

**Chapter 26**  
**Current and resistance**  
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**1. Current and current density**

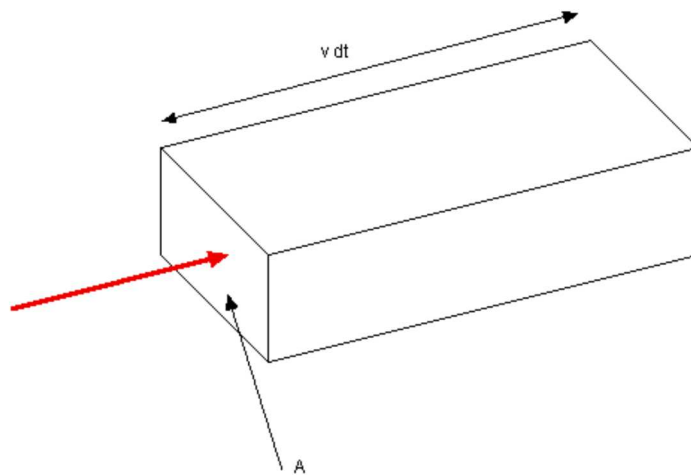
If charge  $dQ$  passes a point in space in time  $dt$ , we define the current at the point as

$$I = \frac{dQ}{dt} \quad [\text{C/s}]$$

Current is measured in A (ampere).

$$1 \text{ A} = 1 \text{ C/s}$$

The direction of current is positive in the direction of motion of positive charges.



There are  $n$  particles per  $\text{m}^3$ , on the average, all moving with the same velocity  $v$  and carrying the same charge  $q$ .

Imagine a small frame of area  $A$  fixed. a time  $\Delta t$ ? The amount of charge passing the frame in a time  $\Delta t$ , is  $\Delta Q = nq(Av\Delta t)$ . So the current  $I$  is

$$I = \frac{\Delta Q}{\Delta t} = nqvA$$

Here we define the current density  $J$  as

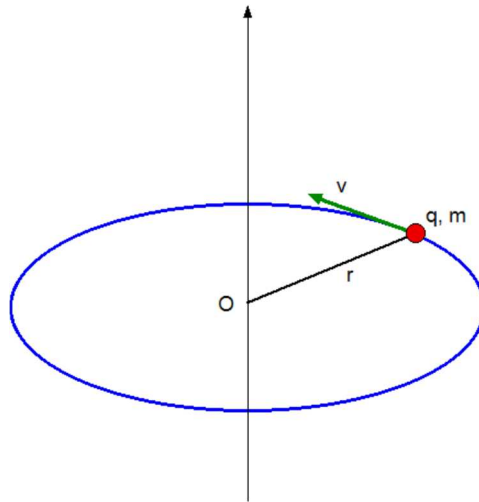
$$J = \frac{I}{A} = nqv = \rho v \quad [\text{A/m}^2]$$

where the charge density  $\rho$  is defined as

$$\rho = nq \quad [\text{C/m}^3]$$

**((Note)) Current due to the orbital motion of particle (charge  $q$ )**

Suppose that one particle (charge  $q$  and mass  $m$ ) rotates with the velocity  $v$  around a circle (radius  $r$ ).



The current  $I$  is given by

$$I = qf = \frac{q}{T}$$

where  $T$  is the period and  $f(=1/T)$  is the frequency. The number of rotation around the orbit is  $1/T$  per unit time (sec). Since  $T = 2\pi/v$ , the current  $I$  is rewritten as

$$I = \frac{qv}{2\pi r}$$

We now calculate the value of the magnetic moment defined by

$$\mu = IA = \frac{qv}{2\pi r} \pi r^2 = \frac{qvr}{2}$$

where  $A$  is the area of the orbit (see Chapter 29). The angular momentum  $L$  is given by

$$L = mvr$$

Then the ratio of the magnetic moment to the angular momentum is

$$\frac{\mu}{L} = \frac{q}{2m} = \text{constant}$$

## 2. Resistivity and conductivity

### 2.1 Definition

The current density  $J$  is proportional to the applied electric field  $E$ ,

$$J = \sigma E$$

where  $\sigma$  is the conductivity. Note that  $J = I/A$ . Assuming that the electric field is constant in the system (conductor), the potential difference over length  $l$  is given by

$$V = El.$$

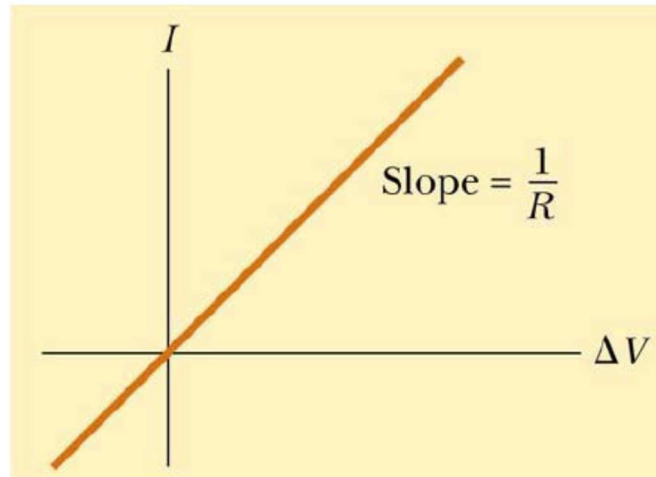
Then we have

$$J = \frac{I}{A} = \sigma \frac{V}{l}$$

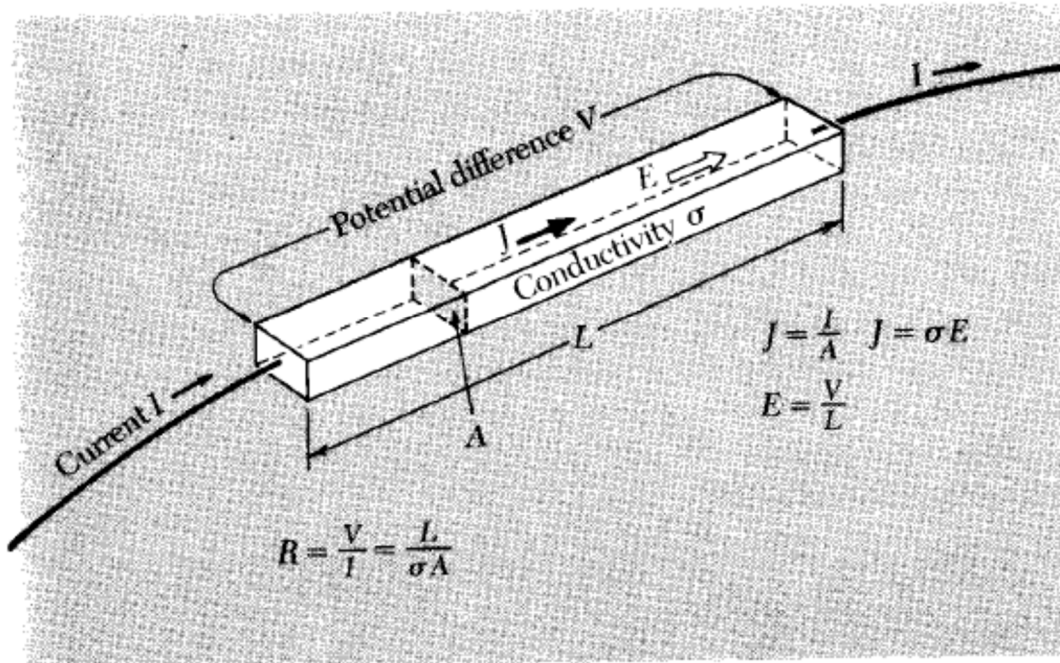
According to the Ohm's law, the resistance  $R$  is defined by

$$R = \frac{V}{I} = \frac{1}{\sigma} \frac{l}{A} = \rho \frac{l}{A} \quad [\Omega, \text{Ohm}].$$

where the resistivity  $\rho = 1/\sigma$  [ $\Omega\text{m}$ ].

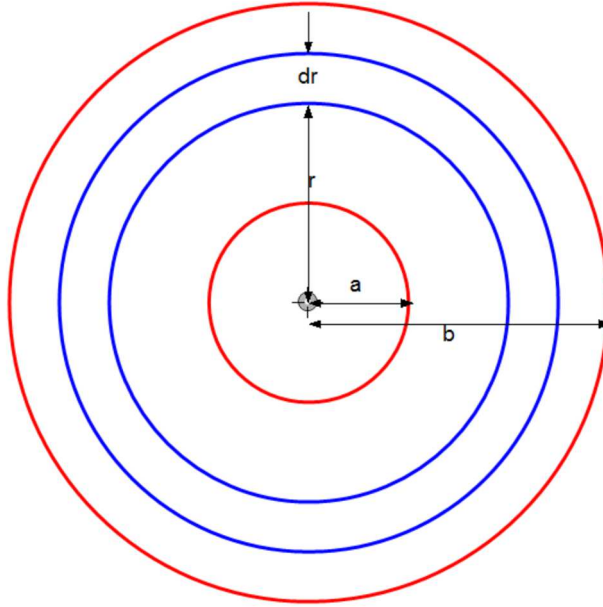


George Simon Ohm (1787 – 1854).



## 2.2 Resistance of metal ring

We consider a metal ring of resistivity  $\rho$  whose inner radius is  $a$ , whose outer radius is  $b$ , and whose length is  $h$ .



To find the electric field in the ring, we note that from the *symmetry*, the current density  $\mathbf{J}$  has a radial component only. Since

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

the electric field  $\mathbf{E}$  is also radial. Then the current density  $J_r$  at the radius  $r$  is

$$J_r = \frac{I}{2\pi r h} = \sigma E_r .$$

The electric field  $E_r$  at the radius  $r$  is

$$E_r = \frac{I}{2\pi r \sigma h} = -\frac{dV}{dr}$$

where  $V$  is the electric potential.

$$V_b - V_a = -\int_a^b \frac{I}{2\pi r \sigma h} dr = \frac{I}{2\pi \sigma h} \ln\left(\frac{b}{a}\right)$$

The resistance  $R$  is

$$R = \frac{V_a - V_b}{I} = \frac{\Delta V}{I} = \frac{1}{2\pi \sigma h} \ln\left(\frac{b}{a}\right) = \frac{\rho}{2\pi h} \ln\left(\frac{b}{a}\right)$$

**((Note)) Another method**

From the definition of the resistance,  $R$  can be also calculated as follows. The resistance  $dR$  between radius  $r$  and  $r + dr$  is given by

$$dR = \rho \frac{dr}{2\pi r h}$$

Then we have

$$R = \int_a^b dR = \frac{\rho}{2\pi h} \int_a^b \frac{dr}{r} = \frac{\rho}{2\pi h} \ln\left(\frac{b}{a}\right)$$

### 2.3 Resistance of metal spherical shell

From the *symmetry*, the current density  $\mathbf{J}$  has a radial component.

$$J_r = \frac{I}{4\pi r^2} = \sigma E_r$$

Then the electric field  $E_r$  at the radius  $r$  is

$$E_r = \frac{I}{4\pi\sigma r^2} = -\frac{dV}{dr}$$

where  $V$  is a electric potential.

$$V_b - V_a = -\int_a^b \frac{I}{4\pi\sigma r^2} dr = -\frac{I}{4\pi\sigma} \left(\frac{1}{a} - \frac{1}{b}\right) = -\frac{I}{4\pi\sigma} \left(\frac{b-a}{ab}\right)$$

The resistance  $R$  is

$$R = \frac{V_a - V_b}{I} = \frac{\Delta V}{I} = \frac{1}{4\pi\sigma} \left(\frac{b-a}{ab}\right) = \frac{\rho}{4\pi} \left(\frac{b-a}{ab}\right)$$

#### ((Note)) Another method

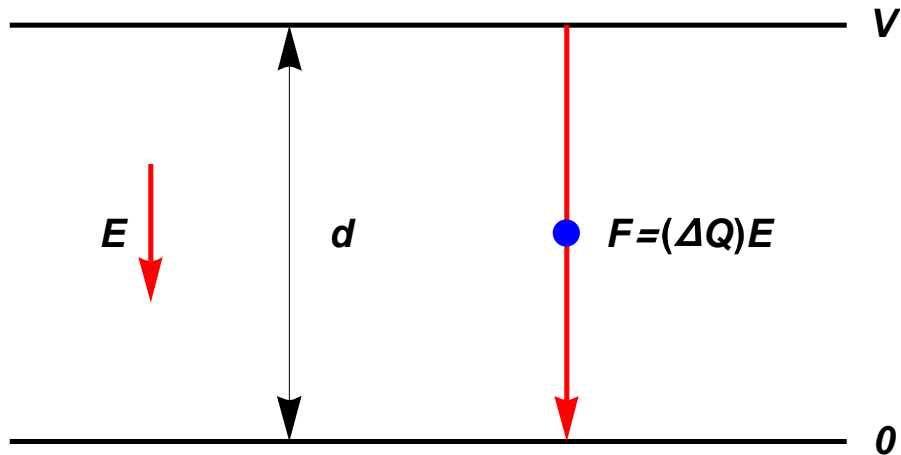
We consider a metal spherical shell of resistivity  $\rho$  whose inner radius  $a$ , whose outer radius is  $b$ . The resistance  $dR$  between radius  $r$  and  $r + dr$  is given by

$$dR = \rho \frac{dr}{4\pi r^2}$$

Then we have

$$R = \int_a^b dR = \rho \int_a^b \frac{dr}{4\pi r^2} = \frac{\rho}{4\pi} \left(\frac{b-a}{ab}\right)$$

### 3. Electric power and Joule heating



Suppose that the potential difference  $V$  set up by the battery is maintained, a steady current  $I$  is produced in the circuit. The amount of charge  $dQ$  moving through the voltage difference  $V$  leads to the the work done on the system

$$\Delta W = Fd = [(\Delta Q)E]d = (\Delta Q)V = -\Delta U$$

Thus the potential energy  $\Delta U$  is

$$\Delta U = -VdQ$$

which is negative. So the dissipated power is obtained as

$$P = -\frac{dU}{dt} = V \frac{dQ}{dt} = IV \quad [\text{W}]$$

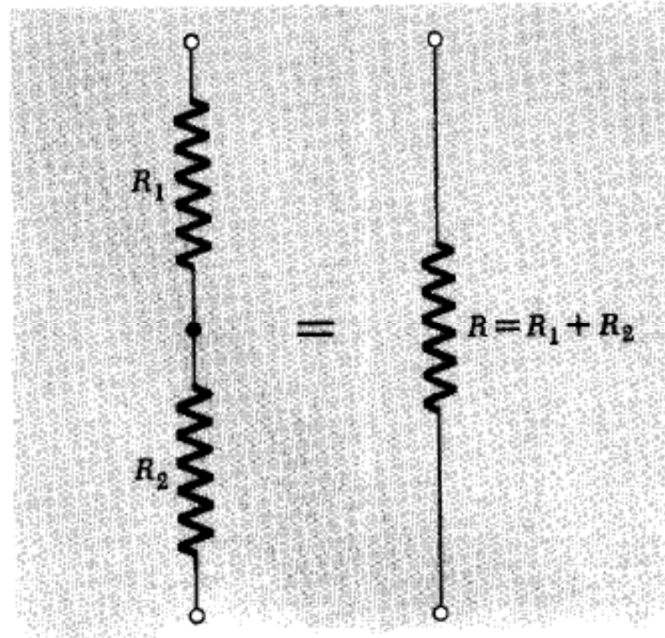
When  $V = IR$  (Ohm's law), the resistive dissipation is

$$P = I^2 R = \frac{V^2}{R}$$

through the resistance  $R$ .

### 4. Resistances in combination

#### 4.1 Series connection



$$V = V_1 + V_2$$

with

$$V_1 = R_1 I$$

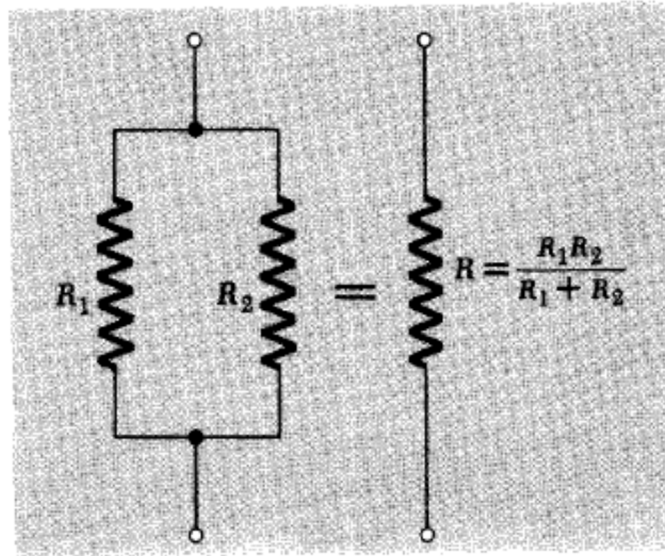
$$V_2 = R_2 I$$

Then we have

$$\frac{V}{I} = R = R_1 + R_2$$

## 4.2 Parallel connection





$$V = R_1 I_1 = R_2 I_2$$

$$I = I_1 + I_2 = \frac{V}{R_1} + \frac{V}{R_2} = \left(\frac{1}{R_1} + \frac{1}{R_2}\right)V$$

Then the resulting resistance  $R$  is such that

$$\frac{1}{R} = \frac{1}{R_1} + \frac{1}{R_2}, \quad \text{or} \quad R = \frac{R_1 R_2}{R_1 + R_2}$$

#### 4. Temperature dependence of resistivity

##### 4.1 Resistivity of metal at high temperatures

Since the electrical resistivity of a conductor such as a Cu wire is dependent upon collisional processes within the wire, the resistivity could be expected to increase with temperature since there will be more collisions. An intuitive approach to temperature dependence leads one to expect a fractional change in resistivity which is proportional to the temperature change:

$$\frac{\Delta\rho}{\rho_0} = \alpha\Delta T$$

or

$$\frac{\rho - \rho_0}{\rho_0} = \alpha(T - T_0)$$

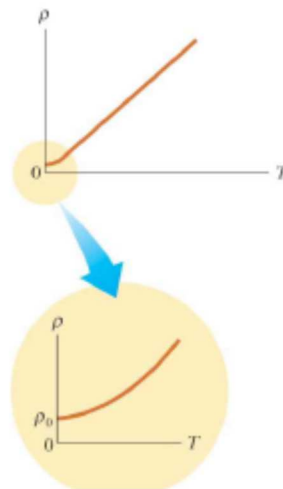
where  $T_0$  is a selected reference temperature,  $\rho_0$  is the resistivity at that temperature, and  $\alpha$  is called the temperature coefficient of resistivity. At  $T_0 = 293 \text{ K}$ ,  $\rho_0 = 1.69 \times 10^{-8} \text{ }\Omega\text{m}$  for Cu.

Since the resistance of a conductor with uniform cross sectional area is proportional to the resistivity, one can find the effect of temperature on resistance.

$$\frac{R - R_0}{R_0} = \alpha(T - T_0)$$

#### 4.2 Resistivity of metal at low temperatures

For metals, the resistivity is nearly proportional to the temperature. A nonlinear region always exists at very low temperatures. The resistivity usually reaches some finite value as the temperature approaches absolute zero



#### ((Matthiessen's rule))

The net resistivity is given by a sum of  $\rho_L$  and  $\rho_i$

$$\rho = \rho_L + \rho_i$$

where  $\rho_L$  and  $\rho_i$  are the resistivities due to the scattering of conduction electrons by phonon (lattice vibration) and by imperfections, respectively.

#### ((Residual resistivity $\rho_i$ ))

The residual resistivity near absolute zero is caused primarily by the collisions of electrons with impurities and imperfections in the metal.

### 5. Classical theory (Drude theory)



Paul Karl Ludwig Drude (July 12, 1863 – July 5, 1906)

A theory of metallic conductivity based on average velocities was developed by Drude in 1900. Lorentz in 1905 reinvestigated the problem, using Boltzmann transport equation and a simplified model of the collisions between the electrons and atoms in the lattice.

We consider a particle (mass  $m$  and charge  $q$ ) in the presence of a uniform electric field. The motion of the particle is described by

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

where  $\tau$  is the relaxation time of the particle. At  $t = \infty$ , the velocity (the drift velocity, the terminal velocity) becomes constant (steady state),

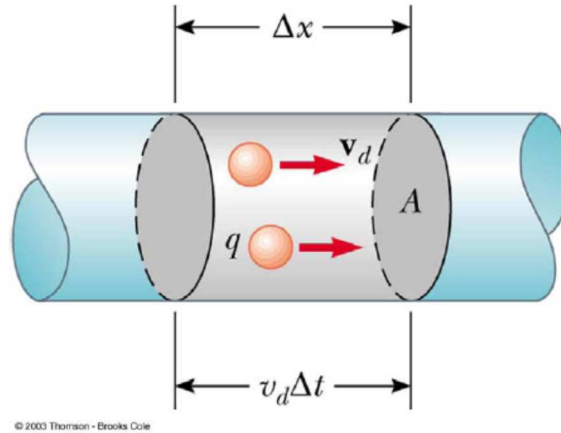
$$v_d = \frac{qE\tau}{m}$$

Then the current density is

$$J = nqv_d = nq\left(\frac{qE\tau}{m}\right) = \frac{nq^2\tau}{m} E$$

This drift velocity is different from the Fermi velocity. The conductivity is obtained as

$$\sigma = \frac{nq^2\tau}{m} \quad (\text{Drude formula})$$



## 6. Classical picture and quantum mechanical picture for the conduction

### 6.1 Quantum mechanical picture (Sommerfeld)

In 1928, Sommerfeld recalculated the conductivities along the lines of Lorentz's theory, but replacing classical statistics by Fermi-Dirac statistics. The Pauli exclusion principle prevents more than two electrons from being present in the lowest energy level. There are two electrons (spins up and down) in each energy level. The kinetic energy of the electrons in that last filled level is called the Fermi energy. The electrons are required to have this value of energy in order to "jump up" to the next, empty energy level. At finite temperatures some electrons will gain energy and move to higher states because of thermal energy, leading to the conduction. In the theory of Sommerfeld, the electrical conductivity is given by

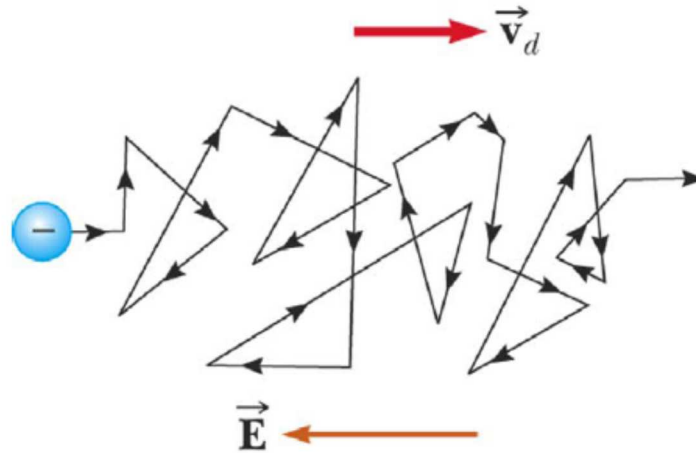
$$\sigma = \frac{ne^2}{m} \tau_F$$

where  $n$  is the number of conduction electrons, and  $\tau_F$  is the relaxation time of electrons having the Fermi energy.

The high conductivity of metals is to be ascribed to the Fermi velocity  $v_F$  at the top of the Fermi distribution, rather than a high density of free electrons, which can be set slowly drifting. The Fermi velocity  $v_F$  is related to the Fermi energy  $E_F$  by

$$E_F = \frac{1}{2} m v_F^2$$

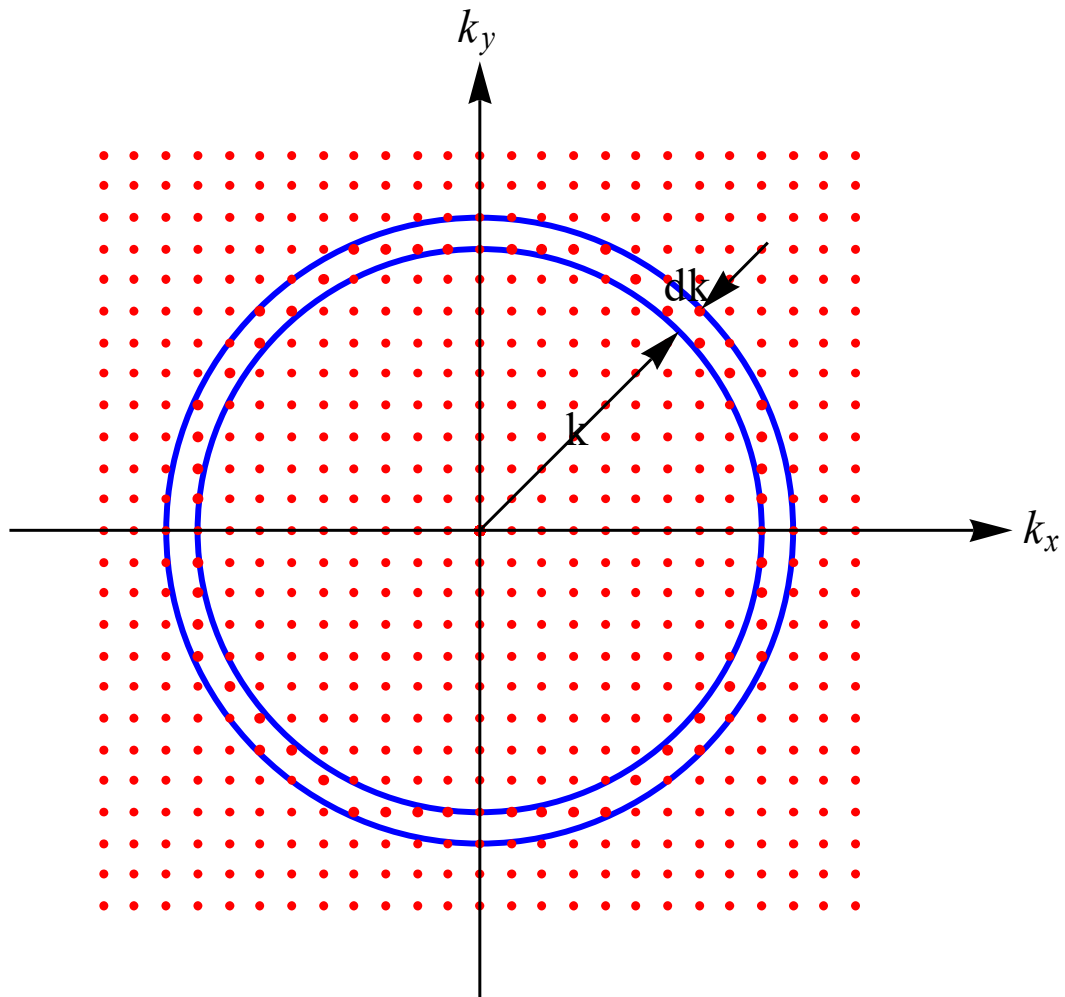
### 6.2 Drift velocity and Fermi velocity



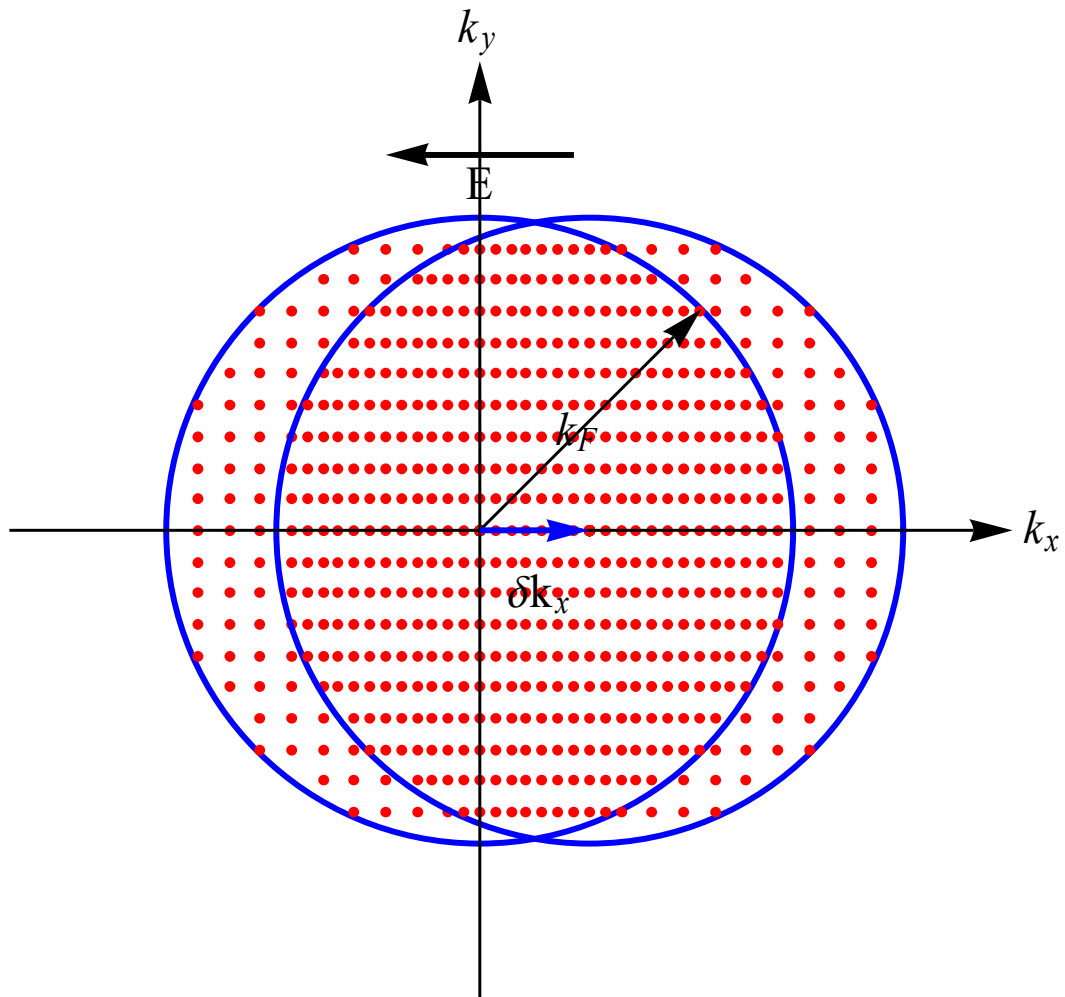
**Fig.** The zig-zag black line represents the motion of charge carrier in a conductor. The net drift speed is small. The sharp changes in direction are due to collisions. The net motion of electrons is opposite the direction of the electric field.

For ordinary currents, the drift velocity  $v_d$  is on the order of mm/s in contrast to the Fermi velocity  $v_F$  of the electrons themselves which are on the order of  $10^6$  m/s.

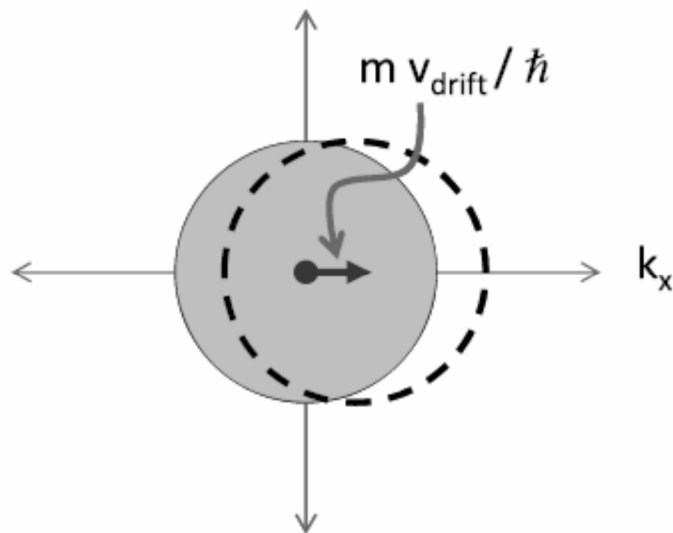
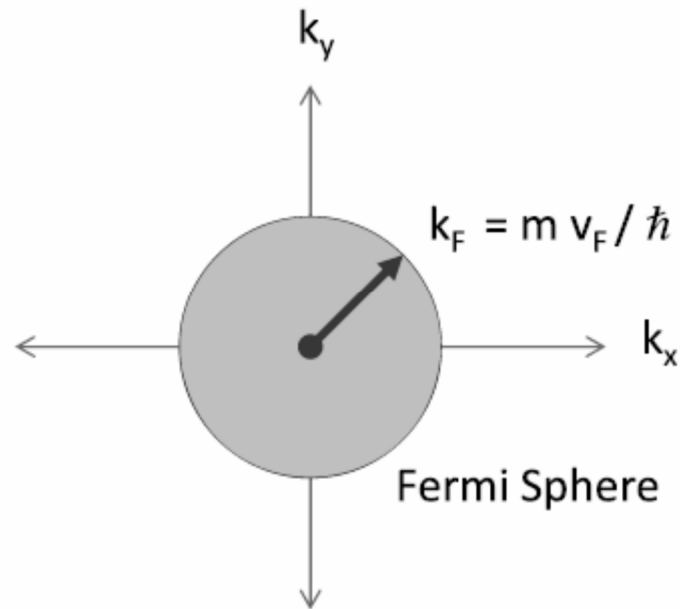
The drift velocity is the average velocity that an electron attains due to an electric field. In general, an electron will rattle around in a conductor at the Fermi velocity randomly. An applied electric field will give this random motion a small net velocity in one direction



**Fig.** Fermi sphere with radius  $k_F$ .

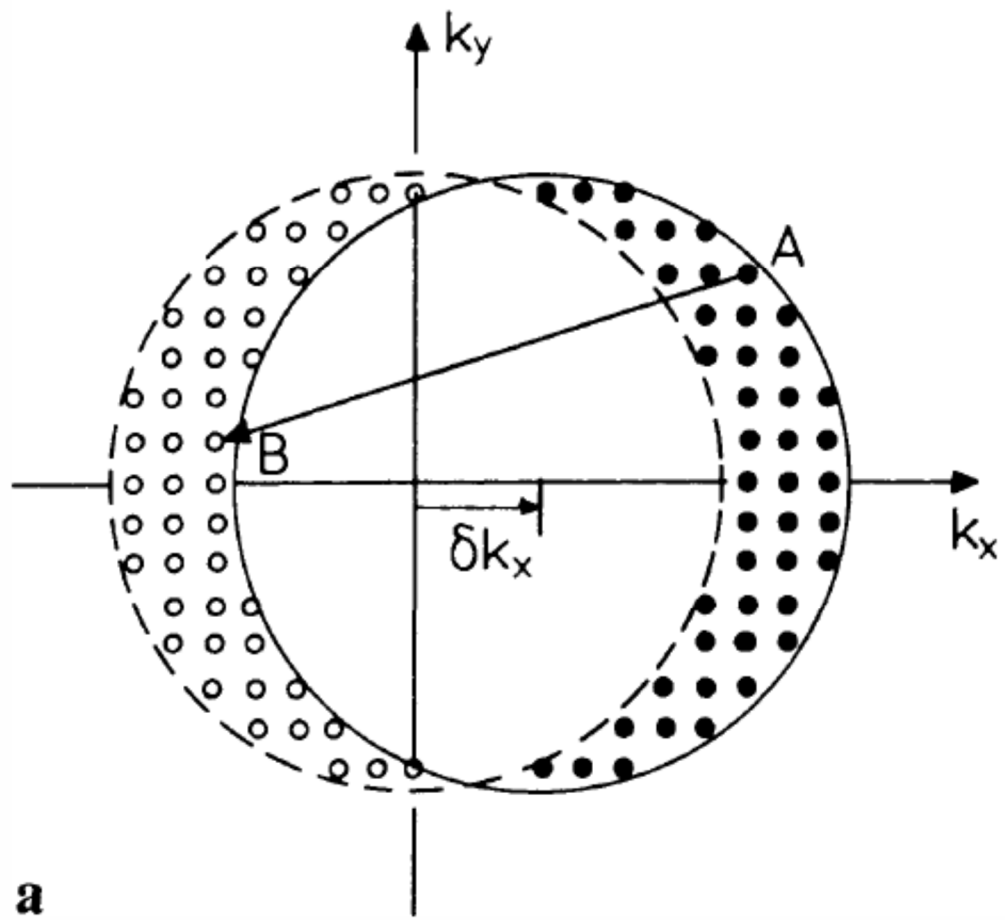


**Fig.** The shift of the Fermi sphere in the presence of an electric field along the negative  $x$  direction.

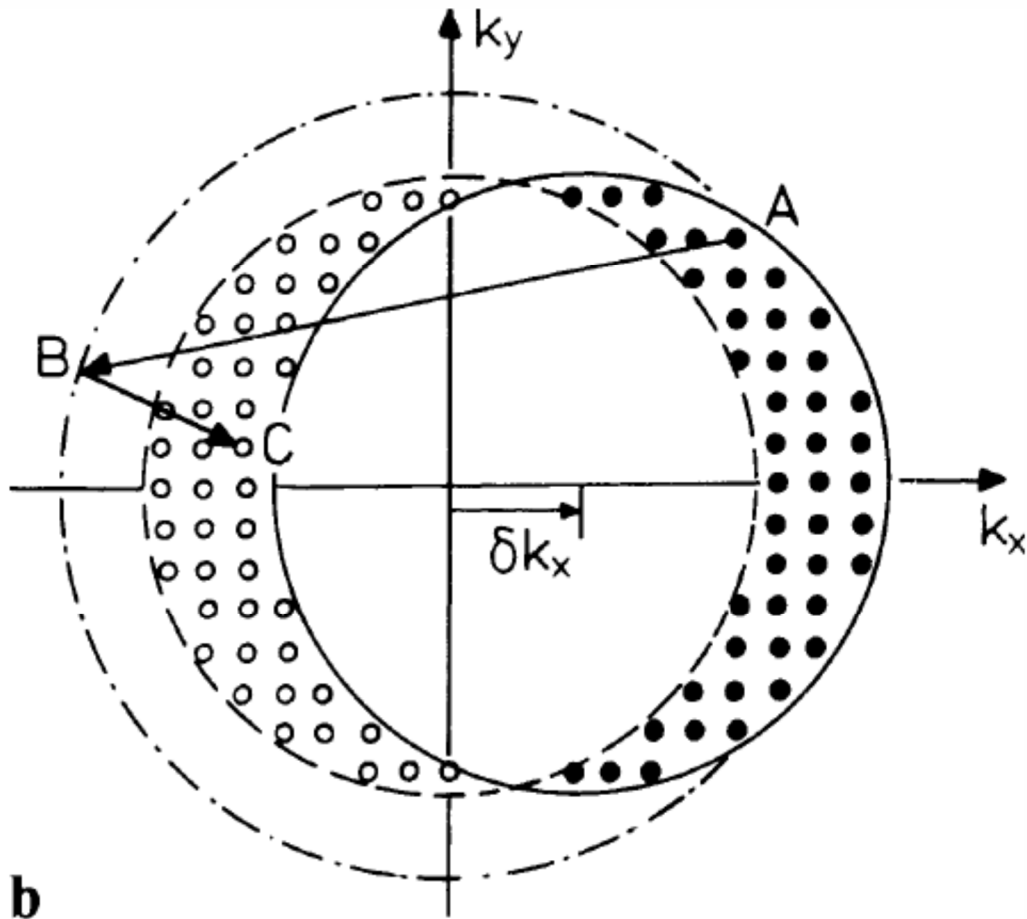


**Fig.** Drift velocity and Fermi velocity. The drift wavevector is the displacement of the entire Fermi sphere (which is generally very very small), whereas the Fermi wavevector is the radius of the Fermi sphere, which can be very large. Drude theory makes sense if one thinks of it as a transport equation for the center of mass of the entire Fermi sphere. i.e., it describes the drift velocity. Scattering of electrons only occurs between the thin crescent that are the difference between the shifted and unshifted Fermi spheres.





**a**



**Fig.** Electron scattering processes in  $k$ -space. The dashed circle represents the Fermi surface in thermodynamic equilibrium ( $E_x = 0$ ). Under the influence of an electric field  $E_x$  and for a constant current, the Fermi surface is displaced as shown by the full circle. (a) When the electric field is switched off, the displaced Fermi surface relaxes back to the equilibrium distribution by means of electron scattering from occupied states ( $\bullet$ ) to unoccupied states ( $\circ$ ). Since the states  $A$  and  $B$  are at different distances from the  $k$ -space origin (i.e., have different energies), the relaxation back to equilibrium must involve inelastic scattering events (e.g., phonon scattering). (b) For purely elastic scattering (from states  $A$  to  $B$ ), the Fermi sphere would simply expand. When the field is switched off, equilibrium can only be achieved by inelastic scattering into states  $C$  within the dashed (equilibrium) Fermi sphere. (H. Ibach and H. Luth, *Solid-State Physics*, 4-th edition (Springer, 2009)).

### 6.3 Evaluation of drift velocity:

The 12-gauge copper wire in a typical residential building has a cross-sectional area of  $A=3.31 \times 10^{-6} \text{ m}^2$ . It carries a constant current of  $I = 10.0 \text{ A}$ . We find the drift velocity of the electrons in the wire. Assume each copper atom contributes one free electron to the current. The density of copper is  $\rho = 8.92 \times 10^3 \text{ kg/m}^3$ . The drift velocity is given by

$$J = \frac{I}{A} = nqv_d$$

or

$$v_d = \frac{I}{nqA}$$

The number density is

$$n = \frac{N_A}{V} = \frac{N_A}{M} \frac{M}{V} = \frac{N_A \rho}{M}$$

where  $V$  is the volume,  $M$  is the molar mass, and  $N_A$  is the Avogadro number. For Cu (monovalent), we have

$$M = 63.5 \times 10^{-3} \text{ kg/mol}, \quad \rho = 8920 \text{ kg/m}^3$$

$$N_A = 6.023 \times 10^{23}$$

Using these values, we have the number density

$$n = 8.461 \times 10^{28} / \text{m}^3$$

Thus the drift velocity is

$$v_d = \frac{I}{nqA}$$

$$= \frac{10.0}{(1.60 \times 10^{-19})(8.461 \times 10^{28})(3.31 \times 10^{-6})}$$

$$= 2.23 \times 10^{-4} \text{ m/s}$$

This velocity is much lower than the Fermi velocity.

**((Note))**

For Cu (fcc), there are 4 Cu atoms per conventional SC unit cell with a lattice constant  $a$ ;  $a = 3.61 \text{ \AA}$ . Each Cu atom has one conduction electron. Thus the number density is

$$n = \frac{4}{a^3} = n = 8.50 \times 10^{22} / \text{cm}^3 = 8.50 \times 10^{28} / \text{m}^3.$$

#### 6.4 Evaluation of thermal velocity of electrons

We note that the drift velocity is amazingly smaller than the root-mean square velocity  $v_{\text{rms}}$  for the conduction electron. The root-mean square velocity of conduction electron can be evaluated as

$$v_{\text{rms}} = \sqrt{\frac{3k_B T}{m}} = 1.168 \times 10^5 \text{ m/s} = 116.8 \text{ km/s}$$

at  $T = 300 \text{ K}$ , from the relation

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

#### 5.5. Relaxation time of conduction electrons in Cu

In quantum mechanics (solid state physics), the conductivity is obtained as

$$\sigma = \frac{ne^2 \tau(E_F)}{m^*}$$

This relation is formally equivalent to that of the Drude model. The relaxation time, is that of electrons at the Fermi level. The effective mass  $m^*$  replaces the free electron mass  $m$ .

Here we estimate the relaxation time  $\tau$  from the above relation. For example, we consider Cu at 300 K.

$$\begin{aligned} \rho &= 1.7 \mu\Omega \text{cm} = 1.7 \times 10^{-8} \Omega \text{m} \\ \sigma &= 5.9 \times 10^5 (\Omega \text{cm})^{-1} = 5.9 \times 10^7 (\Omega \text{m})^{-1} \end{aligned}$$

What is the order of the relaxation time  $\tau$ ?

The density of Cu is given by

$$\rho_{\text{Cu}} = 8.94 \times 10^3 \text{ kg/m}^3.$$

The molar mass of Cu is given by

$$M_{\text{Cu}} = 63.546 \text{ g} = 63.546 \times 10^{-3} \text{ kg/Cu mol}$$

The number of Cu atoms/ $\text{m}^3$  is given by

$$\frac{\rho_{Cu}}{M_{Cu}} N_A$$

where  $N_A$  is the Avogadro number. We assume that each Cu atom contributes to one conduction electron (mass  $m$  and charge  $q = -e$ ). Then the number density  $n$  is obtained as

$$n_{Cu} = \frac{\rho_{Cu}}{M_{Cu}} N_A \times 1 = 8.472 \times 10^{28} / \text{m}^3$$

The relation time  $\tau_{Cu}$  is estimated as

$$\tau_{Cu} = \frac{m \sigma_{Cu}}{n_{Cu} e^2} = 2.5 \times 10^{-14} \text{ s}$$

((Mathematica))

$$\text{Physconst} = \{ \text{NA} \rightarrow 6.02214179 \times 10^{23}, \text{me} \rightarrow 9.1093821545 \times 10^{-31}, \\ \text{qe} \rightarrow 1.602176487 \times 10^{-19} \};$$

$$\text{rule1} = \{ \rho_{Cu} \rightarrow 8.94 \times 10^3, M_{Cu} \rightarrow 63.546 \times 10^{-3}, \sigma_{Cu} \rightarrow 5.9 \times 10^7 \}$$

$$\{ \rho_{Cu} \rightarrow 8940., M_{Cu} \rightarrow 0.063546, \sigma_{Cu} \rightarrow 5.9 \times 10^7 \}$$

$$n_{Cu} = \frac{\rho_{Cu} \text{NA}}{M_{Cu}} /. \text{Physconst} /. \text{rule1}$$

$$8.47228 \times 10^{28}$$

$$\tau_{Cu} = \frac{\text{me} \sigma_{Cu}}{n_{Cu} \text{qe}^2} /. \text{Physconst} /. \text{rule1}$$

$$2.47127 \times 10^{-14}$$

## 6.5 Mean free path

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

$$l = v_F \tau$$

where  $v_F$  is the Fermi velocity;  $v_F = 1.57 \times 10^6$  m/s. Thus the mean free path is given by

$$l(4 \text{ K}) = 3 \times 10^{-3} \text{ m} = 3 \text{ mm}$$

$$l(300 \text{ K}) = 3 \times 10^{-8} \text{ m} = 300 \text{ \AA}.$$

Note that the mean free path is the average distance an electron travels between collisions.

## 6.6 Summary

The drift velocity  $v_d$  is very small compared to the Fermi velocity  $v_F$ ;  $v_d \ll v_F$ ,  $v \approx 10^{-2}$  m/s,  $v_F \approx 10^6$  m/s for Cu. The quantum mechanical picture for the conduction is quite different from the classical one. In the classical picture, the current is carried equally by all electrons, each moving with a very small drift velocity  $v_d$ . On the other hand, In the mechanical picture, the currents is carried only by very small fraction of electrons, all moving with the Fermi velocity  $v_F$ . Since only electrons at the Fermi surface contribute to the conductivity, we can define the mean free path of electrons as  $l = v_F \tau$ . We can estimate the mean free path for metal at room temperature 100 Å.

## 7. Fermi-Dirac statistics of metals

Conduction electrons are Fermions. They obey a **Fermi-Dirac distribution function**

$$f(E) = \frac{1}{\exp\left(\frac{E - E_F}{k_B T}\right) + 1}$$

where  $k_B$  is the Boltzmann constant and  $E_F$  is the Fermi energy. The Fermi velocity  $v_F$  is defined by

$$E_F = \frac{1}{2} m v_F^2$$

where  $m$  is the mass of electron.

According to the Pauli's exclusion principle, each state is occupied by one electron. Only the conduction electrons having the Fermi energy  $E_F$  contribute to the electrical conductivity.

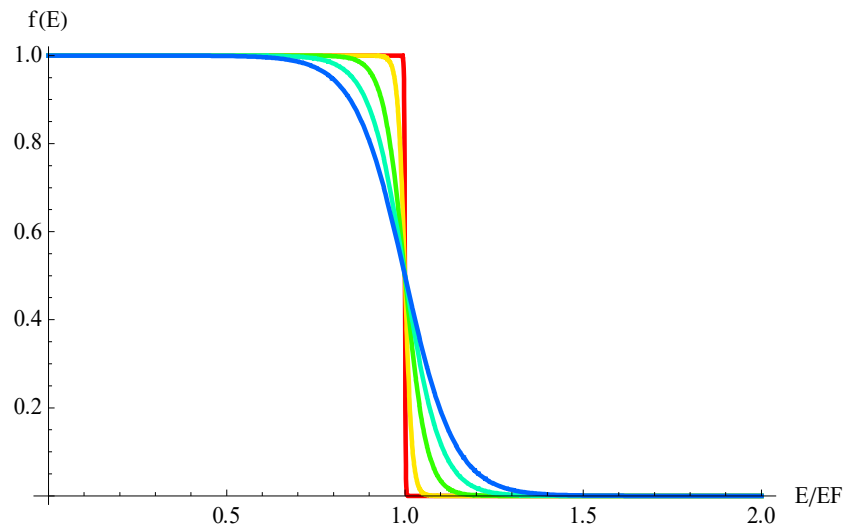


Table 2.1

**FERMI ENERGIES, FERMI TEMPERATURES, FERMI WAVE VECTORS, AND FERMI VELOCITIES FOR REPRESENTATIVE METALS<sup>a</sup>**

ELEMENT	$r_s/a_0$	$\epsilon_F$	$T_F$	$k_F$	$v_F$
Li	3.25	4.74 eV	$5.51 \times 10^4$ K	$1.12 \times 10^8$ cm <sup>-1</sup>	$1.29 \times 10^8$ cm/sec
Na	3.93	3.24	3.77	0.92	1.07
K	4.86	2.12	2.46	0.75	0.86
Rb	5.20	1.85	2.15	0.70	0.81
Cs	5.62	1.59	1.84	0.65	0.75
Cu	2.67	7.00	8.16	1.36	1.57
Ag	3.02	5.49	6.38	1.20	1.39
Au	3.01	5.53	6.42	1.21	1.40
Be	1.87	14.3	16.6	1.94	2.25
Mg	2.66	7.08	8.23	1.36	1.58
Ca	3.27	4.69	5.44	1.11	1.28
Sr	3.57	3.93	4.57	1.02	1.18
Ba	3.71	3.64	4.23	0.98	1.13
Nb	3.07	5.32	6.18	1.18	1.37
Fe	2.12	11.1	13.0	1.71	1.98
Mn	2.14	10.9	12.7	1.70	1.96
Zn	2.30	9.47	11.0	1.58	1.83
Cd	2.59	7.47	8.68	1.40	1.62
Hg	2.65	7.13	8.29	1.37	1.58
Al	2.07	11.7	13.6	1.75	2.03
Ga	2.19	10.4	12.1	1.66	1.92
In	2.41	8.63	10.0	1.51	1.74
Tl	2.48	8.15	9.46	1.46	1.69
Sn	2.22	10.2	11.8	1.64	1.90
Pb	2.30	9.47	11.0	1.58	1.83
Bi	2.25	9.90	11.5	1.61	1.87
Sb	2.14	10.9	12.7	1.70	1.96

**8. Free electron density and electrical resistivity of metals****8.1 Electron configuration in the periodic table**

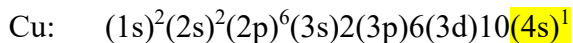
$$(1s)^2|(2s)^2(2p)^6|(3s)^2(3p)^6(3d)^{10}|(4s)^2(4p)^6(4d)^{10}(4f)^{14}|(5s)^2(5p)^6((5d)^{10})\dots$$

Atoms with filled  $n$  shells have a total angular momentum and a total spin of zero. Electrons exterior these closed shells are called valence electrons.

H	(1s)
He	(1s) <sup>2</sup>
Li	(1s) <sup>2</sup> (2s) <sup>1</sup>
Ba	(1s) <sup>2</sup> (2s) <sup>2</sup>
B	(1s) <sup>2</sup> (2s) <sup>2</sup> (2p) <sup>1</sup>
C	(1s) <sup>2</sup> (2s) <sup>2</sup> (2p) <sup>2</sup>
N	(1s) <sup>2</sup> (2s) <sup>2</sup> (2p) <sup>3</sup>

O	$(1s)^2 (2s)^2(2p)^4$
F	$(1s)^2 (2s)^2(2p)^5$
Ne	$(1s)^2 (2s)^2(2p)^6 $
Na	$(1s)^2 (2s)^2(2p)^6 (3s)^1$
Mg	$(1s)^2 (2s)^2(2p)^6 (3s)^2$
Al	$(1s)^2 (2s)^2(2p)^6 (3s)^2(3p)^1$
Si	$(1s)^2 (2s)^2(2p)^6 (3s)^2(3p)^2$
P	$(1s)^2 (2s)^2(2p)^6 (3s)^2(3p)^3$
S	$(1s)^2 (2s)^2(2p)^6 (3s)^2(3p)^4$
Cl	$(1s)^2 (2s)^2(2p)^6 (3s)^2(3p)^5$
Ar	$(1s)^2 (2s)^2(2p)^6 (3s)^2(3p)^6$
K	$(1s)^2 (2s)^2(2p)^6 (3s)^2(3p)^6(3d)^1$
Ca	$(1s)^2 (2s)^2(2p)^6 (3s)^2(3p)^6(3d)^2$
Sr	$(1s)^2 (2s)^2(2p)^6 (3s)^2(3p)^6(3d)^3$
Ti	$(1s)^2 (2s)^2(2p)^6 (3s)^2(3p)^6(3d)^4$
V	$(1s)^2 (2s)^2(2p)^6 (3s)^2(3p)^6(3d)^5$
Cr	$(1s)^2 (2s)^2(2p)^6 (3s)^2(3p)^6(3d)^6$
Mn	$(1s)^2 (2s)^2(2p)^6 (3s)^2(3p)^6(3d)^7$
Fe	$(1s)^2 (2s)^2(2p)^6 (3s)^2(3p)^6(3d)^8$
Co	$(1s)^2 (2s)^2(2p)^6 (3s)^2(3p)^6(3d)^9$
Ni	$(1s)^2 (2s)^2(2p)^6 (3s)^2(3p)^6(3d)^{10} $
Cu	$(1s)^2 (2s)^2(2p)^6 (3s)^2(3p)^6(3d)^{10} (4s)^1$

What is the conduction electron in metals? We consider a metal such Cu. The electron configuration of Cu is given by



The  $s$  electron in the outermost shell becomes conduction electrons.

## 8.2 Free electron density of metallic elements

$$n \text{ (10}^{22}\text{/cm}^3\text{)} = n \text{ (10}^{28}\text{/m}^3\text{)}$$



Table 1.1  
**FREE ELECTRON DENSITIES OF SELECTED METALLIC ELEMENTS<sup>a</sup>**

ELEMENT	Z	$n$ ( $10^{22}/\text{cm}^3$ )	$r_s(\text{\AA})$	$r_s/a_0$
Li (78 K)	1	4.70	1.72	3.25
Na (5 K)	1	2.65	2.08	3.93
K (5 K)	1	1.40	2.57	4.86
Rb (5 K)	1	1.15	2.75	5.20
Cs (5 K)	1	0.91	2.98	5.62
Cu	1	8.47	1.41	2.67
Ag	1	5.86	1.60	3.02
Au	1	5.90	1.59	3.01
Be	2	24.7	0.99	1.87
Mg	2	8.61	1.41	2.66
Ca	2	4.61	1.73	3.27
Sr	2	3.55	1.89	3.57
Ba	2	3.15	1.96	3.71
Nb	1	5.56	1.63	3.07
Fe	2	17.0	1.12	2.12
Mn ( $\alpha$ )	2	16.5	1.13	2.14
Zn	2	13.2	1.22	2.30
Cd	2	9.27	1.37	2.59
Hg (78 K)	2	8.65	1.40	2.65
Al	3	18.1	1.10	2.07
Ga	3	15.4	1.16	2.19
In	3	11.5	1.27	2.41
Tl	3	10.5	1.31	2.48
Sn	4	14.8	1.17	2.22
Pb	4	13.2	1.22	2.30
Bi	5	14.1	1.19	2.25
Sb	5	16.5	1.13	2.14

(Ashcroft and Mermin, Solid State Physics)

### 8.3 Measured resistivity of metals

The electrical resistivity of metals  $\rho$  ( $\Omega\text{cm}$ ) [=  $10^{-2}\rho$  ( $\Omega\text{ m}$ )].

Table 1.2  
ELECTRICAL RESISTIVITIES OF SELECTED ELEMENTS<sup>a</sup>

ELEMENT	77 K	273 K	373 K	$\frac{(\rho/T)_{373\text{ K}}}{(\rho/T)_{273\text{ K}}}$
Li	1.04	8.55	12.4	1.06
Na	0.8	4.2	Melted	
K	1.38	6.1	Melted	
Rb	2.2	11.0	Melted	
Cs	4.5	18.8	Melted	
Cu	0.2	1.56	2.24	1.05
Ag	0.3	1.51	2.13	1.03
Au	0.5	2.04	2.84	1.02
Be		2.8	5.3	1.39
Mg	0.62	3.9	5.6	1.05
Ca		3.43	5.0	1.07
Sr	7	23		
Ba	17	60		
Nb	3.0	15.2	19.2	0.92
Fe	0.66	8.9	14.7	1.21
Zn	1.1	5.5	7.8	1.04
Cd	1.6	6.8		
Hg	5.8	Melted	Melted	
Al	0.3	2.45	3.55	1.06
Ga	2.75	13.6	Melted	
In	1.8	8.0	12.1	1.11
Tl	3.7	15	22.8	1.11
Sn	2.1	10.6	15.8	1.09
Pb	4.7	19.0	27.0	1.04
Bi	35	107	156	1.07
Sb	8	39	59	1.11

## 9. Classification by the energy scheme

Energy band of insulator, metal, semimetal, and semiconductor

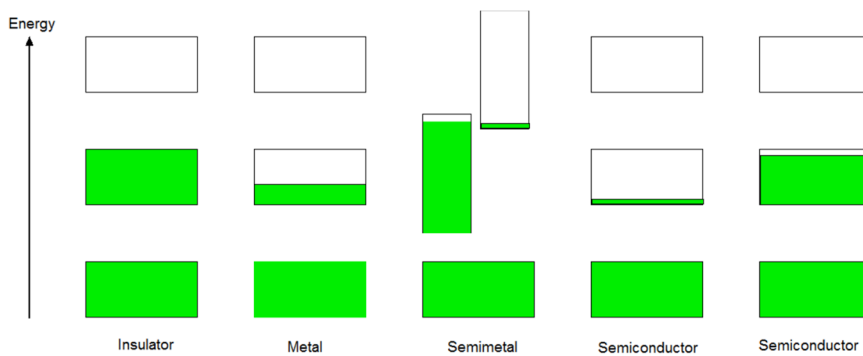
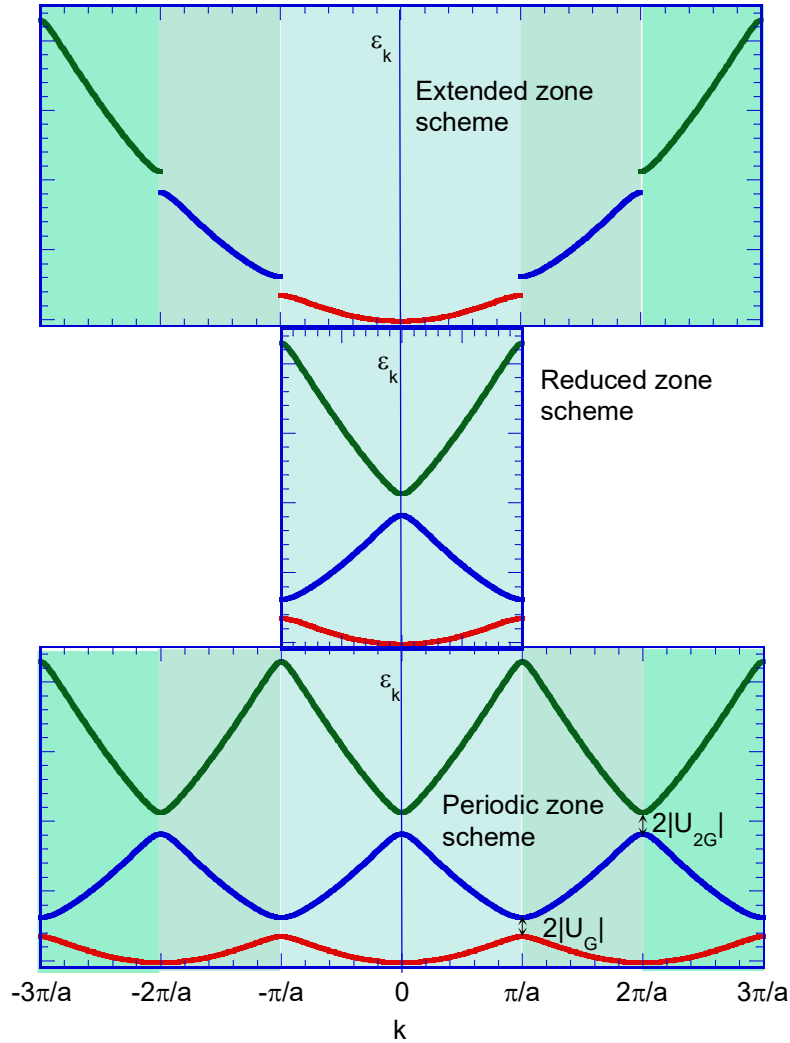


Fig. Schematic electron occupancy of allowed energy bands for an insulator, metal, semiconductor, and semiconductor. The vertical extent of the boxes indicates the

allowed energy regions. The shaded areas indicate the regions filled with electrons. In a semimetal (such as Bi) one band is almost filled and another band is nearly empty. The left of the two semiconductors shown is at a temperature, with carriers excited thermally. The other semiconductor is electron-deficient because of impurities.

### Energy band structure electron for one dimensional metal



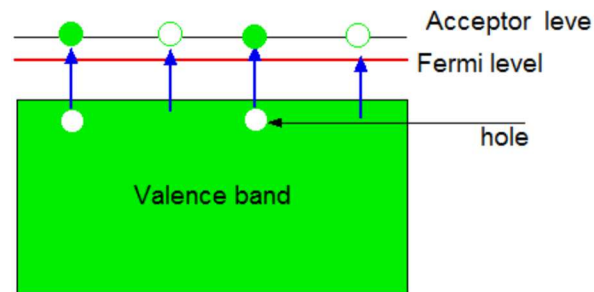
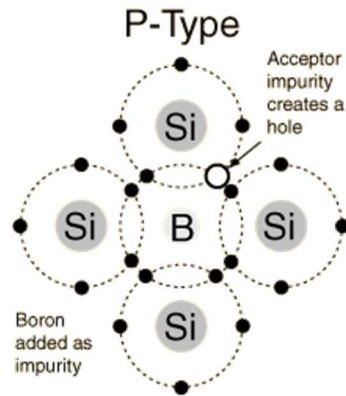
## 10. Semiconductor

### 10.1 The Doping of Semiconductors

The addition of a small percentage of foreign atoms in the regular crystal lattice of silicon or germanium produces dramatic changes in their electrical properties, producing n-type and p-type semiconductors.

### 10.2 p-Type Semiconductor

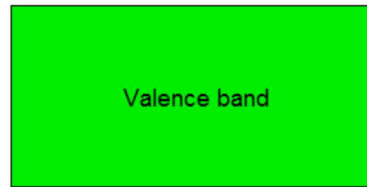
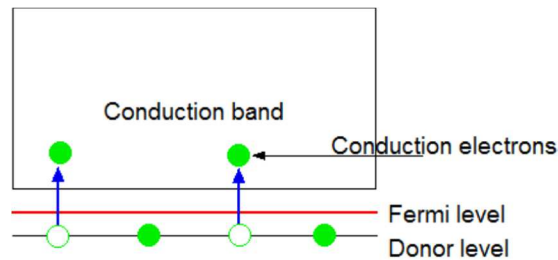
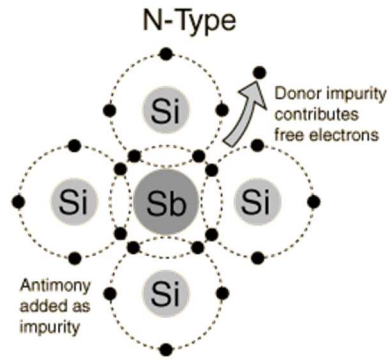
The addition of trivalent impurities such as boron, aluminum or gallium to an intrinsic semiconductor creates deficiencies of valence electrons, called "holes".



p-type semiconductor

### 10.3 n-type Semiconductor

The addition of pentavalent impurities such as Sb, As or P contributes free electrons, greatly increasing the conductivity of the intrinsic semiconductor.



n-type semiconductor

## 11. Superconductors

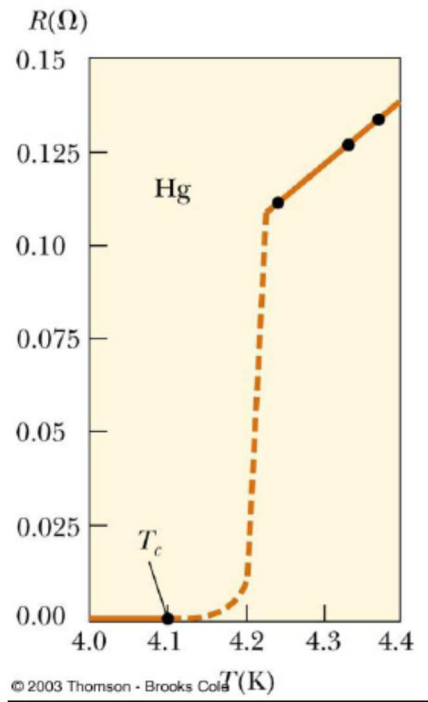
### 11.1 Nature of superconductivity

If mercury is cooled below 4.1 K, it loses all electric resistance. This discovery of superconductivity by [H. Kammerlingh Onnes](#) in 1911 was followed by the observation of other metals which exhibit zero resistivity below a certain critical temperature. The fact that the resistance is zero has been demonstrated by sustaining currents in superconducting lead rings for many years with no measurable reduction. An induced current in an ordinary metal ring would decay rapidly from the dissipation of ordinary resistance, but superconducting rings had exhibited a decay constant of over a billion years!

One of the properties of a superconductor is that it will exclude magnetic fields, a phenomenon called the Meissner effect. The disappearance of electrical resistivity was modeled in terms of electron pairing in the crystal lattice by John Bardeen, Leon Cooper, and Robert Schrieffer in what is commonly called the BCS theory. A new era in the study of superconductivity began in 1986 with the discovery of high critical temperature superconductors.

### 11.2 The disappearance of the resistivity

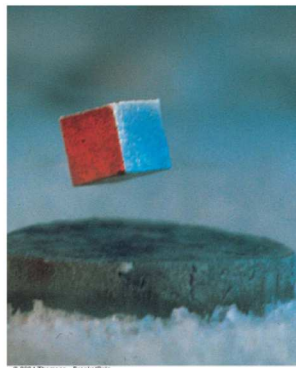
The electrical resistivity  $\rho$  of many metals and alloys drops suddenly to zero when the specimen is cooled to sufficiently low temperature.

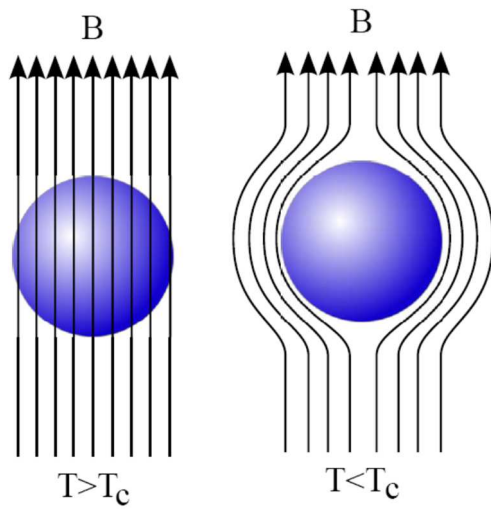


### 11.3 Meissner effect

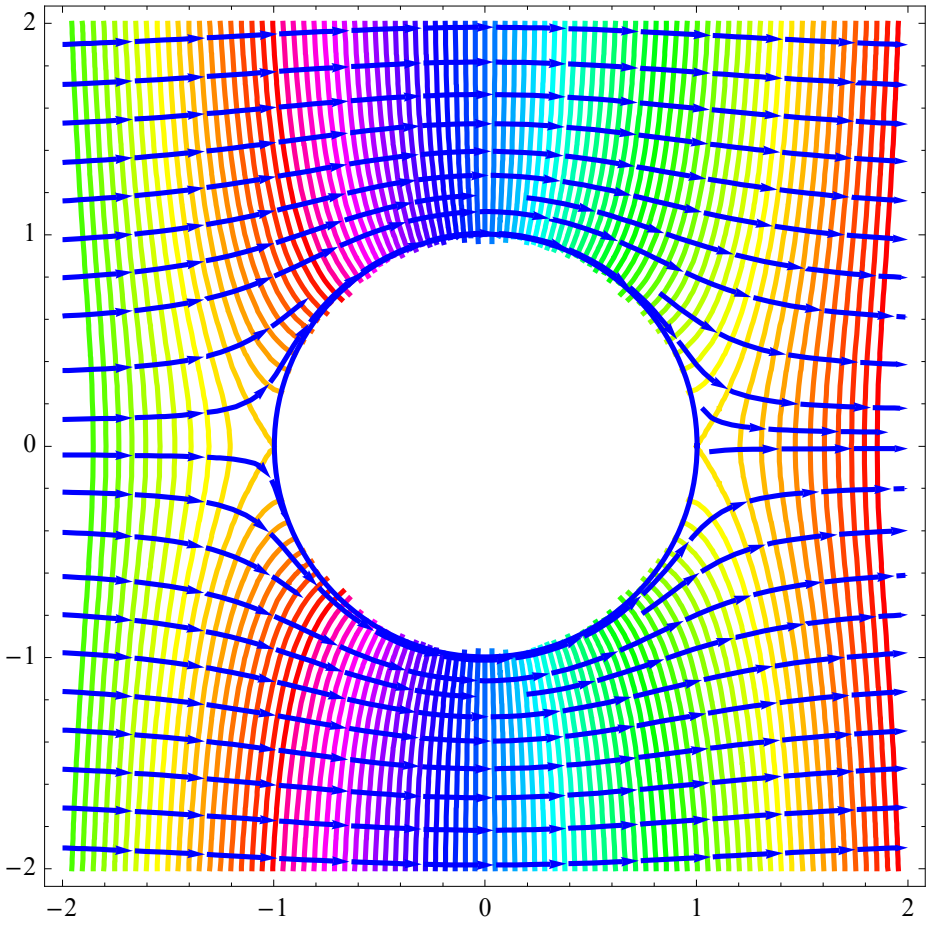
[Meissner & Ochsenfeld (1933)]

A bulk superconductor in a weak magnetic field will act as a perfect diamagnetism, with zero magnetic induction in the interior.





**Fig.** Meissner effect in a superconducting sphere cooled in a constant applied magnetic field; on passing below the transition temperature the lines of induction  $B$  are ejected from the sphere



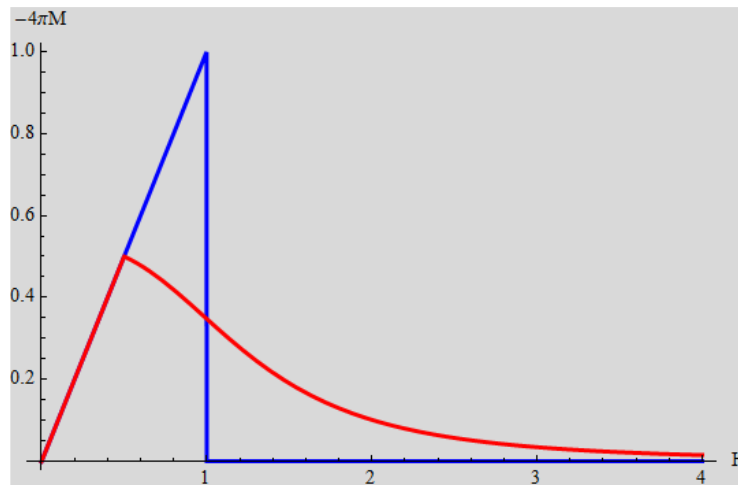
**Fig.** Magnetic field distribution around a superconducting sphere of radius  $R$ . For an external magnetic field which is relatively low, there is a complete Meissner effect. The length of arrows does not corresponds to the magnitude of  $\mathbf{B}$ .

When a specimen is placed in a magnetic field and is then cooled through the critical temperature for superconductivity, the magnetic flux originally present is ejected from the specimen. The demagnetizing field contribution is negligible (cylinder).

$$B = H + 4\pi M = 0 \quad (\text{CGS units})$$

or

$$M = -\frac{1}{4\pi} H \quad (\text{CGS units})$$



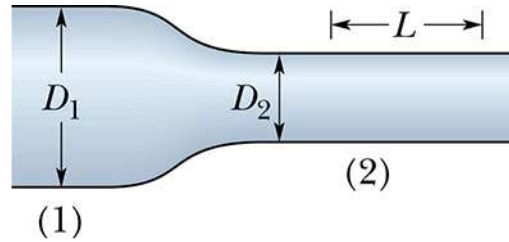
Magnetization vs magnetic field for the Type-I (blue) and type-II (red) superconductors. Meissner phase in the type I superconductors, the Meissner and mixed phases in type II superconductors.

## 12. Typical examples

### 12.1 Problem 26-36 (SP-26)

Figure shows wire section 1 of diameter  $D_1 = 4.00 R$  and wire section 2 of diameter  $D_2 = 2.00 R$  connected by a tapered section. The wire is copper ( $\rho = 1.69 \times 10^{-8} \Omega\text{m}$ ) and carries a current. Assume that the current is uniformly distributed across any cross-section area through the wire's width. The electric potential change  $V$  along the length  $L = 2.00 \text{ m}$  shown in section 2 is  $10.0 \mu\text{V}$ . The number of charge carriers per unit volume is  $8.49 \times 10^{28} \text{ m}^{-3}$ . What is the drift speed of the conduction electrons in section 1





**((Solution))**

$$D_1 = 4R$$

$$D_2 = 2R$$

$$L = 2 \text{ m}$$

$$n = 8.49 \times 10^{28} \text{ m}^{-3}$$

$$V_2 = 10 \text{ } \mu\text{V}$$

$$\rho = 1.69 \times 10^{-8} \text{ } \Omega\text{m}$$

Equation of continuity for the current,

$$I_1 = J_1 A_1 = nq v_1 A_1$$

$$I_2 = J_2 A_2 = nq v_2 A_2$$

Since  $I_1 = I_2$ , we have

$$v_1 = \frac{nq v_2 A_2}{nq A_1} = \frac{v_2 A_2}{A_1} \quad (1)$$

Ohm's law

$$V_2 = \rho \frac{L}{A_2} I_2 = \rho \frac{L}{A_2} (nq v_2 A_2) = \rho L (nq v_2)$$

or

$$v_2 = \frac{V_2}{\rho L n q} \quad (2)$$

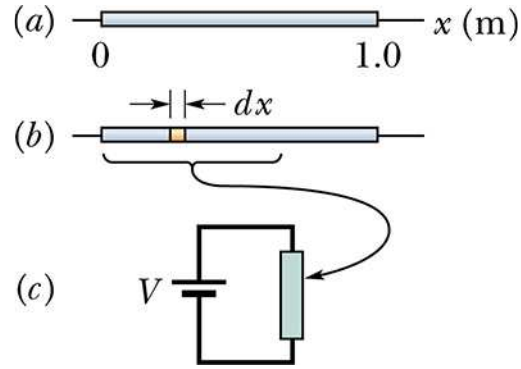
Then the drift velocity  $v_1$  in the section 1 is

$$v_1 = \frac{A_2}{A_1} \cdot \frac{V_2}{\rho L n q} = 5.438 \times 10^{-9} \text{ m/s}$$

## 12.2 Problem 26-54 (SP-26)

Figure (a) shows a rod of resistive material. The resistance per unit length of the rod increases in the positive direction of the  $x$  axis. At any position  $x$  along the rod, the resistance  $dR$  of a narrow (differential) section of width  $dx$  is given by  $dR = 5.00 x dx$ , where  $dR$  is in ohms and  $x$  is in meters. Figure (b) shows such a narrow section. You are to

slice off a length of the rod between  $x = 0$  and some position  $x = L$  and then connect that length to a battery with potential difference  $V = 5.0 \text{ V}$  (Fig.(c)). You want the current in the length to transfer energy to thermal energy at the rate of  $200 \text{ W}$ . At what position  $x = L$  should you cut the rod?



**((Solution))**

$$dR = 5x dx$$

$$R = \int dR = \int_0^L 5x dx = \frac{5}{2} L^2$$

When  $V = 5 \text{ V}$ , and  $P = 200 \text{ W}$ , we have

$$P = IV = \frac{V^2}{R}$$

$$R = \frac{V^2}{P} = \frac{5}{2} L^2 = \frac{25}{200}$$

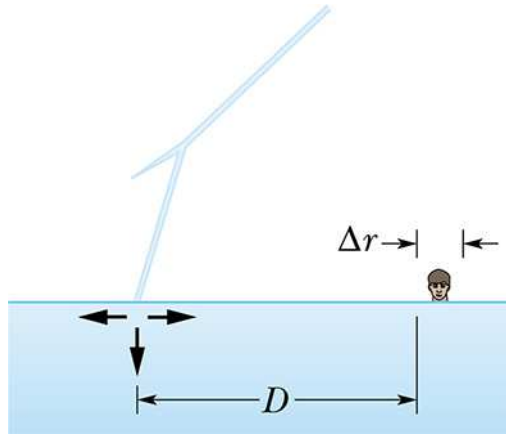
or

$$L = 0.224 \text{ m}$$

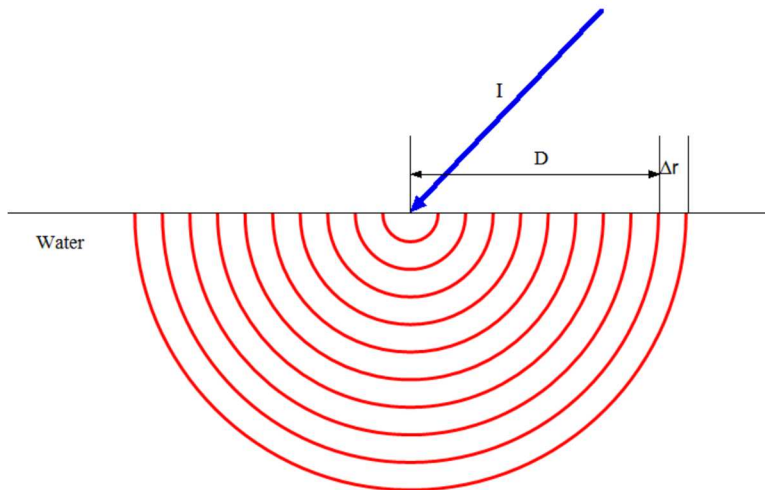
### 13 Hint of home work (HW-26)

#### 13.1 HW26-34

Swimming during a storm. Figure shows a swimmer at distance  $D = 35.0 \text{ m}$  from a lightning strike to the water, with current  $I = 78 \text{ kA}$ . The water has resistivity  $30 \Omega\text{m}$ , the width of the swimming along a radial line from the strike is  $0.70 \text{ m}$ , and his resistance across the width is  $4.00 \text{ k}\Omega$ . Assume that the current spread through the water over a hemisphere centered on the strike point. What is the current through the swimmer?



**((Hint))**



$r = 0.7 \text{ m}$   
 $R = 4 \text{ k}\Omega$   
 $I = 78 \text{ kA}$   
 $D = 35.0 \text{ m}$   
 $\rho_w = 30 \text{ }\Omega\text{m}$

The current density:

$$J = \frac{I}{2\pi r^2}$$

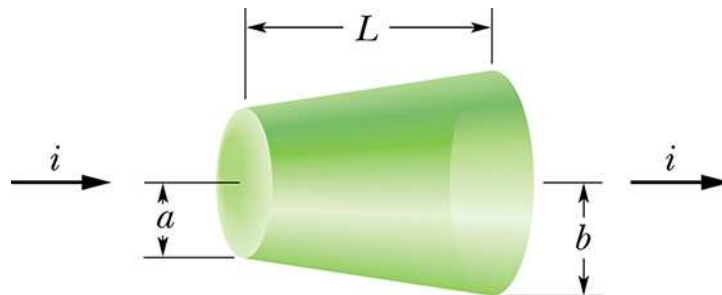
The electric field  $E_r$  in the water

$$E_r = \rho_w J = \rho_w \frac{I}{2\pi r^2} = -\frac{dV}{dr}$$

$$\Delta V = - \int_D^{D+\Delta r} E_r dr$$

### 13.2 HW 26-35 (\*\*\*)

In Fig., current is set up through a truncated right circular cone of resistivity  $731 \Omega\text{m}$ , left radius  $a = 2.00 \text{ mm}$ , right radius  $b = 2.30 \text{ mm}$  and length  $L = 1.94 \text{ cm}$ . Assume that the current density is uniform across any cross section taken perpendicular to the length. What is the resistance of the cone?



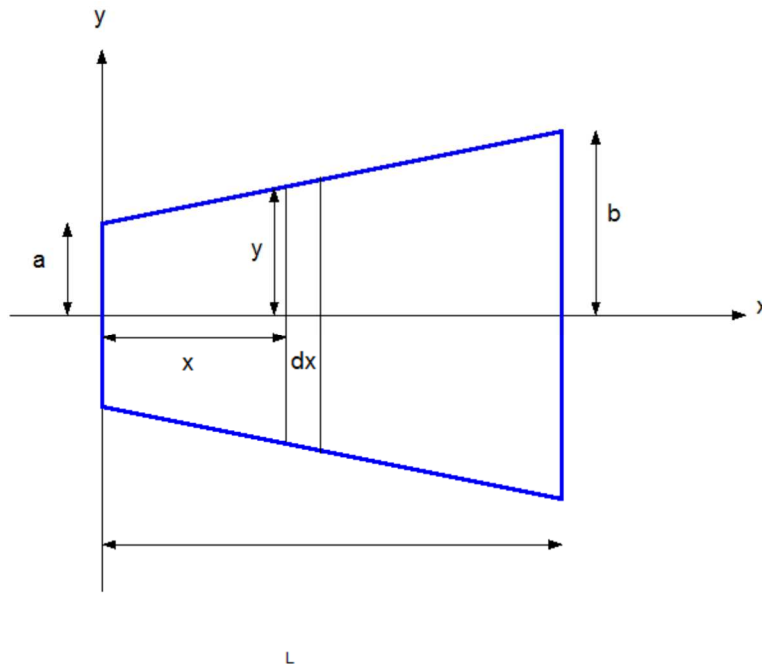
((Hint))

$$\rho = 731 \Omega\text{m}$$

$$a = 2.00 \text{ mm}$$

$$b = 2.30 \text{ mm}$$

$$L = 1.94 \text{ cm}$$



The expression of the straight line AB:

$$y = \frac{b-a}{L}(x-0) + a$$

The resistance  $dR$  between  $x$  and  $x+dx$ ,

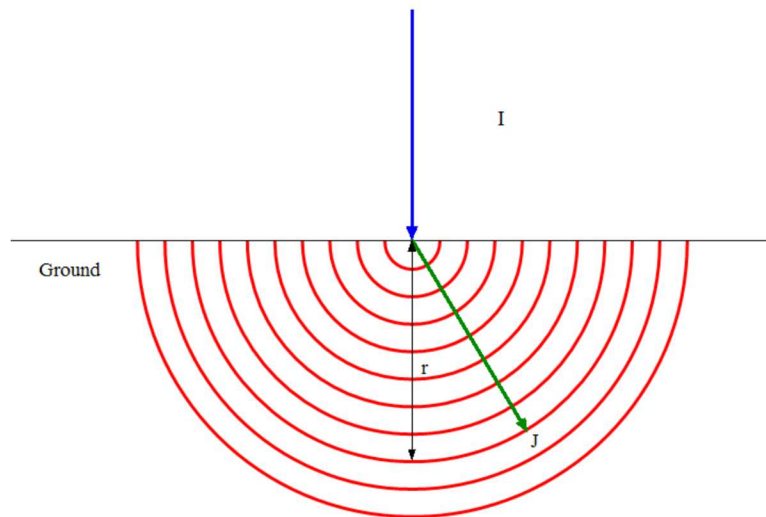
$$dR = \rho \frac{dx}{\pi y^2} = \rho \frac{dx}{\pi \left[ \left( \frac{b-a}{L} \right) x + a \right]^2}$$

## APPENDIX-A

### Measurement of the resistance of the ground using the four probes methods

#### A.1 Electric potential $V$

We consider a point source of current at the surface of the ground at the origin. What is the electric potential  $V$  at a distance  $r$  from the origin in the ground?



From the symmetry, the current density  $J_r$  has the radial component,

$$J_r = \frac{I}{2\pi r^2}$$

The electric field  $E_r$  is defined by

$$E_r = \rho J = \rho \frac{I}{2\pi r^2} = -\frac{dV}{dr}$$

from the Ohm's law, where  $\rho$  is the resistivity. Then the potential  $V$  at a distance  $r$  away from the source point is

$$V = -\int_{\infty}^r \frac{\rho I}{2\pi r^2} dr = \frac{\rho I}{2\pi} \frac{1}{r}$$

Next we consider two point sources of the current  $I_1$  and  $I_2$  on the surface of the ground. From the principle of superposition, the potential  $V$  at a point from the point source 1 (current  $I_1$ ) at the distance  $r_1$  and from the point source 2 (current  $I_2$ ) at the distance  $r_2$ , is obtained as

$$V = \frac{\rho I_1}{2\pi r_1} + \frac{\rho I_2}{2\pi r_2}.$$

When  $I_1 = I$  and  $I_2 = -I$  (the special case), we have

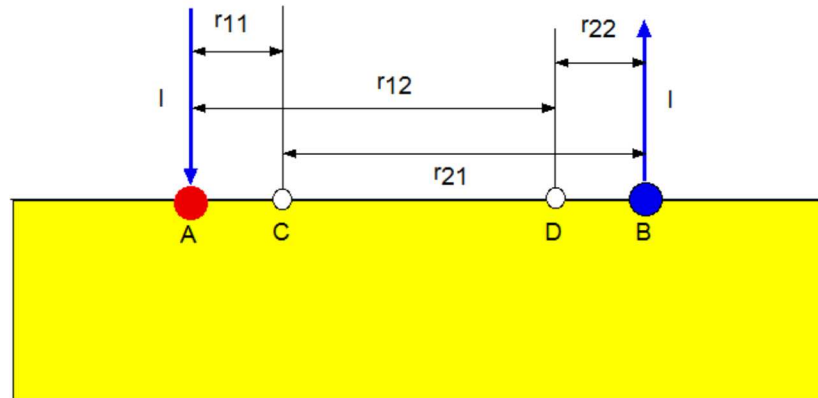
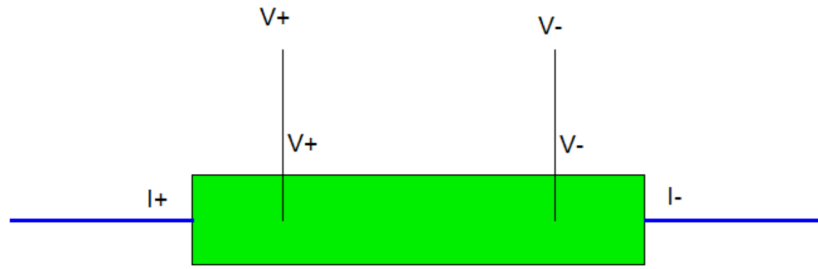
$$V = \frac{\rho I}{2\pi} \left( \frac{1}{r_1} - \frac{1}{r_2} \right)$$

## **A.2 Four-probes method**

We want to measure the resistance between two points on the surface of the ground. We use the four probes methods, where there are two current probes and two voltage probes. The resistance  $R$  is obtained as

$$R = \frac{V}{I}$$

where  $V$  is the voltage between the voltage probes (C and D) and  $I$  is the current flowing between two current probes (A and B).



The potential at the point C is

$$V_C = \frac{\rho I}{2\pi} \left( \frac{1}{r_{11}} - \frac{1}{r_{21}} \right),$$

while the potential at the point D is

$$V_D = \frac{\rho I}{2\pi} \left( \frac{1}{r_{12}} - \frac{1}{r_{22}} \right)$$

Then the voltage difference between the points C and D is

$$\begin{aligned} \Delta V &= V_C - V_D \\ &= \frac{\rho I}{2\pi} \left( \frac{1}{r_{11}} - \frac{1}{r_{21}} \right) - \frac{\rho I}{2\pi} \left( \frac{1}{r_{12}} - \frac{1}{r_{22}} \right) \\ &= \frac{\rho I}{2\pi} \left( \frac{1}{r_{11}} - \frac{1}{r_{21}} - \frac{1}{r_{12}} + \frac{1}{r_{22}} \right) \end{aligned}$$

We define the array constant or geometrical factor k as

$$\frac{1}{k} = \frac{1}{r_{11}} - \frac{1}{r_{21}} - \frac{1}{r_{12}} + \frac{1}{r_{22}}.$$

The resistivity  $\rho$  is expressed by

$$\rho = 2\pi k \frac{\Delta V}{I}$$

(a) **Werner array**

We assume that

$$\begin{aligned} r_{11} &= a \\ r_{22} &= a \\ r_{12} &= 2a \\ r_{21} &= 2a, \end{aligned}$$

Then we have

$$\frac{1}{k} = \frac{1}{a} - \frac{1}{2a} - \frac{1}{2a} + \frac{1}{a} = \frac{1}{a}$$

and

$$\rho = 2\pi a \frac{\Delta V}{I}$$

(b) **Schlumberger array**

We assume that

$$\begin{aligned} r_{11} &= r_{22} = s - a \\ r_{12} &= r_{21} = s + a, \end{aligned}$$

$$\frac{1}{k} = \frac{2}{s-a} - \frac{2}{s+a} = \frac{4a}{s^2 - a^2}$$

Then we have

$$\rho = 2\pi \left( \frac{s^2 - a^2}{4a} \right) \frac{\Delta V}{I}$$

## APPENDIX B Bloch electron in a periodic potential of quantum box

We discuss the energy band of conduction electron (spin 1/2 fermion) in metal, which is one-dimensional. In a quantum box with a well potential, the wave number of electrons becomes discrete due to the Heisenberg's principle of uncertainty. The energy dispersion of electrons is quantized. In a real metal, the electrons are not completely free but move in a weak periodic potential due to atoms in the unit cells of lattice. These electrons are called



Bloch electrons. For a monovalent metal, there is one electron per unit cell, contributing to Bloch electrons. For a divalent metal, there are two electron per unit cell. The energy dispersion of the Bloch electrons is periodic as a function of wave number with the periodicity of the reciprocal lattice, forming an energy band. The energy gap is formed at the boundary of the Brillouin zone, as a result of the Bragg reflection of electrons. The electrons are fermions and obey the Pauli's exclusion principle. All the states below the Fermi energy are occupied by electrons at  $T = 0$  K. If the number of electrons per unit cell is even, the Fermi energy coincides with the energy gap. The system becomes insulator. If the number of electrons per unit cell is odd, the Fermi energy is not equal to energy gap. The system is still metallic.

### **B 1. Energy dispersion for free electron**

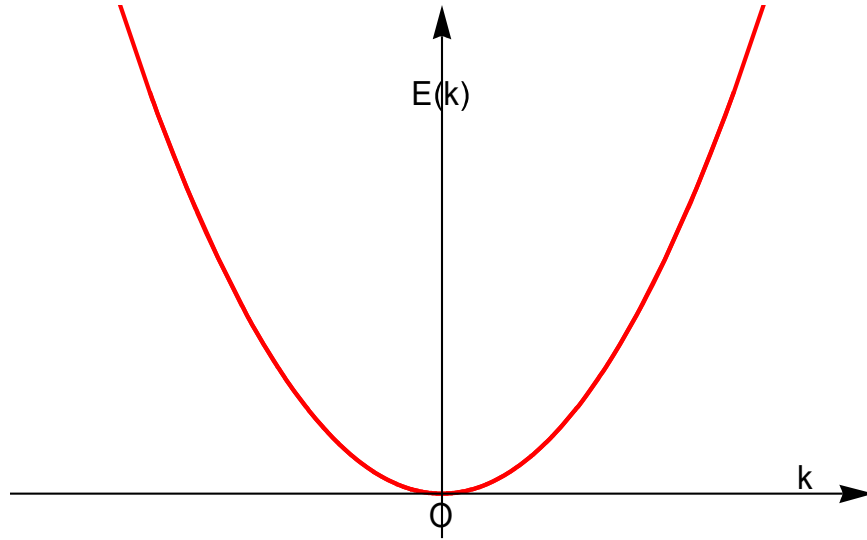
Electrons are quantum mechanical particles (fermions). They behave like a particle as well as a wave. The momentum  $p$  ( $= mv$ ) of the electron is related to the Broglie wavelength  $\lambda$  as

$$p = \frac{h}{\lambda} = \hbar k,$$

where  $k$  ( $= \frac{2\pi}{\lambda}$ ) is the wave number,  $h$  is the Planck constant and  $\hbar$  is the Dirac constant ( $\hbar = \frac{h}{2\pi}$ ). The energy  $E$  of electron is given by the energy dispersion

$$\varepsilon_k = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m},$$

in a free space, where  $k$  is the wave number and  $k$  is continuous.



**Fig.** Plot of energy versus wavenumber for a free electron, where  $k$  is the wave number and is continuous.

## **B 2. Quantum box: Heisenberg's principle of uncertainty**

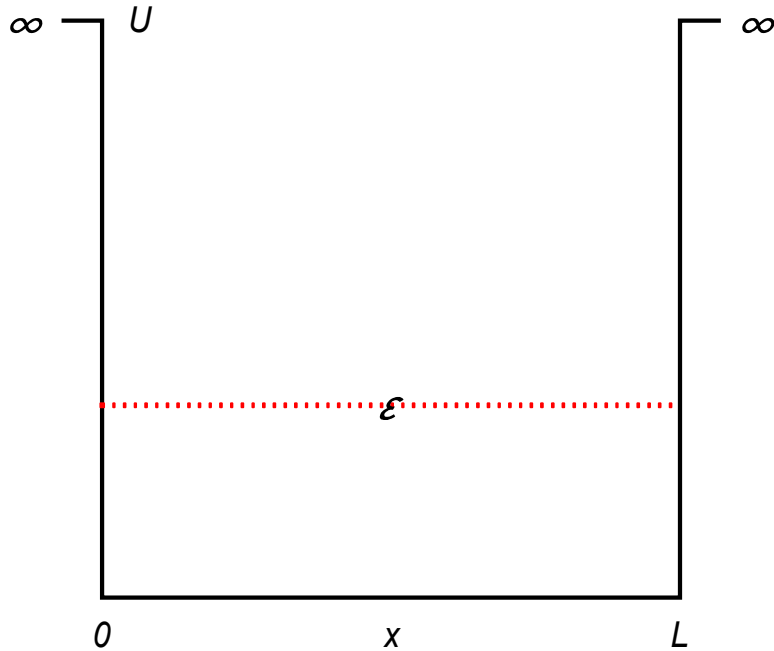
We consider a free electron gas in 1D system. The Schrödinger equation is given by

$$H\psi_k(x) = \frac{p^2}{2m}\psi_k(x) = -\frac{\hbar^2}{2m} \frac{d^2\psi_k(x)}{dx^2} = \varepsilon_k\psi_k(x), \quad (1)$$

where

$$p = \frac{\hbar}{i} \frac{d}{dx},$$

and  $\varepsilon_k$  is the energy of the electron in the orbital.



**Fig.** Electrons in a well-potential with size  $L$ . The potential is infinity outside the box. The determination of the energy eigenvalue of such an electron by using Schrödinger equation is called the quantum box problem.

The orbital is defined as a solution of the wave equation for a system of only one electron: ⟨⟨one-electron problem⟩⟩. Using a periodic boundary condition:  $\psi_k(x+L) = \psi_k(x)$ , we have

$$\psi_k(x) \sim e^{ikx}, \quad (2)$$

with

$$\varepsilon_k = \frac{\hbar^2}{2m} k^2 = \frac{\hbar^2}{2m} \left( \frac{2\pi}{L} n \right)^2,$$

$$e^{ikL} = 1$$

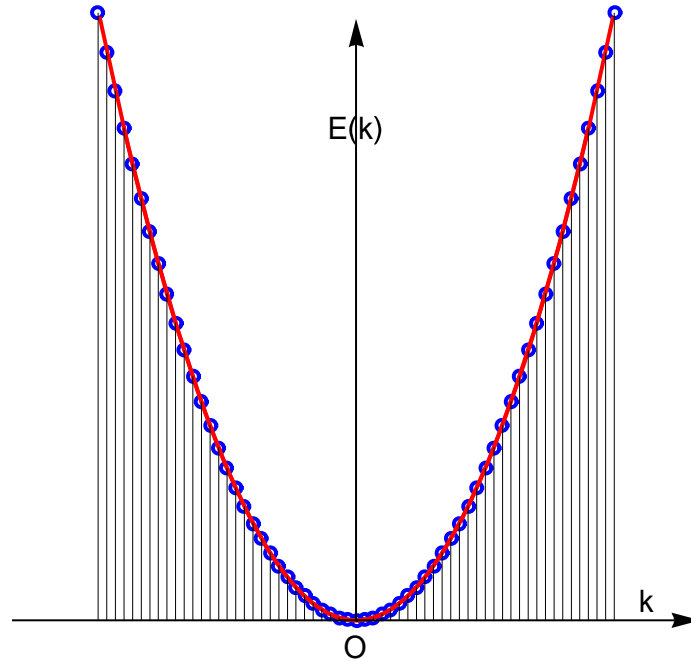
or

$$k = \frac{2\pi}{L} n$$

where  $k$  has a discrete value

$$\Delta k = \frac{2\pi}{L}$$

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



**Fig.** Energy dispersion curve for the electron in a quantum box.

The wave number is no longer continuous. It takes discrete values of  $k$  whose division is given by

$$\Delta k = \frac{2\pi}{L},$$

or

$$k_x = \frac{2\pi}{L} n_x \quad (n = 0, \pm 1, \pm 2, \pm 3, \dots)$$

**((Heisenberg's uncertainty of principle))**

The discreteness of the wave number is derived from the Heisenberg's principle of uncertainty.

$$\Delta x \Delta k \approx 2\pi$$

When  $\Delta x = L$ , we have

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

### **((The Pauli's exclusion principle))**

The one-electron levels are specified by the wavevectors  $k$  and by the projection of the electron's spin along an arbitrary axis, which can take either of the two values  $\pm\hbar/2$ . Therefore associated with each allowed wave vector  $k$  are two levels:

$$|k, \uparrow\rangle, |k, \downarrow\rangle.$$

### **B.3. Periodic potential: Bloch theorem**

In metals, there are many atoms. They are periodically arranged, forming a lattice with the lattice constant  $a$ . We consider conduction electron in the presence of periodic potential (due to a Coulomb potential of positive ions). The electrons undergo movements under the periodic potential as shown below. Such electrons are called the Bloch electrons. According to Bloch, the wave function of the Bloch electrons can be expressed by

$$\psi_k(x) = e^{ikx} u_k(x)$$

where  $u_k(x)$  is a periodic function of  $x$  with the periodicity  $a$ ,

$$u_k(x+a) = u_k(x).$$

So we have

$$\psi_k(x+a) = e^{ik(x+a)} u_k(x+a) = e^{ika} e^{ikx} u_k(x) = e^{ika} \psi(x)$$

Note that the wave function satisfies the boundary condition

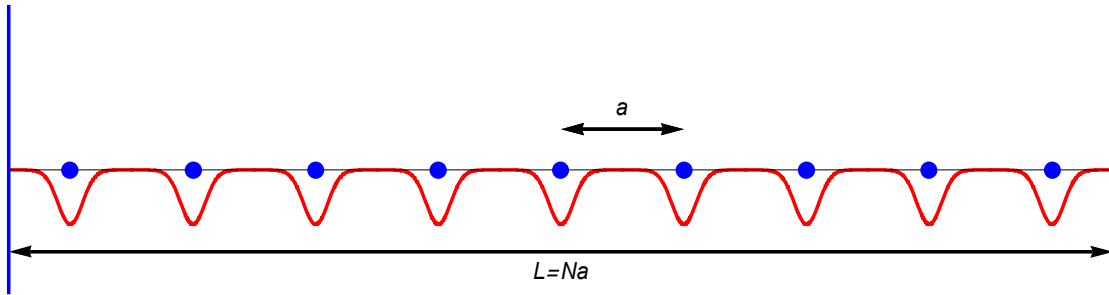
$$\psi_k(x+L) = e^{ikL} \psi(x) = \psi(x).$$

since  $e^{ikL} = 1$ . We note that  $u_k(x)$  can be expressed

$$u_k(x) = \sum_G u_{k-G} \exp(-iGx),$$

by using the Fourier series, where  $G$  is the reciprocal lattice

$$G = \frac{2\pi}{a} n \quad (n \text{ is integer}).$$



**Fig.** Periodic lattice of lattice constant  $a$ . The form of potential energy of an electron in a one-dimensional lattice. The positions of the ion cores are indicated by the points (blue solid circles) with the separation  $a$  (lattice constant).

When  $k$  is replaced by  $k + G$ ,

$$\psi_{k+G}(x+a) = e^{i(k+G)a} \psi_{k+G}(x) = e^{ika} \psi_{k+G}(x),$$

since  $e^{iGa} = e^{i2\pi n} = 1$ . This implies that  $\psi_{k+G}(x)$  is the same as  $\psi_k(x)$ ,

$$\psi_{k+G}(x) = \psi_k(x).$$

So the energy eigenvalue of  $\psi_{k+G}(x)$  is the same as that of  $\psi_k(x)$ , leading to the periodicity of  $E_k$  as

$$E_{k+G} = E_k.$$

We also note that the relation  $\varepsilon_k = \varepsilon_{-k}$  is always valid, whether or not the system is centrosymmetric. Then the energy dispersion of  $\varepsilon_k$  vs  $k$  can be obtained by the superposition of the curve of  $E_{k+G}$  vs  $k$  with  $G$  changed as a parameter.

$$\varepsilon_{k+G} = \frac{\hbar^2}{2m}(k+G)^2$$

Since

$$k = \frac{2\pi}{L}n = \frac{2\pi}{Na}n = \frac{\pi}{a}\left(\frac{2n}{N}\right),$$

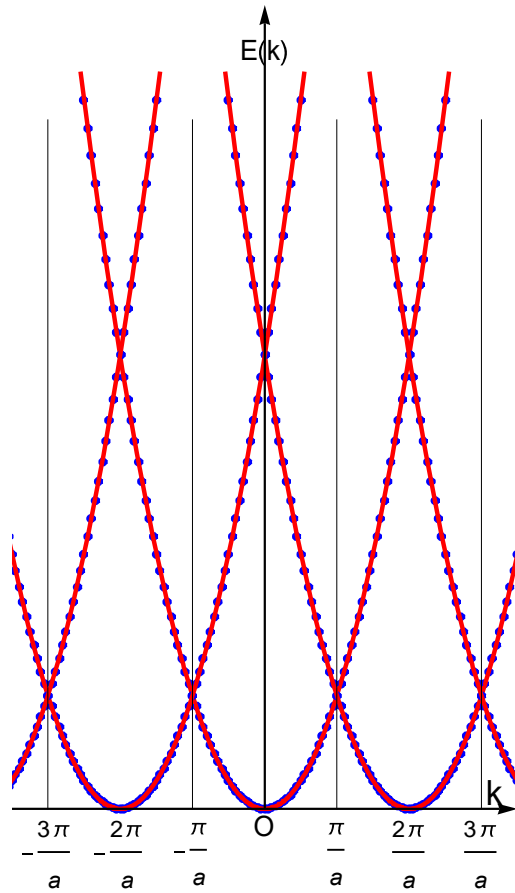
the value of  $k$  is chosen as

$$-\frac{\pi}{a} \leq k \leq \frac{\pi}{a}, \quad (\text{the first Brillouin zone})$$

or

$$-\frac{N}{2} \leq n \leq \frac{N}{2}, \quad (\text{the total number is } N, \text{ the number of unit cell}).$$

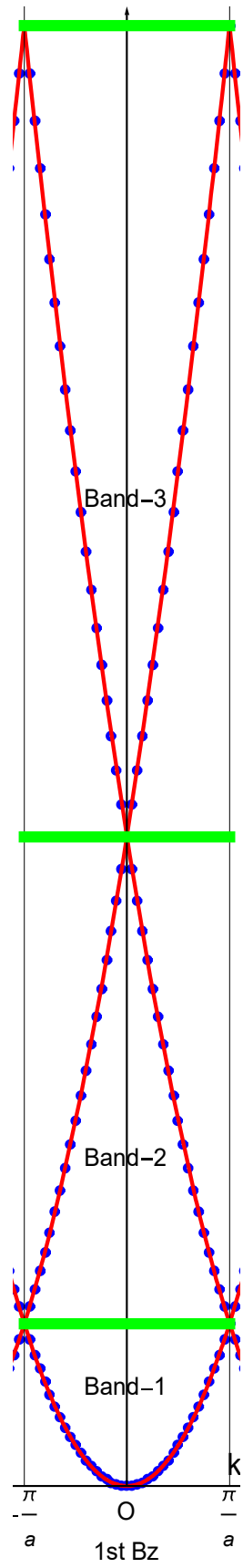
The energy dispersion thus obtained is shown in the Fig. as shown below.



**Fig.** The parabolic energy curves of a free electron in one dimension, periodically continued in reciprocal space. The periodicity in real space is a periodic lattice with a vanishing periodic potential (empty lattice). The first Brillouin zone (

The energy vs  $k$  consists of branches denoted by the number of band (band-1, band-2, band-3,...) in the first Brillouin zone. As we discuss later, there are energy gaps between adjacent bands.





The first Brillouin zone is defined as  $|k| \leq \frac{\pi}{a}$ . There are  $N$  states in the first Brillouin zone.

When the spin of electron is taken into account, there are  $2N$  states in the first Brillouin zone. Suppose that the number of electrons per unit cell is  $n_c$  ( $= 1, 2, 3, \dots$ ). Then the number of the total electrons is  $n_c N$ .

(a)  $n_c = 1$ . So there are  $N$  electrons.  $N/2N = 1/2$  (band-1: half-filled).

(b)  $n_c = 2$ .  $2N/2N = 1$  (band-1: filled).

(c)  $n_c = 3$ .  $3N/2N = 1.5$  (band-1: filled, band-2: half-filled).

(d)  $n_c = 4$ .  $4N/2N = 2$  (band-1: filled, band-2: filled).

When there are even electrons per unit cell, bands are filled. Then the system is an insulator. When there are odd electrons per unit cell, bands are not filled. Then the system is a conductor.

#### **B.4. Bragg reflection at the boundary of the Brillouin zone**

Just like x-ray, the electrons undergo a Bragg reflection under the condition of

$$\Delta k = k' - k = G.$$

This can occur when

$$k = \frac{\pi}{a} \text{ and } k' = -\frac{\pi}{a} \text{ (boundary of the Brillouin zone)}$$

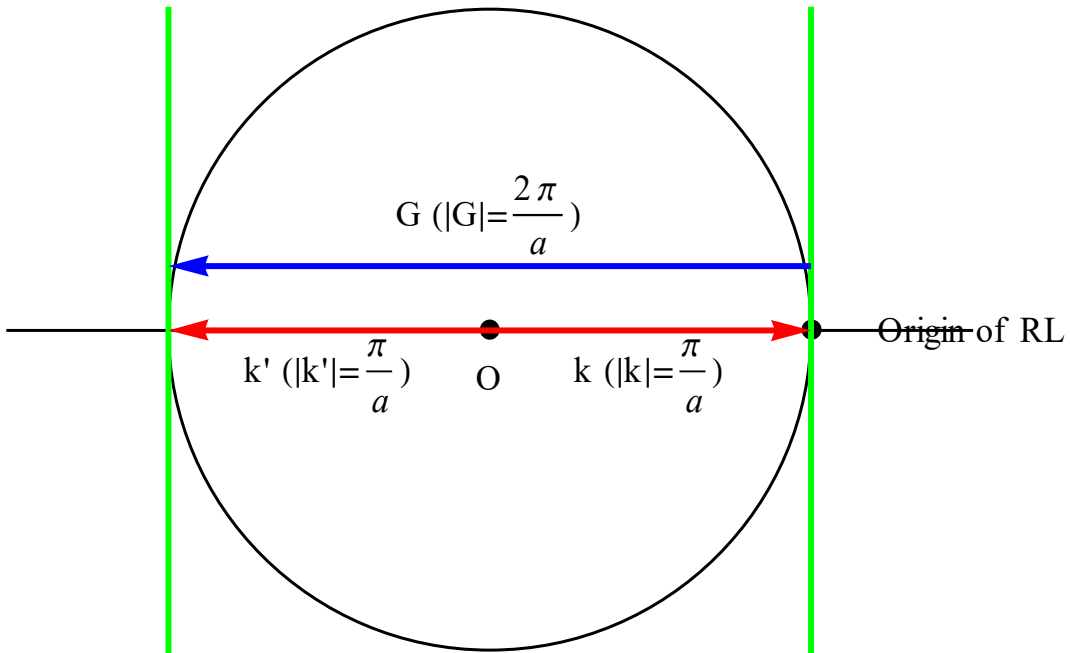
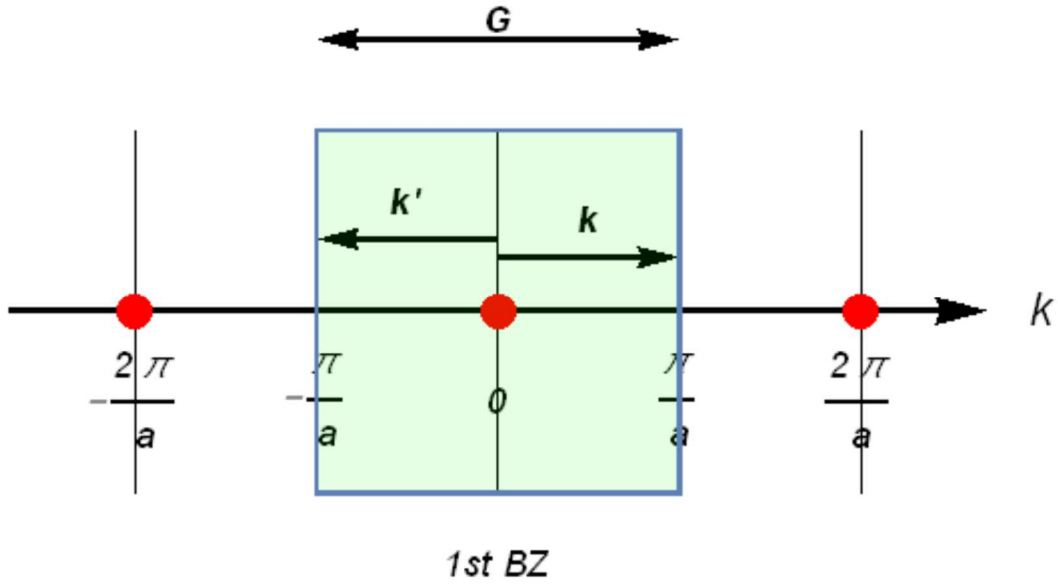
where  $G$  is the reciprocal lattice,

$$G = \frac{2\pi}{a}n \quad (n: \text{integer}).$$

As a result of the Bragg reflection, one can find a standing wave, leading to the energy gap at the boundary of the first Brillouin zone. We note that the magnitude of the energy gap can be evaluated from the time-dependent perturbation with the degenerate system. In the unperturbed system, the two independent states  $\left| k = \frac{\pi}{a} \right\rangle$  and  $\left| k' = -\frac{\pi}{a} \right\rangle$  are degenerate in energy. In the presence of weak perturbation due to the Fourier component of a periodic potential, these two states are combined into two different states with different energy. The difference of the energy leads to the energy gap.

**1D system:**

For For the 1D system this condition at the zone boundary at  $k = G/2 = \pm\pi/a$ .



**Fig.** Condition of the Bragg reflection for the 1D case.  $|k| = |k - G|$ .  $G = 2\pi/a$ .  $k^2 = k - G$ .

**B 5. The zone scheme of energy band**

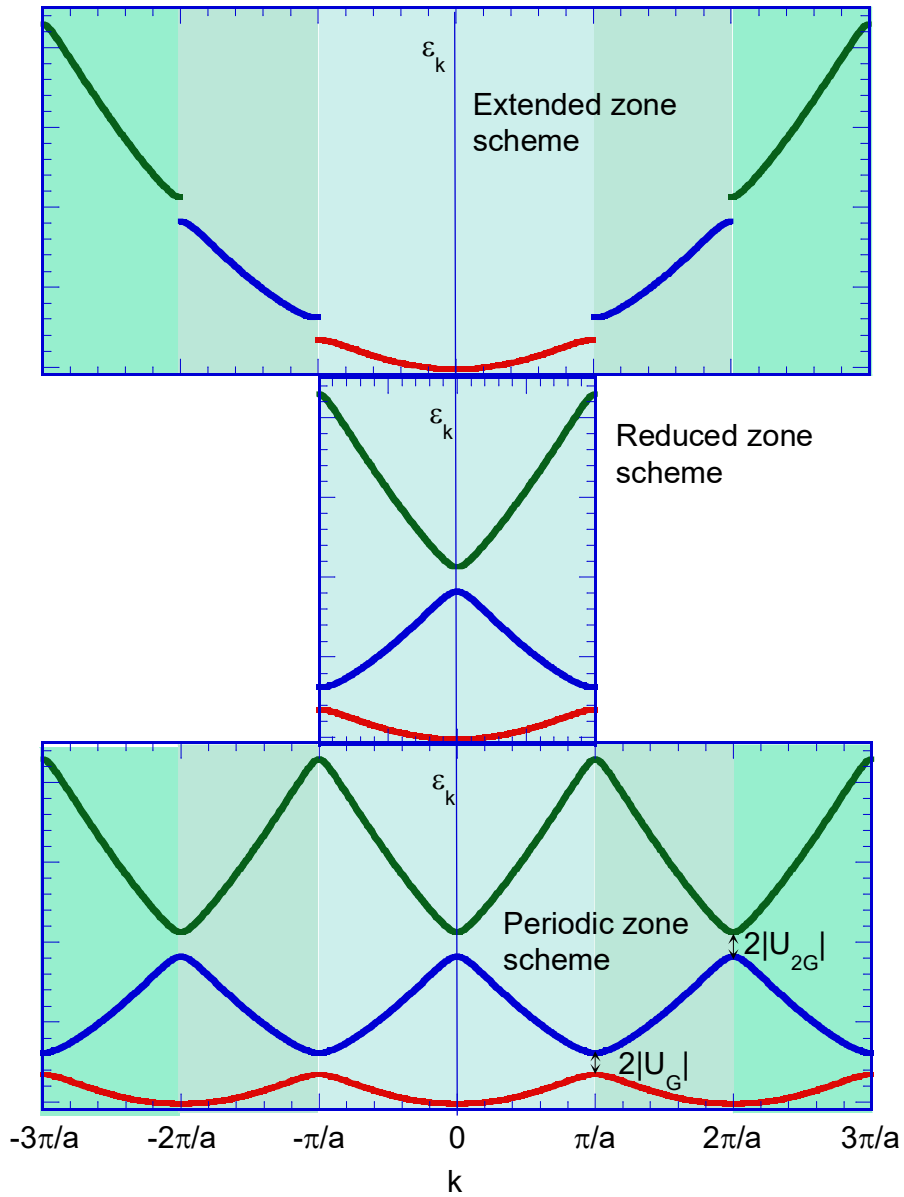
There are several zone schemes of energy band

- (a) Extended zone scheme.
- (b) Reduced zone scheme.
- (c) Periodic zone scheme.

These three schemes are equivalent because of the two features,

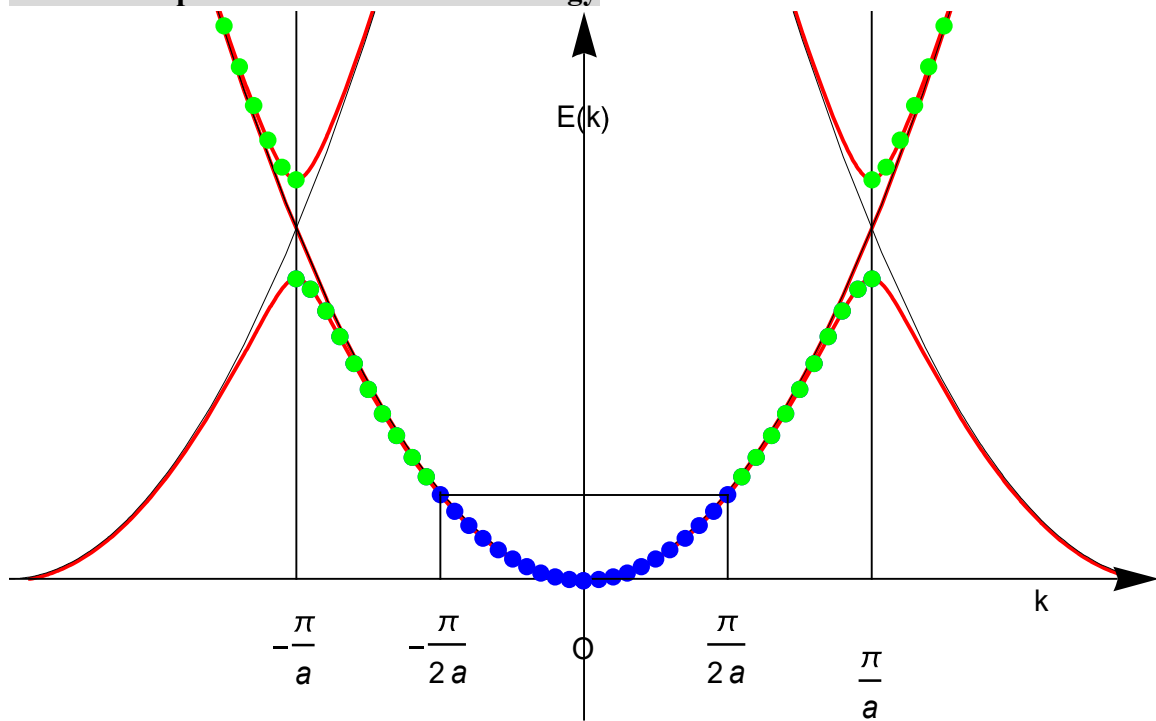
$$\varepsilon_{k+G} = \varepsilon_k, \quad \varepsilon_{-k} = \varepsilon_k$$

for the Bloch electrons.

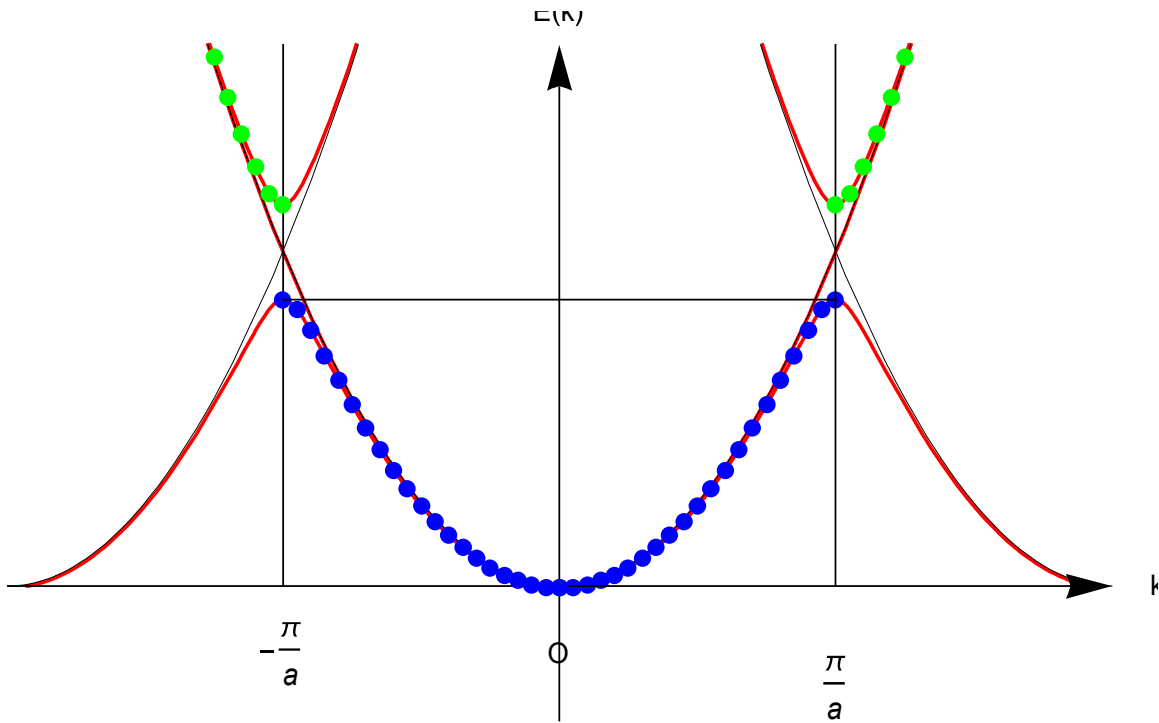


**Fig.** Three zone schemes for the 1D system. Extended zone scheme. Reduced zone scheme. Periodic zone scheme.

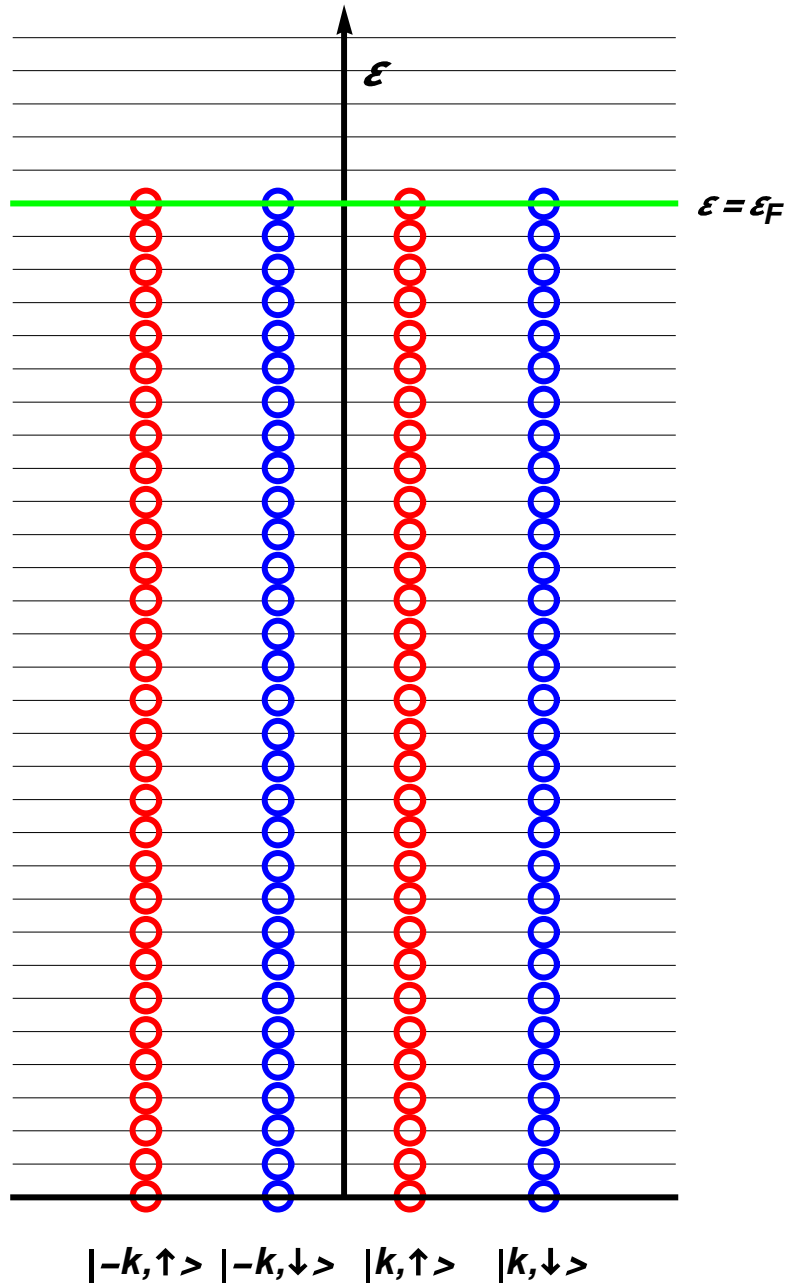
**B 6. Occupied states below Fermi energy**



**Fig.** 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.



**Fig.** Energy band with  $2N$  filled states (full filled state) in the first Brillouin zone. The  $2N$  states are allowed in the first Brillouin zone. The energy gap is associated with the Bragg reflection at the boundary of the first Brillouin zone  $k = \pm \frac{\pi}{a}$ .



**Fig.** Occupation of energy states below the Fermi energy.

### B.7 Metal and insulator

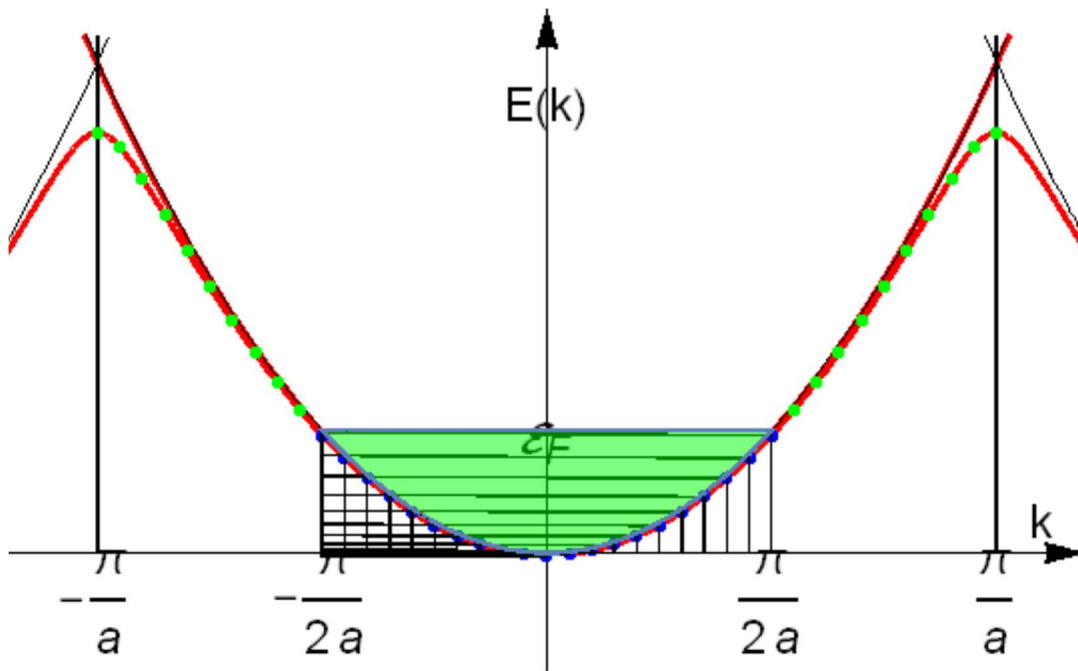
$N$  is the number of unit cell. The size of the system is  $L = Na$ , where  $a$  is the lattice constant. The number of states in the Brillouin zone is equal to  $2N$ , where the factor 2 comes from the spin  $1/2$ .

Suppose that there is one conduction electron per atom. In this case there are  $N$  electrons. Since there are  $2N$  states in the first Brillouin zone, a half of states in the Brillouin zone are occupied.

When there is one conduction electron per atom. In this case there are  $N$  electrons. Since there are  $2N$  states in the first Brillouin zone, a half of states in the Brillouin zone are occupied. So the system is metallic.

When there are two conduction electrons per atom. In this case there are  $2N$  electrons. Since there are  $2N$  states in the first Brillouin zone, all states in the first Brillouin zone are occupied. The system is insulator.

When there are three conduction electrons per atom. In this case there are  $3N$  electrons. Since there are  $2N$  states in the first Brillouin zone, all states in the first band are occupied. A half of the states in the second band are occupied by the remaining electrons. The system is metallic.



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## REFERENCES

S.L. Altman, Band Theory of Metals (Pergamon, 1970)

C. Kittel, Introduction to Solid State Physics 8-th edition (John Wiley and Sons, 2005).