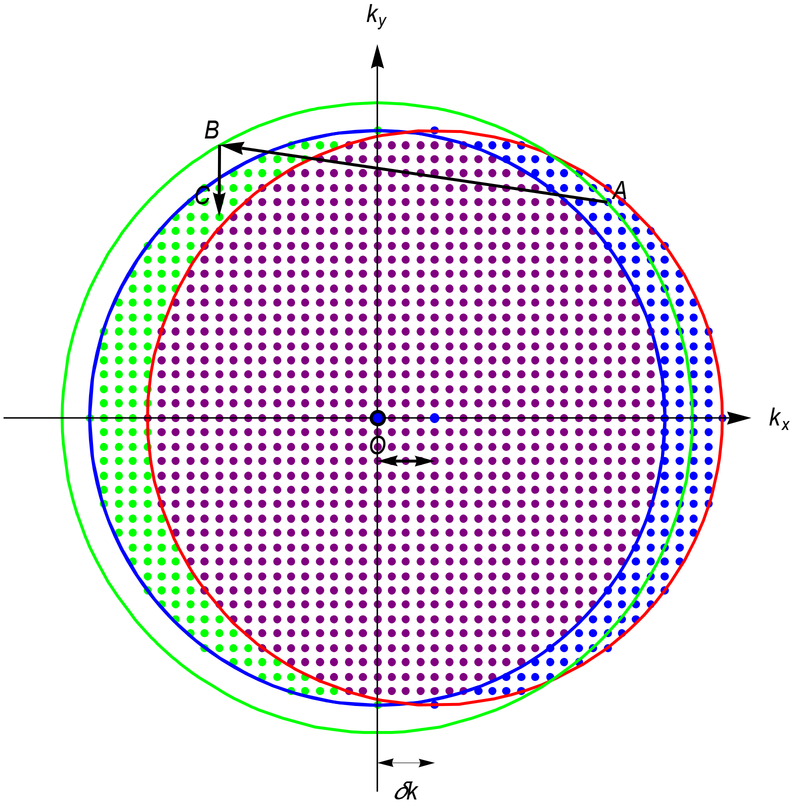


Fig.9(b) The effect of a constant electric field E_x on the ***k***-space distribution of quasi-free electrons. Red circle denotes the 2D Fermi surface when the electric field is applied along the negative *x* axis. The center of the Fermi surface is displaced to the positive k_x axis well after the relaxation time τ. Such an asymmetric distribution becomes stable. Note that the displaced Fermi distribution only differs significantly from the equilibrium distribution in the vicinity of the Fermi energy (Fermi radius). What happens to the distribution when the case when the electric field is turned off ? Elastic scattering of an electron at *A* by a static imperfection or impurity can carry the electron to any point such as *B* (on the green circle) which lies above the sphere of constant energy $\varepsilon_A = \varepsilon_B (> \varepsilon_F)$. Inelastic scattering will reduce the total momentum to zero by redistribution the occupied states (*C*, denoted by blue dots) with energy $\varepsilon_C (< \varepsilon_F)$, but phonon processes such as $B \rightarrow C$ are needed to relax back to the original distribution centered at ***k*** = 0.

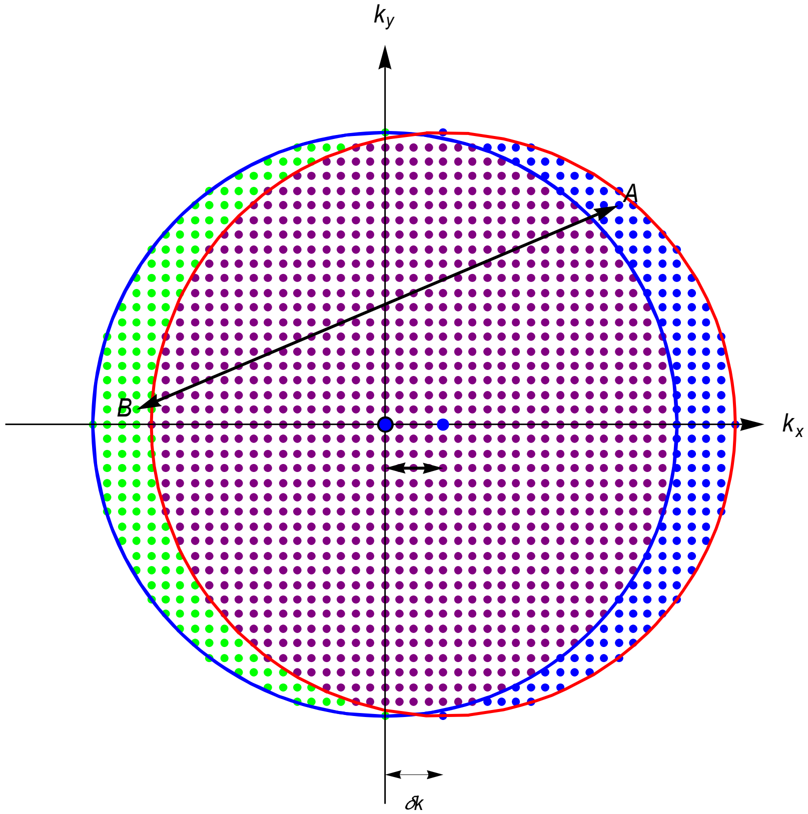


Fig.9(c) When the applied force is turned off, collision processes tend to return the system to the ground state. The electrons are transferred from those filled states (denoted by blue dots) to those empty states (denoted by green dots). An electron at A can make a transition to an empty state, say B, by the emission of a phonon of suitable wavevector and angular frequency.

Here we assume that the Fermi surface is a circle in the 2D $\boldsymbol{k}$-space. However, the following discussion is also true for the Fermi sphere in the 3D $\boldsymbol{k}$-space.

(a) The case of $E = 0$

When the electric field is equal to $E = 0$, the center of the 2D Fermi surface is at $k = 0$. It means that as many electrons would be travelling to the right as there would be to the left. The contribution from all of the free electrons would give an average electron velocity of zero, and no net electric current.

(b) The case of $E \neq 0$

By contrast, what happens to the surface of a 2D Fermi surface an electric field, E , is applied to the system. Every electron in the Fermi gas will be accelerated in a direction opposite to the field, so there will now be more electrons travelling in one direction than the other. The center of the Fermi surface is shifted to the direction of force due to the applied electric field, leading to a current flow.

When current flows in a conductor it does not just keep increasing in magnitude with the same electric field applied. Instead it quickly rises up to a central value that depends on the magnitude of the field, then remains steady as that value. This can be explained in terms of the Fermi surface.

Free electrons in the energy states near to the Fermi surface (which has the energy ε_F) suffer collisions with other electrons, lattice ions, and defects, which causes them to be scattered. This in turn will mean that their wave vector will change, or in other words, the change in direction and speed that their scattering produces means they have to go to a new ***k*** state. It is only those electrons near the Fermi surface that can find vacant states into which they can be scattered. The vacant *k* states that the scattered electrons take are those with a lower value of energy situated to the left side of the Fermi sphere. The current does not therefore increase indefinitely in size, because to do so the electrons would have to keep increasing in energy (so they could travel along faster). This would mean they would have to move to ***k*** states with higher and higher energies rather than moving into states with lower energies. For example, an electron in state B will move into state A rather than a higher energy state, limiting the current.

14. Density of states of electrons (Sommerfeld)

The density of states for conduction electrons (the 3D system) is given by

$$D(\varepsilon) = \alpha\sqrt{\varepsilon} \,,$$

where α is constant. The electron states are fully occupied below the Fermi energy ε_F (Fermi-Dirac statistics). The total number density of electrons below ε_F is

$$n = \frac{N}{V} = \int_0^{\varepsilon_F} D(\varepsilon) d\varepsilon = \alpha \int_0^{\varepsilon_F} \sqrt{\varepsilon} d\varepsilon = \frac{2\alpha}{3} \varepsilon_F^{3/2} .$$

Note that

$$\frac{n}{D(\varepsilon_F)} = \frac{2a\varepsilon_F^{3/2}}{3a\varepsilon_F^{1/2}} = \frac{2}{3}\varepsilon_F \,,$$

or

$$n = \frac{2}{3}\varepsilon_F D(\varepsilon_F) .$$

The conductivity is given by

$$\sigma = \frac{ne^2\tau(\varepsilon_F)}{m} .$$

since only the electrons at the Fermi level undergo collisions, where $\tau(\varepsilon_F)$ is the relaxation time. Using the expression of *n* described above, the conductivity can be rewritten as

$$\begin{aligned}\sigma &= \frac{2e^2}{3m}\tau(\varepsilon_F)\varepsilon_F D(\varepsilon_F) \\ &= \frac{e^2}{3}v_F \Lambda(\varepsilon_F) D(\varepsilon_F)\end{aligned}$$

where $\Lambda(\varepsilon_F) = v_F \tau(\varepsilon_F)$ is the mean-free path. This shows that the conductivity depends only on the properties of the electrons at the Fermi level. The high conductivity of metals is to be ascribed to the high current carried by the electrons at the top of the Fermi distribution

15. Significance of the drift velocity

When a current flows in a conductor, it does not just keep increasing in magnitude with the same electric field applied. Instead it quickly rises up to a central value that depends on the magnitude of the field, then remains steady as that value (the terminal velocity). This can be explained in terms of the Fermi surface. Free electrons in the energy states near the Fermi surface (which has the energy ε_F) suffer collisions with other electrons, lattice ions, and defects, which causes them to be scattered. This in turn will mean that their wave vector will change, or in other words, the change in direction and speed that their scattering produces means they have to go to a new *k* state. It is only those electrons near the Fermi surface that can find vacant states into which they can be scattered. The vacant ***k*** states that the scattered electrons take are those with a lower value of energy situated to the left side of the Fermi sphere.

The current does not therefore increase indefinitely in size, because to do so the electrons would have to keep increasing in energy (so they could travel along faster). This would mean they would have to move to ***k*** states with higher and higher energies rather than moving into states with lower energies. For example, an electron in state *B* will move into state *A* than a higher energy state, limiting the current.

The change of momentum:

$$\boldsymbol{F} = q\boldsymbol{E} = \hbar\frac{d\boldsymbol{k}}{dt}.$$

The energy change:

$$\Delta\varepsilon = \hbar\boldsymbol{v}_k \cdot \Delta\boldsymbol{k}.$$

16. Root-mean square velocity

We now consider why conduction electrons in metals have such a large intrinsic velocity, the Fermi velocity. We first note that the Fermi velocity is not simply the thermal velocity of the electrons. In a classical gas of particles of mass *m* at temperature *T*, the average root-mean square velocity v_{rms} of the particle is given by

$$\frac{1}{2}m{v_{rms}}^2 = \frac{3}{2}k_B T \ .$$

For electrons at room temperature, this root-mean velocity is about 10^5 m/s, factor of 10 smaller than the Fermi velocity. Another difference between the thermal velocity and Fermi velocity is as follows. The Fermi velocity is independent of temperature, while the thermal velocity rises with increasing temperature.

17. Validity of the Ohm's law in electrical conductivity

The fact that the electrical conductivity of a metal is independent of the applied electric field *E* is surprising for the following reason. The conductivity depends on the collision time τ according to the Drude formula. At first glance, it might seem that the collision time τ should depend on the field *E*. After all, if the field *E* is increased, the acceleration *a* of a conduction electron will increase (according to $a = qE/m$); and if the electron accelerates more quickly, it will surely encounter an impurity or phonon more quickly, resulting in a shorter collision time and a smaller conductivity σ. The argument, which implies that σ depends on *E*, would be correct if conduction electrons had zero initial velocity after a collision. However, because of the Pauli's exclusion principle, the electrons in a metal always have a very large intrinsic velocity, called the Fermi velocity v_F. The Fermi velocity is about 0.3 % of the speed of light ($v_F = 0.003\,c \approx 10^6$ m/s). In contrast, the magnitude of the drift velocity v_d (the mean velocity due to the applied field *E*), is minuscule (mm/s). Consequently, the increase in velocity due to the *E* field is completely negligible compared to the initial huge Fermi velocity of the conduction electron, and the collision time is almost completely independent of the field *E*. The fact that τ is independent of *E* is the origin of Ohm's law.

18. Definition of mean-free path

The motion of conduction electrons is thus one of extremely rapid motion due to the large Fermi velocity and, superimposed on this, a very small bias toward one direction due to the tiny drift velocity. A conduction electron in a metal follows a random zigzag path even with zero applied field ($E = 0$), regardless of the temperature. This is an example of random-walk diffusive motion. The mean free path is defined as the mean distance an electron travels between collisions, that is, the step length in the random walk. The mean free path related to the Fermi velocity and the collision time $\tau$by

$$\Lambda(\varepsilon_F) = \tau v_F \, .$$

The mean free path depends on the purity and temperature of the sample. Vey dirty samples, such as alloys, or metals at very high temperatures, may have a mean free path of nanometers or less. Metals of ordinary purity at room temperatures may have a mean free path of roughly 10-100 nm. While high-purity (clean) samples at low temperatures may have a mean free path of many micrometers or even millimeters.

19. The Boltzmann equation (Ziman, Chambers)

Here we discuss the Boltzmann equation to derive the formula of conductivity based on the quantum mechanics. We know that a uniform electric field, acting for a relaxation time $\tau_{\boldsymbol{k}}$, would displace an electron in the ***k***-space by the (extremely small) amount

$$\begin{aligned} f(\boldsymbol{k}) &= f_0(\boldsymbol{k}) - \hbar \boldsymbol{k}_d \cdot \boldsymbol{v}_k \frac{\partial f_0}{\partial \varepsilon} \\ &= f_0(\boldsymbol{k}) + f_1(\boldsymbol{k}) \\ &= f_0(\boldsymbol{k}) - q\tau_{\boldsymbol{k}} \boldsymbol{E} \cdot \boldsymbol{v}_k \frac{\partial f_0}{\partial \varepsilon} \end{aligned}$$

where $q = -e$, $f_0(\boldsymbol{k})$ is the Fermi distribution function in thermal equilibrium, and drift velocity is defined by

$$\hbar \boldsymbol{k}_d = m v_d = q\tau_{\boldsymbol{k}} \boldsymbol{E} \cdot$$

Note that if the electric field is turned off, the distribution function would decay to the distribution function in thermal equilibrium with the same relaxation time $\tau_{\boldsymbol{k}}$;

$$f_1(\boldsymbol{k}) = e\tau_{\boldsymbol{k}} \boldsymbol{E} \cdot \boldsymbol{v}_k \frac{\partial f_0}{\partial \varepsilon}.$$

In the case of free particle with $\varepsilon = \frac{1}{2m} \boldsymbol{p}^2$,

$$f \approx f_0(\varepsilon - q\tau \boldsymbol{v} \cdot \boldsymbol{E}) \simeq f_0(\frac{1}{2m}(\boldsymbol{p} - q\tau \boldsymbol{E})^2)$$

The center of the Fermi circle is displaced from the origin to $q\tau \boldsymbol{E}$.

20. Boltzmann transport theory: Fermi-Dirac distribution

In order to evaluate the electrical conductivity, we need the corresponding current density:

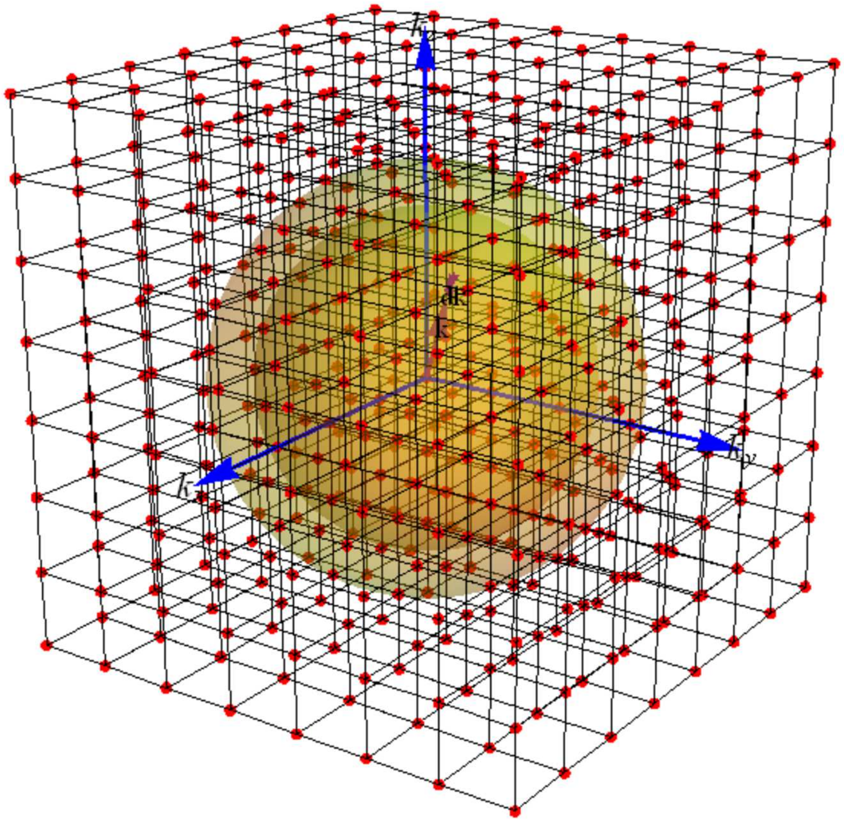
$$
\begin{aligned}
\boldsymbol{J} &= \frac{1}{V}\sum_{\boldsymbol{k}}(-e)\boldsymbol{v}_{\boldsymbol{k}} f_1(\boldsymbol{k}) \\
&= \frac{1}{V}\frac{2V}{(2\pi)^3}\int d\boldsymbol{k}(-e)\boldsymbol{v}_{\boldsymbol{k}} f_1(\boldsymbol{k}) \\
&= (-e)\frac{2}{4\pi^3}\int d\boldsymbol{k}\boldsymbol{v}_{\boldsymbol{k}}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

where V is the volume of the system and

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

and

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



s

Fig.10 Density of states in the 3D ***k***-space. There are 2 states per $(2\pi / L_0)^3$; 2 for spin factor.

The factor 2 arises from the spin freedom (spin of electron is 1/2). 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 *S*). We use the deviation of the distribution function from that in thermal equilibrium, which is given by

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

where $q = -e$ is the charge of electron, and $e>0$.

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

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

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

The density of states is

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

or

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

Then the conductivity is obtained as

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

with

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

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

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

where

$$-\frac{\partial f_0}{\partial \varepsilon_{\boldsymbol{k}}} \approx \delta(\varepsilon_{\boldsymbol{k}} - \varepsilon_F) \qquad \text{(Dirac delta function)}$$

Noting that

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

we have the conductivity

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

Using the number density given by

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

$$\sigma_{qn} = \sigma_{xx} = \frac{ne^2\tau(\varepsilon_F)}{m}\,.$$

In summary, only the electrons near the Fermi energy is partially filled bands have to be considered to calculate the conductivity. So the mass in a semiclassical version would be replaced by the effective mass at the Fermi energy and the relaxation time would be that for electrons at the Fermi energy. The electron density *n* would still appear but not because all the electrons contribute to the current. The reason for having *n* is that the number of electrons at the Fermi energy depends on the electron density (**Hoffmann, 2015**).

21. Physical meaning of the role in the drift velocity

Now we imagine the same system in an infinitesimal electric field. Since the electric field is capable of changing the electron energy by only infinitesimal amounts, the contribution to the total current from electrons of a particular energy will depend only on the distribution function for that and immediately adjacent values of the energy.

We consider the electron state whose energy is very close to the Fermi energy ε_F. When the electric field *E* is applied to the system, the wave vector of the electron changes as

$$\boldsymbol{k} \to \boldsymbol{k} + \delta\boldsymbol{k}\,,$$

with $\delta\boldsymbol{k} = \frac{q\boldsymbol{E}}{\hbar}\tau(\varepsilon_F)$ and the energy changes as

$$\varepsilon(\boldsymbol{k}) \to \varepsilon(\boldsymbol{k}) + \delta\varepsilon(\boldsymbol{k})$$

with

$$\begin{aligned}\delta\varepsilon(\boldsymbol{k}) &= \hbar\boldsymbol{v}_{\boldsymbol{k}}\cdot\Delta\boldsymbol{k}\\ &= \hbar\boldsymbol{v}_{\boldsymbol{k}}\cdot\frac{q\boldsymbol{E}}{\hbar}\tau(\varepsilon_F)\\ &= q\tau(\varepsilon_F)\boldsymbol{v}_{\boldsymbol{k}}\cdot\boldsymbol{E}\end{aligned}$$

where $|\boldsymbol{v}_{\boldsymbol{k}}| \approx v_F$ and v_F is the Fermi velocity

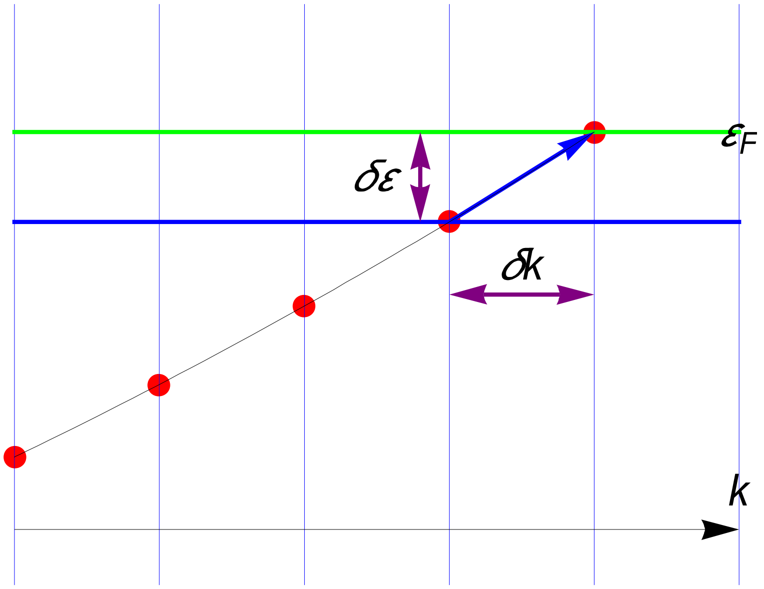


Fig.11 The change of wave number $\delta\boldsymbol{k} = \tau(\varepsilon_F)q\boldsymbol{E}$ and the change of energy $\delta\varepsilon = \hbar\boldsymbol{v}_k \cdot \delta\boldsymbol{k}$, where $q = -e$ and the electric field $\boldsymbol{E}$ is applied. The separation between adjacent vertical blue lines is $2\pi / L_0$, where L_0 is the size of the system. This discreteness of k comes from the plane wave form $\psi(x) = e^{ikx}$ with the periodic boundary condition; $\psi(x + L_0) = \psi(x + L_0)$.

Here we consider the electron system with the finite size (L_0 is the side for cubic system). In the periodic boundary condition, the wave function of electron can be described by the plane-wave form

$$\langle \boldsymbol{r} | \boldsymbol{k} \rangle = \exp(i\boldsymbol{k} \cdot \boldsymbol{r}),$$

with the energy eigenvalue

$$\varepsilon(\boldsymbol{k}) = \frac{\boldsymbol{p}^2}{2m} = \frac{\hbar^2}{2m}\boldsymbol{k}^2,$$

with the discrete values of k_x, k_y, and k_z;

$$k_x = \frac{2\pi}{L_0} n_x, \qquad k_y = \frac{2\pi}{L_0} n_y, \qquad k_z = \frac{2\pi}{L_0} n_z,$$

where n_x, n_y, and n_z are integers.

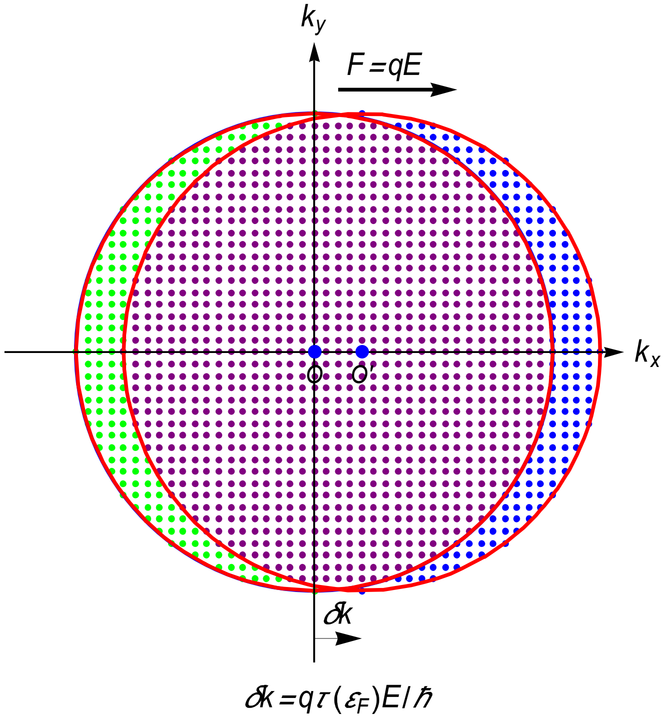


Fig.12 Displaced 2D Fermi surface. The force $\boldsymbol{F} = q\boldsymbol{E}$ is applied along the positive x axis.

21. Evaluation of Δk and $\Delta \varepsilon$

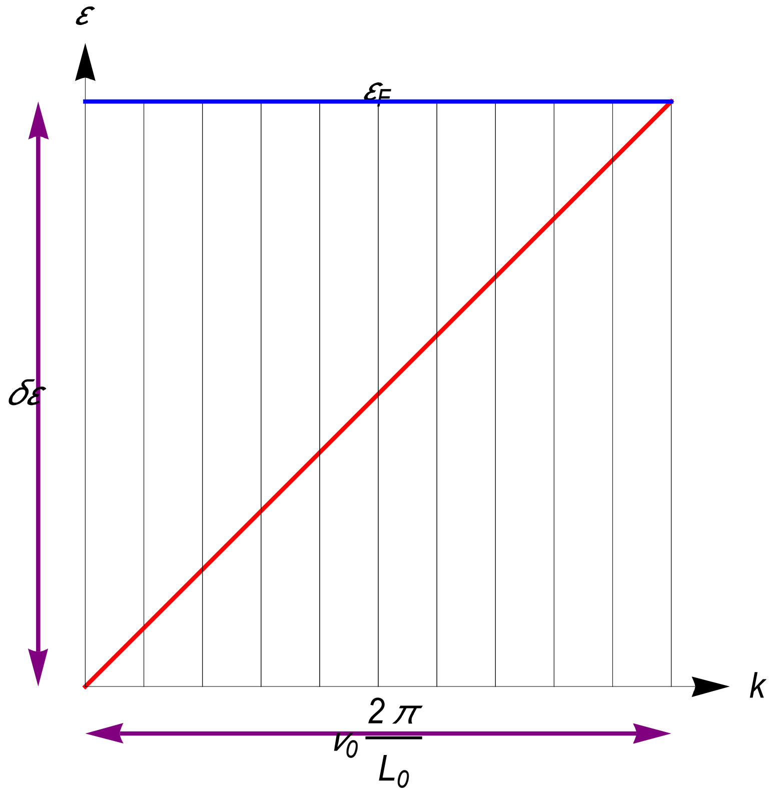


Fig.13 Energy ε vs the wave number k for the 1D system in the vicinity of ε_F. $\Delta k = \frac{2\pi}{L_0}\nu_0$. ν_0 is a positive integer. The separation between adjacent vertical lines is $\frac{2\pi}{L_0}$. L_0 is the size of the system.

Suppose that we use the electric field E as

$$E = 1.72 \times 10^{-2}\,\text{V/m} \qquad \text{(typical experimental value)}$$

Then we get the value of Δk

$$\Delta k = \frac{q}{\hbar}\tau E = 15.1927 E = 0.261\,/\text{m}$$

We note that L_0 is the size of the system. We now consider a possibility that the state of the electron changes from $|\boldsymbol{k}\rangle$ to $|\boldsymbol{k} + d\boldsymbol{k}\rangle$. Such a change in state can occur only if

$$\Delta k > \frac{2\pi}{L_0}\nu_0,$$

where k is very close to k_F, ν_0 is a finite positive integer (ν_0=1, 2,3,…). This may be related to the Heisenberg's principle of uncertainty:

$$\hbar\Delta k\left(\frac{L_0}{4\pi\nu_0}\right) > \frac{\hbar}{2}, \qquad \text{or} \qquad \Delta x\Delta p > \frac{\hbar}{2},$$

where $\Delta x = \frac{L_0}{4\pi\nu_0} = \frac{24.08}{4\pi} = 1.915$ m, and $\Delta p = \hbar\Delta k$. When $\Delta k = 0.261$ /m, the lower limit of the size (L_0) is obtained as

$$\frac{2\pi}{L_0} = \frac{0.261}{\nu_0},$$

or

$$L_0 = 24.08\ \nu_0\ \text{(m)},$$

leading that L_0 is at least larger than 24.08 (m). Using this value of L_0, we can estimate the energy separation between the states $|\boldsymbol{k}\rangle$ to $|\boldsymbol{k}+d\boldsymbol{k}\rangle$. The condition for the energy separation is

$$\Delta\varepsilon > \hbar v_F\Delta k = \hbar v_F\frac{2\pi}{L_0}\nu_0 = \hbar v_F\frac{2\pi}{24.08} = 27.05\ \text{neV},$$

where $v_F = 1.575\times10^6$ m/s for Cu. This may bealso related to the Heisenberg's principle uncertainty as

$$\Delta\varepsilon\left(\frac{L_0}{4\pi\nu_0 v_F}\right) > \frac{\hbar}{2}, \qquad \text{or} \qquad \Delta\varepsilon\,\Delta t > \frac{\hbar}{2},$$

where

$$\Delta t = \frac{L_0}{4\pi\nu_0 v_F} = \frac{24.08}{4\pi v_F} = 12.17\ \text{ns}.$$

22. Heisenberg's principle uncertainty and Pauli exclusion principle

((**R.P. Peierls, 1955**)) **Quantum Theory of Solids, p.52**

The modern electron theory of metals started with the remark by Pauli that the exclusion principle, and hence Fermi-Dirac statistics, must be applied to all the electrons, in particular, all the conduction electrons, in a piece of metal. This removed at once the difficulty about the paramagnetism of metals (Pauli paramagnetism).

By Fermi-Dirac statistics, most electrons are in orbital states already containing two electrons of opposite spin. They cannot therefore align themselves with the external field without violating the exclusion principle. This is possible only for electrons in states of motion which are not completely filled, i.e., those with energies within a distance k_BT from the Fermi energy, ε_F. Their number is less than the total number of electrons by a factor of the order of k_BT/ε_F and this factor explains both the temperature independence and the small value of the susceptibility. This step opened the way to the solution of many other paradoxes of a similar kind. However, although the application of the Pauli principle to all the electrons in the system was clearly required by the basic rules of quantum mechanics, and confirmed by empirical knowledge, it left people with a rather uncomfortable feeling: if two electrons are at opposite ends of a metal wire of macroscopic dimensions (such as the size of the system L_0) , say a meter in length, is it not surprising that they can manage to avoid being in the same state of motion? How can each of them know what the other is doing? The answer to this question is that it would indeed be difficult for two electrons located far from each other to affect each other's motion, but that this is also not required by the exclusion principle. In this law, "state of motion" comprises both position and momentum, as far as the uncertainty relation allows us to know then; if we can specify that the two electrons are in different regions of space, this is enough to ensure that they are in distinct states of motion, and thus to satisfy the Pauli principle. No further restriction on their motion is required.

23. The electrical conductivity: spherical symmetry

We consider a simple case: free electron Fermi gas model. The electrical conductivity based on this model is found to be equivalent to that derived by Kubo (**Kubo, 1965**), using Kubo formula. The density of states:

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

$$\varepsilon = \frac{\hbar^2}{2m}k^2, \qquad k = \sqrt{\frac{2m\varepsilon}{\hbar^2}}, \qquad dk = \frac{1}{2}\sqrt{\frac{2m}{\hbar^2}}\frac{1}{\sqrt{\varepsilon}}d\varepsilon,$$

where V is the volume of the system. Thus we have the expression of the density of states,

$$D(\varepsilon)d\varepsilon = \frac{V}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\sqrt{\varepsilon}d\varepsilon$$

or

$$D(\varepsilon) = \frac{V}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\sqrt{\varepsilon} = \frac{V\sqrt{2\varepsilon}}{\pi^2\hbar^3}m^{3/2}$$

We note that

$$\overline{v_\alpha v_\beta} = \frac{2\varepsilon}{3m} .$$

The number density *n*:

$$n = \frac{N}{V} = \frac{1}{V}\int_0^{\varepsilon_F} D(\varepsilon)d\varepsilon = \frac{1}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\int_0^{\varepsilon_F}\sqrt{\varepsilon}d\varepsilon ,$$

or

$$n = \frac{1}{3\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\varepsilon_F^{\ 3/2},$$

$$\frac{D(\varepsilon_F)}{N} = \frac{3}{2\varepsilon_F} .$$

The conductivity can be obtained as

$$\begin{aligned}\sigma_{\alpha\beta} &= \frac{1}{V}e^2\tau(\varepsilon_F)\overline{v_\alpha v_\beta}^F D(\varepsilon_F)\\ &= \frac{1}{V}e^2\tau(\varepsilon_F)\frac{2\varepsilon_F}{3m}\delta_{\alpha\beta}\frac{3N}{2\varepsilon_F}\\ &= \frac{ne^2\tau(\varepsilon_F)}{m}\delta_{\alpha\beta}\end{aligned}$$

which agrees with the Drude formula for the electrical conductivity. The component of the electrical conductivity tensor is

$$\sigma_{\alpha\beta} = \frac{e^2}{V}\int \tau\overline{v_\alpha v_\beta}\left(-\frac{\partial f_0}{\partial\varepsilon}\right)D(\varepsilon)d\varepsilon,$$

where $D(\varepsilon)$ is the density of states, and $\overline{v_\alpha v_\beta}$ the average of $v_\alpha v_\beta$ taken over the energy surface ε. This formula is the same as that derived from the Kubo formula (as will be discussed later).

24. Kubo formula for the electrical conductivity (Kubo, 1957)

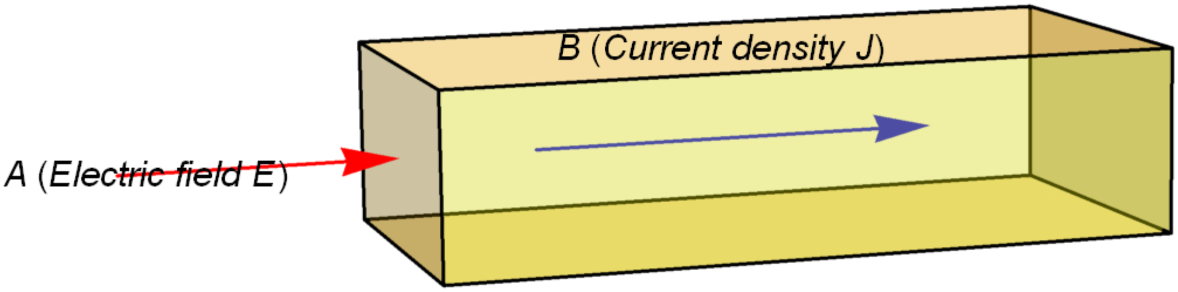


Fig.14 Kubo formula for the electrical conductivity. External field ***A*** (*E*) and response *B* (*J*).

In 1957, Ryogo Kubo (久保 亮五) discussed how the linear response to a small perturbation of a system in equilibrium can be expressed in terms of the fluctuations of dynamic variables of the unperturbed system. His linear response theory, which extended and unified work on the statistical description of transport properties, has since become an important tool in fields such as condensed matter physics.

The fundamental concept of the electrical conductivity is to observe a current density ***J***, when an external field ***E*** (electric field) is applied to the system. The state of the system is deviated from the thermal equilibrium state in the presence of this electric field. Thus, it enters into the non-equilibrium state. Theoretically it is very difficult to treat directly such a non-equilibrium state. However, in the range of linear response where the electric field is linearly proportional to the response (the current density), *the deviation of the state of the system from thermal equilibrium is equivalent to the thermal fluctuation in the thermal equilibrium state*. Based on this concept, the Kubo formula is a general formula of the statistical mechanics where the exact physical quantity can be calculated from microscopic Hamiltonian.

We now consider the conduction electrons in metals in the presence of the electric field. The un-perturbed Hamiltonian is given by

$$H_0 = \frac{1}{2m}\sum_i \boldsymbol{p}_i^2,$$

where m is the mass of electron, and $\boldsymbol{p}_i$ is the momentum. The perturbation Hamiltonian is given by

$$H_{ext} = -q\sum_i \boldsymbol{r}_i \cdot \boldsymbol{E} \,,$$

where $q = -e$ (charge of electron) and the electric field is given by $\boldsymbol{E}$, and the μ-component of the vector $\boldsymbol{A}$ is defined by

$$A_\mu = q\sum_1 (\boldsymbol{r}_i)_\mu = q\sum_i x_{i\mu} \,,$$

with

$$x_{i\mu} = (\boldsymbol{r}_i)_\mu \,.$$

and $\boldsymbol{J}$ is the current density,

$$\boldsymbol{J} = \frac{1}{V}\frac{q}{m}\sum_i \boldsymbol{p}_i \,.$$

where V is the volume of the system. The Kubo formula for the electrical conductivity is derived as

$$J_\mu = \sigma_{\mu\nu} E_\nu$$

and

$$\sigma_{\mu\nu} = V\int_0^\infty dt \int_0^\beta d\lambda \left\langle J_\nu(-i\hbar\lambda) J_\mu(t) \right\rangle_{eq} \,, \qquad \text{(Kubo formula)}$$

where J_μ is the μ -component of current density (response), E_ν is the ν-component of electric field, and $\langle ... \rangle_{eq}$ is the average in the thermal equilibrium;

$$\beta = \frac{1}{k_B T} \,,$$

where k_B is the Boltzmann constant and T is the temperature. Note that $J(t)$ is the quantum mechanical operator of current of the current density in the Heisenberg picture.

$$J(t) = \exp(\frac{itH_0}{\hbar}) J \exp(-\frac{itH_0}{\hbar}).$$

When $[J, H_0] = 0$, the conductivity can be rewritten as

$$\sigma_{\mu\nu} = V\int_0^\infty dt \int_0^\beta d\lambda \langle J_\nu(0) J_\mu(t) \rangle_{eq} ,$$

or simply, for $\mu = \nu = x$, we have

$$\sigma_{xx} = V\int_0^\infty dt \int_0^\beta d\lambda \langle J_x(0) J_x(t) \rangle_{eq} .$$

(a) Application of the Kubo formula to the quantum case (Sommerfeld formula)

We consider the quantum case. The current density $J_x(0)$ is given by

$$J_x(0) = \frac{1}{V}\sum_{\boldsymbol{k}} \frac{q\hbar}{m} k_\mu a_{\boldsymbol{k}}^+ a_{\boldsymbol{k}} ,$$

For simplicity we assume that $J_x(t)$ has the exponential decay form as

$$J_x(t) = \frac{1}{V}\sum_{\boldsymbol{k}} e^{-t/\tau_k} \frac{q\hbar}{m} k_\mu a_{\boldsymbol{k}}^+ a_{\boldsymbol{k}} ,$$

where $a_{\boldsymbol{k}}^+$ and $a_{\boldsymbol{k}}$ are the creation and annihilation operators.

Now we calculate the conductivity using the Kubo formula;

$$\begin{aligned}\sigma_{xx} &= V\int_0^\infty dt \int_0^\beta d\lambda \left\langle \frac{1}{V}\sum_{\boldsymbol{k}'} \frac{q\hbar}{m} k_\nu^{'} a_{\boldsymbol{k}'}^+ a_{\boldsymbol{k}'} \sum_{\boldsymbol{k}} e^{-t/\tau_k} \frac{q\hbar}{m} k_\mu a_{\boldsymbol{k}}^+ a_{\boldsymbol{k}} \right\rangle_{eq} \\ &= \int_0^\infty dt \int_0^\beta d\lambda \left(\frac{q\hbar}{m}\right)^2 \sum_{\boldsymbol{k},\boldsymbol{k}'} e^{-t/\tau_k} k_\mu k_\nu^{'} \langle a_{\boldsymbol{k}'}^+ a_{\boldsymbol{k}'} a_{\boldsymbol{k}}^+ a_{\boldsymbol{k}} \rangle_{eq}\end{aligned} .$$

Here we use the Bloch-De Deminicis theorem for the expansion of $\langle a_{\boldsymbol{k}'}^+ a_{\boldsymbol{k}'} a_{\boldsymbol{k}}^+ a_{\boldsymbol{k}} \rangle_{eq}$ (**Kubo, Toda, and Hashitsume**, **1978**);

$$\begin{aligned}\left\langle a_{\boldsymbol{k}'}{}^{+} a_{\boldsymbol{k}'} a_{\boldsymbol{k}}{}^{+} a_{\boldsymbol{k}} \right\rangle_{eq} &= \left\langle a_{\boldsymbol{k}'}{}^{+} a_{\boldsymbol{k}} \right\rangle_{eq} \left\langle a_{\boldsymbol{k}'} a_{\boldsymbol{k}}{}^{+} \right\rangle_{eq} \\ &= \delta_{\boldsymbol{k}',\boldsymbol{k}} n_{\boldsymbol{k}} (1 - n_{\boldsymbol{k}})\end{aligned}$$

with

$$\left\langle a_{\boldsymbol{k}}{}^{+} a_{\boldsymbol{k}} \right\rangle_{eq} = n_{\boldsymbol{k}}\,, \qquad \left\langle a_{\boldsymbol{k}} a_{\boldsymbol{k}}{}^{+} \right\rangle_{eq} = 1 - n_{\boldsymbol{k}}$$

$$\left\langle a_{\boldsymbol{k}} a_{\boldsymbol{k}'} \right\rangle_{eq} = 0\,, \qquad \left\langle a_{\boldsymbol{k}}{}^{+} a_{\boldsymbol{k}'}{}^{+} \right\rangle_{eq} = 0$$

Note that $n_{\boldsymbol{k}}$ is the Fermi distribution function and is expressed by $f(\varepsilon)$,

$$n_{\boldsymbol{k}} = f(\varepsilon) = \frac{1}{e^{\beta(\varepsilon - \varepsilon_F)} + 1}\,,$$

$$n_{\boldsymbol{k}}(1 - n_{\boldsymbol{k}}) = f(\varepsilon)[1 - f(\varepsilon)] = \frac{e^{\beta(\varepsilon - \varepsilon_F)}}{[e^{\beta(\varepsilon - \varepsilon_F)} + 1]^2}\,,$$

and

$$\beta f(\varepsilon)[1 - f(\varepsilon)] = -\frac{\partial f}{\partial \varepsilon} \approx \delta(\varepsilon - \varepsilon_F)\,,$$

where ε_F is the Fermi energy and $\delta(\varepsilon - \varepsilon_F)$ is the Dirac-delta function. Using this, the conductivity can be rewritten as

$$\begin{aligned}
\sigma_{xx} &= \frac{e^2\hbar^2}{m^2V}\sum_{\boldsymbol{k}}\tau(\varepsilon)k_x^{\;2}\beta f(\varepsilon)[1-f(\varepsilon)] \\
&= \frac{e^2\hbar^2}{m^2V}\int_0^\infty d\varepsilon\tau(\varepsilon)D(\varepsilon)\frac{1}{3}\boldsymbol{k}^2\beta f(\varepsilon)[1-f(\varepsilon)] \\
&= \frac{e^2\hbar^2}{m^2V}\int_0^\infty d\varepsilon\tau(\varepsilon)D(\varepsilon)\frac{2m\varepsilon}{3\hbar^2}[-\frac{\partial f(\varepsilon)}{\partial\varepsilon}] \\
&= \frac{e^2\hbar^2}{m^2V}\int_0^\infty d\varepsilon\tau(\varepsilon)D(\varepsilon)\frac{2m\varepsilon}{3\hbar^2}\delta(\varepsilon-\varepsilon_F) \\
&= \frac{e^2\hbar^2}{m^2V}\frac{2m}{3\hbar^2}\varepsilon_F\tau(\varepsilon_F)D(\varepsilon_F) \\
&= \frac{2e^2}{3mV}\varepsilon_F\tau(\varepsilon_F)D(\varepsilon_F)
\end{aligned}$$

where $k_x^{\;2} \to \frac{1}{3}\boldsymbol{k}^2$. We note that $D(\varepsilon_F)$ is the density of states. For the above calculation we use the following relations;

$$\frac{\varepsilon_F D(\varepsilon_F)}{V} = a_0\varepsilon_F^{\;3/2}, \qquad n = \frac{2}{3}a_0\varepsilon_F^{\;3/2},$$

or

$$\frac{\varepsilon_F D(\varepsilon_F)}{V} = \frac{3n}{2},$$

with

$$a_0 = \frac{1}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}.$$

Finally, we get the expression of the conductivity as

$$\sigma_{qm} = \frac{2e^2}{3m}\tau(\varepsilon_F)\frac{\varepsilon_F D(\varepsilon_F)}{V} = \frac{ne^2}{m}\tau(\varepsilon_F) \qquad \text{(Sommerfeld, 1927)}$$

which agrees with the Sommerfeld result.

((**Hoddeson et. al. 1992**)): **Result of Fermi liquid theory**

One of the mysterious of the Fermi surface was the fact that states inside are fully occupied, whereas those outside are completely empty in the ground state. This puzzling property known as the sharpness of the Fermi surface. The scattering lifetimes of electrons at the Fermi surface grow longer as the temperature falls. Such a sharpness was eventually answered in 1951 by V. Weisskopf, who showed the increase in lifetimes of particles close to the Fermi surface was a consequence of the Pauli exclusion principle. Not until 1957 did Luttinger, Kohn, and Migdal more fully explain the sharpness of the Fermi surface within the context of Landau's Fermi liquid theory.

(b) Application of the Kubo formula to the classical case (Drude formula)

For convenience we assume that $J_x(t)$ is defined by the exponential decay form

$$J_x(t) = J_x(0)\exp(-\frac{t}{\tau})$$

Thus we get

$$\begin{aligned}\sigma &= V\int_0^\infty e^{-t/\tau}dt\int_0^\beta d\lambda\left\langle J_x^2\right\rangle_{eq} \\ &= V\beta\tau\left\langle J_x^2\right\rangle_{eq}\end{aligned}$$

We note that

$$J_x = \frac{1}{V}\sum_i qv_{ix},$$

and

$$\begin{aligned}\left\langle J_x^2\right\rangle &= \frac{1}{V^2} < \sum_i qv_{ix}\sum_j qv_{jx} >_{eq} \\ &= \frac{q^2}{V^2}\sum_i\left\langle v_{ix}^2\right\rangle_{eq} \\ &= \frac{q^2}{V^2}\sum_i\frac{1}{3}\left\langle \boldsymbol{v}_i^2\right\rangle_{eq} \\ &= \frac{q^2N}{3V^2}\left\langle \boldsymbol{v}^2\right\rangle_{eq}\end{aligned}$$

Since the root-mean square velocity v_{rms} is defined as

$$\frac{m}{2}\left\langle \boldsymbol{v}^2\right\rangle_{eq} = \frac{3}{2}k_BT = \frac{3}{2\beta},$$

with $v_{rms} = \sqrt{\left\langle \boldsymbol{v}^2 \right\rangle_{eq}}$, we get

$$\left\langle J_x^{\,2} \right\rangle = \frac{q^2 N}{3V^2} \frac{3}{m\beta} = \frac{q^2 n}{mV\beta},$$

and

$$\sigma_{cl} = V\beta\tau \left\langle J_x^{\,2} \right\rangle_{eq} = V\beta\tau \frac{q^2 n}{mV\beta} = \frac{nq^2\tau}{m} \qquad \text{(Drude, 1900)}$$

which agrees with the Drude formula.

25. CONCLUSION

Drude's work was done well before the appearance of quantum mechanics, so there was no way for Drude to calculate the Fermi velocity or the mean free path. Why then was Drude's model immediately successful? It was because Drude's calculations contained two large mistakes that cancelled out! From the known values of the conductivity of metals. Drude used his formula

$$\sigma_{cl} = \frac{ne^2\tau}{m},$$

to correctly compute the collision time τ. He also computed the collision time using $\tau = \Lambda / v$, where Λ is the mean free path and v is the mean electron velocity. But his values for l and τ were both too small by an order of magnitude. He assumed, incorrectly that the electrons scattered from individual ions, so his estimate of the mean free path Λ was a few nanometers – smaller by a factor of at least 10 than the correct value for metals at room temperature. He also incorrectly that the velocity of the electrons is given by the thermal velocity of about 10^5 m/s, which is about 10 times smaller than the correct Fermi velocity. Because both numbers were wrong by about the same factor, the ratio, τ, was correctly evaluated. Consequently, the model appeared to be nicely self-consistent and it was immediately accepted by physicists. More than 30 years passed before enough quantum mechanics was known for the correct picture to emerge. Today we remember Drude because his simple but wrong model leads to the correct formula $\sigma = ne^2\tau / m$

Finally, we discuss the physics on the electrical resistivity of metals. In the general physics, it is based on the Drude theory where the electrons in metals are discussed in terms of a classical gas model. First, we consider an electron of mass m and the relaxation time τ,

$$m\left(\frac{dv}{dt} + \frac{v}{\tau}\right) = qE$$

where m is the mass and q is the charge of electrons. When $E = 0$ is at $t = 0$, the solution of this differential equation is

$$v = v(0)\exp(-\frac{t}{\tau}) .$$

The velocity exponentially decays to zero with the relaxation time τ. Next we consider the case when the electric field E is turned on at $t = 0$. In the steady state ($dv/dt = 0$) in the limit of $t \to \infty$, the terminal velocity (or drift velocity) is obtained as

$$v_d = \frac{qE}{m}\tau .$$

This drift velocity is proportional to E and τ. We note that the relaxation time is the same as that of the terminal velocity.

(a) Shift of the wave number due to the electric field

$$\hbar\frac{d\boldsymbol{k}}{dt} = q\boldsymbol{E} \qquad \Delta\boldsymbol{k} = \frac{q}{\hbar}\boldsymbol{E}\tau \qquad \text{(the change of wave number vector)}$$

$$\Delta\varepsilon = \hbar\boldsymbol{v}\cdot\Delta\boldsymbol{k} = q\tau(\boldsymbol{v}\cdot\boldsymbol{E}) \qquad \text{(the change of energy)}$$

When $v = v_F$ (the Fermi velocity),

$$\Delta\varepsilon \approx qv_F\tau E = q\Lambda(\varepsilon_F)E$$

(b) Fermi-Dirac statistics

What happens to the conduction of electrons in metals? Electrons are fermions, obey the Fermi-Dirac statistics. We consider the Fermi sphere
In the ***k***-space, all the electrons are occupied below the Fermi momentum. These electrons do not contribute to the conduction of electrons in the presence of electric field.

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APPENDIX-I Definitions

		SI units
$\hbar$	Dirac constant ($=\dfrac{h}{2\pi}$)	(J s)
h	Planck constant	(J s)
k_B	Boltzmann constant	(J/K)
c	Velocity of light	(m/s)
$q=-e$	Charge of electron; e>0	(C)
p	Momentum ($p=mv$)	
k	Wave number ($k=p/\hbar$)	
m	Mass of electron	(kg)
ε	Energy of electron	(J)

N	Total number of particles	
V	Volume of the system	(m^3)
T	Temperature	(K)
β	$\beta = \dfrac{1}{k_B T}$	(1/J)
$\boldsymbol{v}$	Velocity	(m/s)
v_{rms}	Root-mean square velocity	(m/s)
$\boldsymbol{J} = nq\boldsymbol{v} = \dfrac{1}{V} Nq\boldsymbol{v}$	Current density	(A/m^2)
n	Number density	(m^{-3})
Λ	Mean-free path	(m)
τ	Relaxation time	(s)
L_0	Size of the system (side of cubic system)	(m)
R	Resistance	(Ω)
ρ	Resistivity	(Ω m)
σ	Conductivity	$[(\Omega m)^{-1}]$
ρ_c	Charge density	(C/m^3)

$\boldsymbol{F} = q\boldsymbol{E} = -\nabla \tilde{V} = -\nabla(q\phi)$,

Force on charge q due to the applied electric field

$\tilde{V}$: Potential energy; $\tilde{V} = -q\boldsymbol{E} \cdot \boldsymbol{r}$

ϕ: Electric potential ($\tilde{V} = q\phi$)

$\boldsymbol{E}$: Electric field

APPENDIX-II Units of physical quantities in the cgs units

Conductivity	σ	1/s	$(\Omega\mathrm{m})^{-1}$
Resistivity	ρ	s	Ωm

1s (cgs) = 8.98756 × 10^9 Ωm (SI).

APPENDIX-III Ground state of hydrogen atom (for comparison)

In order to understand the magnitudes of the Fermi velocity and the relaxation times for Cu, for comparison, here we put the information on the velocity and period t_{orbit} of electron in the ground state (the inner most orbit) of hydrogen. The velocity v is given by

$$v_1 = \frac{e^2}{\hbar} = \frac{e^2}{\hbar c} c = \alpha c = 2.18769 \times 10^6 \text{ m/s}$$

with α is the fine structure constant. The Bohr radius r_B is

$$r_B = \frac{\hbar^2}{me^2} = 0.529177 \text{ Å}$$

with

$$\frac{1}{\alpha} = 137.035999084 .$$

The period t_{orbit} is

$$t_{orbit} = \frac{2\pi r_B}{v_1} = 2\pi \frac{\hbar^3}{me^4} = 1.51983 \times 10^{-16} \text{ s}$$

The energy of the ground state:

$$\varepsilon_0 = -\frac{me^4}{2\hbar^2} = -13.6057 \text{ eV}$$