Unit-3

Electrical Conductivity in Metals

Reference Material

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- Arthur Beiser, “Perspectives of Modern Physics”, S.Chand Publications, 3rd Edition, 2004.
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- G.K. Shivakumar “Engineering Physics”, Prism Publications, 2007-08.

VTU Syllabus

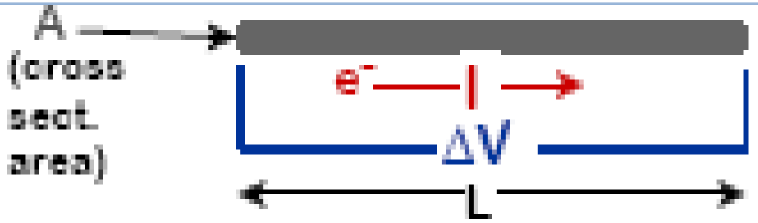
- Free-electron concept
- Classical free-electron theory- Assumptions
- Drift Velocity
- Mean collision time and mean free path; Relaxation time
- Expression for drift velocity
- Expression for electrical conductivity in metals
- Effect of impurity and temperature on electrical resistivity of metals.
- Failure of classical free-electron theory

- Quantum free-electron theory- Assumptions
- Fermi-Dirac Statistics
- Fermi energy- Fermi factor
- Density of states (With derivation)
- Expression for electrical resistivity/conductivity
- Temperature dependence of resistivity of metals
- Merits of quantum free-electron theory.

7 Hrs

- Ohm's Law:

R depends on specimen geometry



$$\Delta V = I\,R$$

voltage drop (volts)

current (amps)

resistance (Ohms)

- Resistivity, ρ and Conductivity, σ:

→ geometry-independent forms of Ohm's Law

$$\frac{\Delta V}{L} = \frac{I}{A}\,\rho$$

Elelectric Field intensity

resistivity (Ohm-m)

J: current density

Conductivity:

$$\sigma = \frac{1}{\rho}$$

- Resistance: $R = \dfrac{\rho L}{A} = \dfrac{L}{A\sigma}$

Resistance, Resistivity, and Conductivity

- **Resistance is defined as *R* = *V*/*i***
  - Resistance is higher for
    - Longer wires and for wires with smaller cross section
- ***R* ~ *L*/*A* ⇒ *R* = ρ·(*L*/*A*)**
  - ρ is called resistivity. The units are [Ω·m]
  - "Conductivity" is inverse of resistivity $\sigma = 1/\rho$
  - *Conductivity and Resistivity are material properties, and do not depend on the size or geometry*

$$\boxed{R=\rho\frac{L}{A}=\frac{1}{\sigma}\frac{L}{A}}$$

Examples of Resistivity (ρ)

- **Ag (Silver): 1.59×10^{-8} Ω·m**
- **Cu (Copper): 1.68×10^{-8} Ω·m**
- **Graphite (C): (3 to 60)$\times10^{-5}$ Ω·m**
- **Diamond (C): ~10^{14} Ω·m**
- **Glass: ~10^{10} - 10^{14} Ω·m**
- **Pure Germanium: ~ 0.5 Ω·m**
- **Pure Silicon: ~ 2300 Ω·m**

Classical Free-electron Theory of Conductivity in Metals

It is proposed by Drude and Lorentz is based on the following assumptions:

- Atoms in a metal are considered to be made up of ion cores which are nuclei surrounded by inner electrons excluding the valance electrons and the valence electrons which are free to move anywhere inside the sample.

- The effect of electric potential due to positive ion cores on the electrons is considered to be constant and hence neglected.

- The electrostatic repulsion between the electrons is neglected.

- The electrons in the metal are considered equivalent to molecules in a gas and the gas laws are made applicable to the electrons in a metal. Accordingly the distribution of energy and velocity is assumed to follow Maxwell-Boltzman statistics.

Electrical Conduction: “Macroscopic” View

- Current density, conductivity, electric field: $J = \sigma E$
- resistance of material: $R = \dfrac{\rho \ell}{A} = \dfrac{\ell}{\sigma A}$

σ : electrical conductivity
ρ : electrical resistivity

- voltage drop across material:

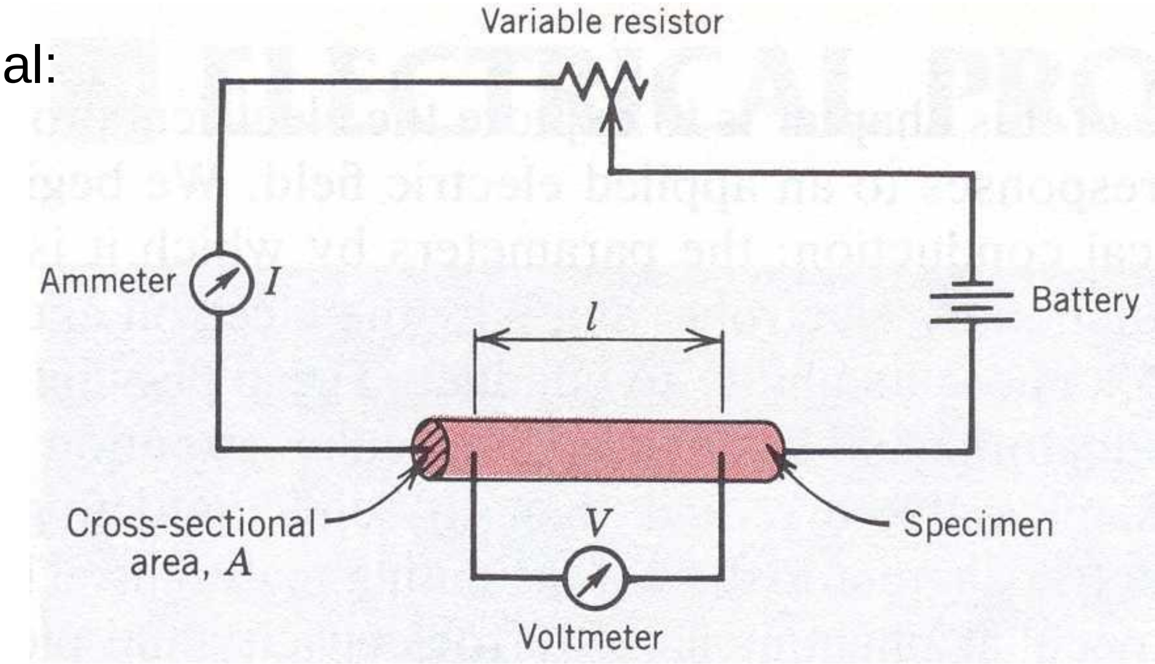
$$V = E\ell$$

- current through material:

$$I = JA$$

- $\Rightarrow$ Ohm’s law:

$$V = IR$$



Electrical Conduction: “Microscopic” View [Callister 19.2]

$$\sigma = ne|z|\mu$$

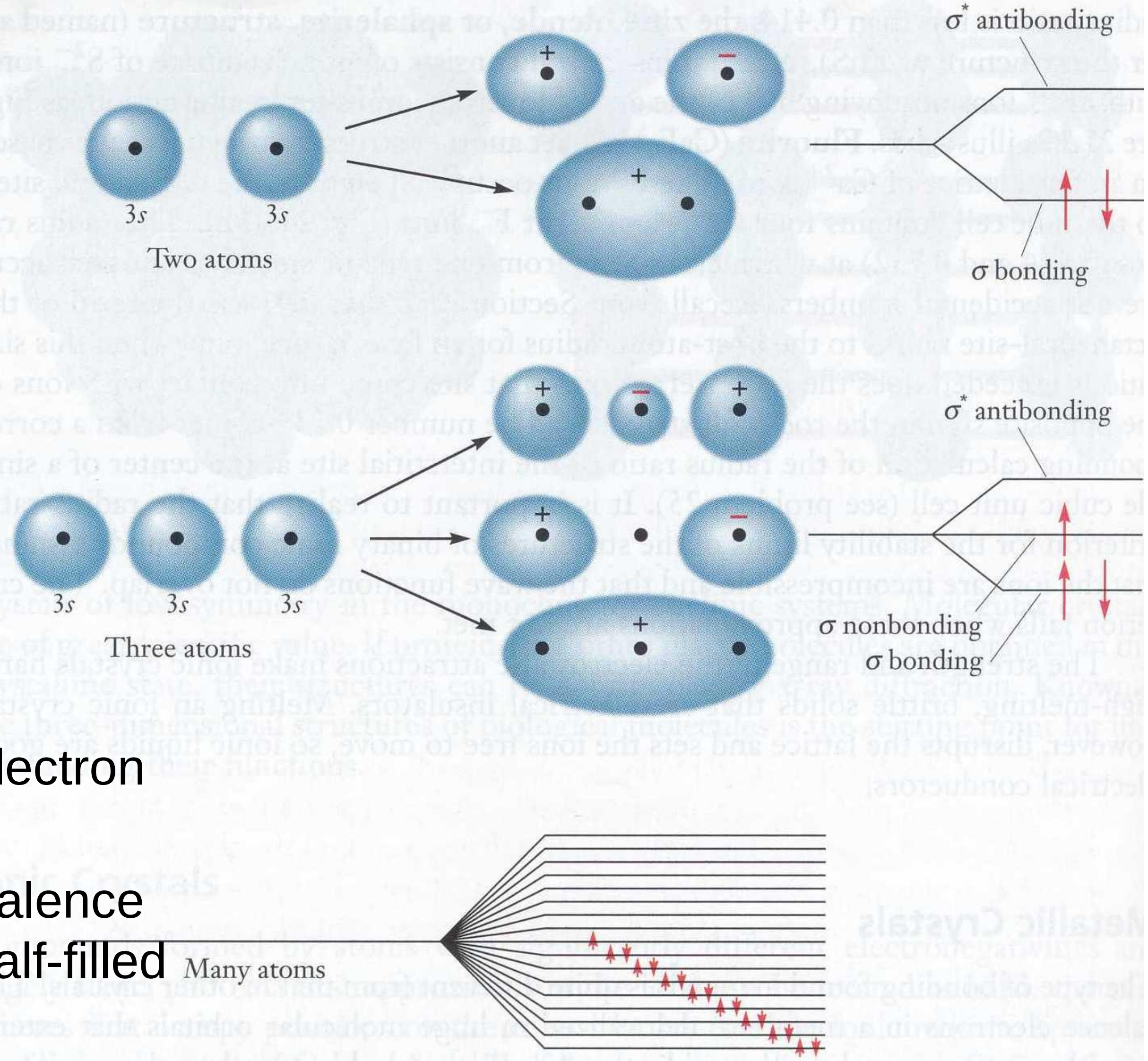
- σ: ***electrical conductivity*** $[\Omega^{-1}m^{-1}]=Cm^{-1}V^{-1}s^{-1}$
- n: ***concentration of charge carriers*** $[m^{-3}]$
- e: charge on an electron — a constant [C]
- z: valence of charge carriers (±1, ±2, …) z=1 for electrons and holes, 2 for O^{2-} ions, …
- μ: ***mobility*** of charge carriers $[m^2V^{-1}s^{-1}]$

- This expression holds for ***all substances***
- Electrical conductivity varies by ***>22 orders of magnitude*** in ordinary materials , because of differences in n and μ
- If material has more than one type of charge carrier:

$$\sigma_{tot} = \sum_{all\ \ carrier\ \ types} ne\,|\,z\,|\,\mu$$

Energy Bands in Metals

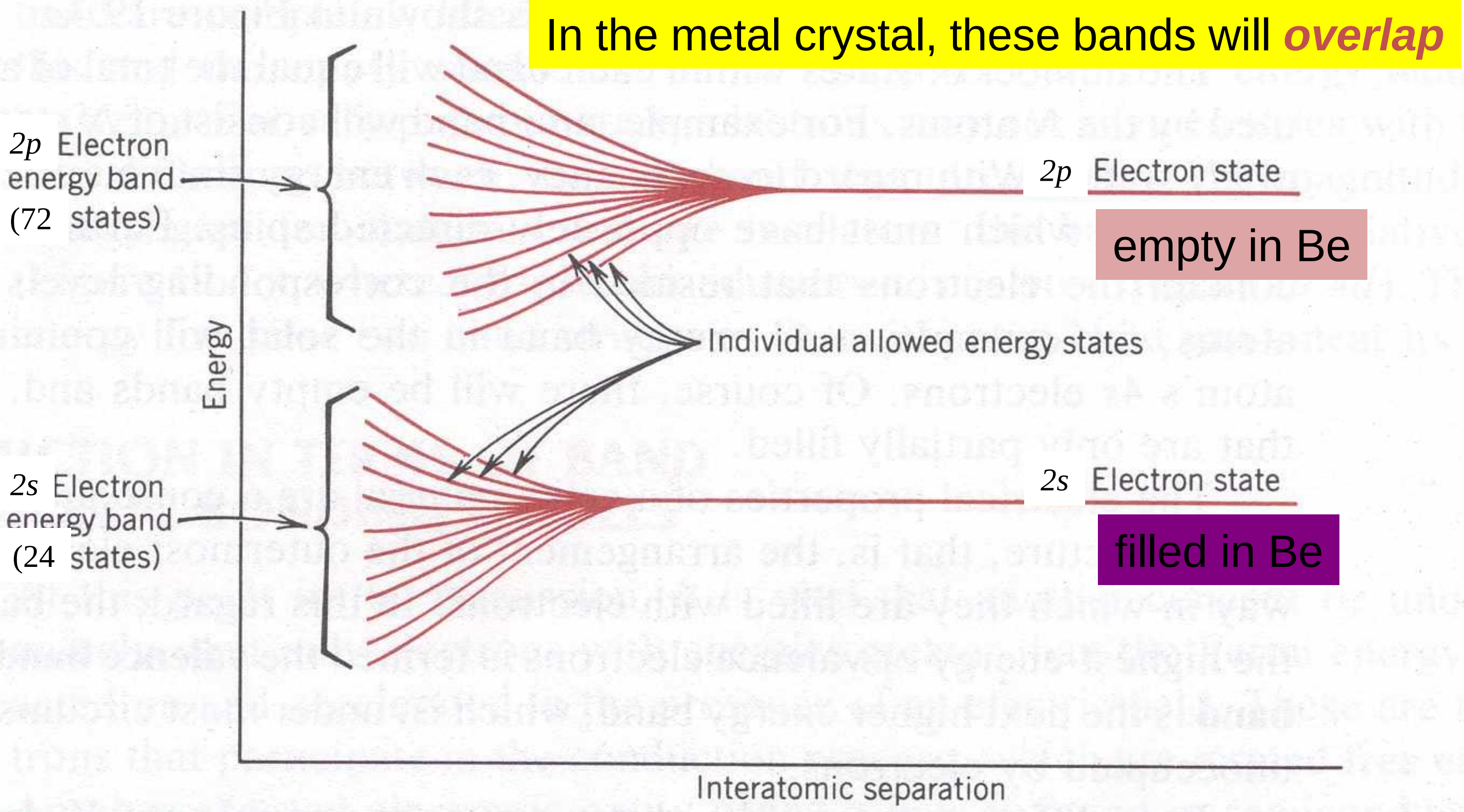
FIGURE 21.20 As sodium atoms are brought together, the molecular orbitals formed from their 3*s* atomic orbitals spread out into a band of levels, half occupied by electrons.



Energy bands:

- Many closely spaced electron states
- Li, Na, K, Cu, Ag, Au: valence orbital in free atom is half-filled ⇒ band is half-filled

Bands in Metal Crystals

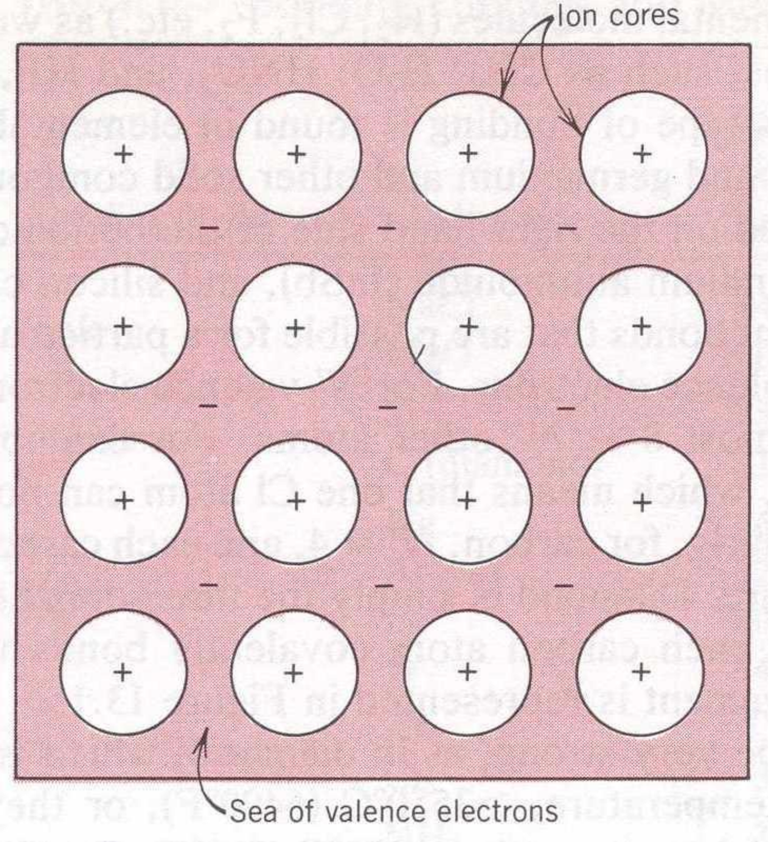


In the metal crystal, these bands will *overlap*

Figure 19.2 Schematic plot of electron energy versus interatomic separation for an aggregate of 12 atoms ($N = 12$). Upon close approach, each of the 1*s* and 2*s* atomic

Carrier Concentration in Metals

- The charge carriers in metals are the valence electrons
  - Not bound to particular atoms (ionic bonds)
  - Not shared by specific atoms (covalent bonds)
  - Rather, shared throughout the crystal (metallic bond) — “free electron gas” or “sea of valence electrons”



- Usually 1-3 per atom
  - Depending on element
  - ~Independent of …
    - temperature
    - dislocations
    - grain size

Expression for Electrical Conductivity in metals

The force on the electron is F=e E (1)

If m is the mass of the electron, then from Newton's law of motion, the force on the electron can be

$$F = m\frac{dv}{dt} \qquad (2)$$

$$eE = m\frac{dv}{dt}$$

$$or$$

$$dv = \frac{eE}{m}dt$$

$$Integrating\ on\ both\ sides$$

$$\int dv = \int \frac{eE}{m}dt$$

Expression for Electrical Conductivity in metals

$$or\ \ v = \frac{eE}{m} t$$

Where t is the time of traverse.

Is t is taken as equal to the collision time τ which is the average value, the corresponding velocity becomes the average velocity

$$\bar{v} = \frac{eE}{m} \tau$$

The expression for electrical conductivity σ is

$$\sigma = \frac{J}{E}$$

Where J is the current density

Expression for Electrical Conductivity in metals

But J= I/A

Where I is the current in the conductor and A is the area of cross section of the conductor

$$\therefore \sigma = \frac{I}{AE}$$

The quantity of charge crossing a given point in the conductor/unit area/unit time is

$$I = ne\bar{v}A$$

$$\therefore \sigma = \frac{ne\bar{v}}{E}$$

Expression for Electrical Conductivity in metals

Substituting the value of $\bar{v}$

$$\sigma = \frac{ne}{E}\left(\frac{eE}{m}\right)\tau$$

$$or\ \ \sigma = \frac{ne^2\tau}{m}$$

Mobility of Electrons:

The mobility of electrons is defined as the magnitude of the drift velocity acquired by the electrons in a unit field. Thus, if ***E*** is the applied electric field in which the electrons acquire a drift velocity v_d , then the mobility of electrons μ is given by,

$$\mu = \frac{v_d}{E}$$

$$J = \sigma E$$

$$\therefore \sigma = \frac{J}{E} = \frac{I}{AE} = \frac{nev_d A}{AE} = ne\mu$$

$$or, \mu = \frac{\sigma}{ne}$$

By substituting for σ we have,

$$\mu = \frac{e\tau}{m}$$

Mobility of Electrons:

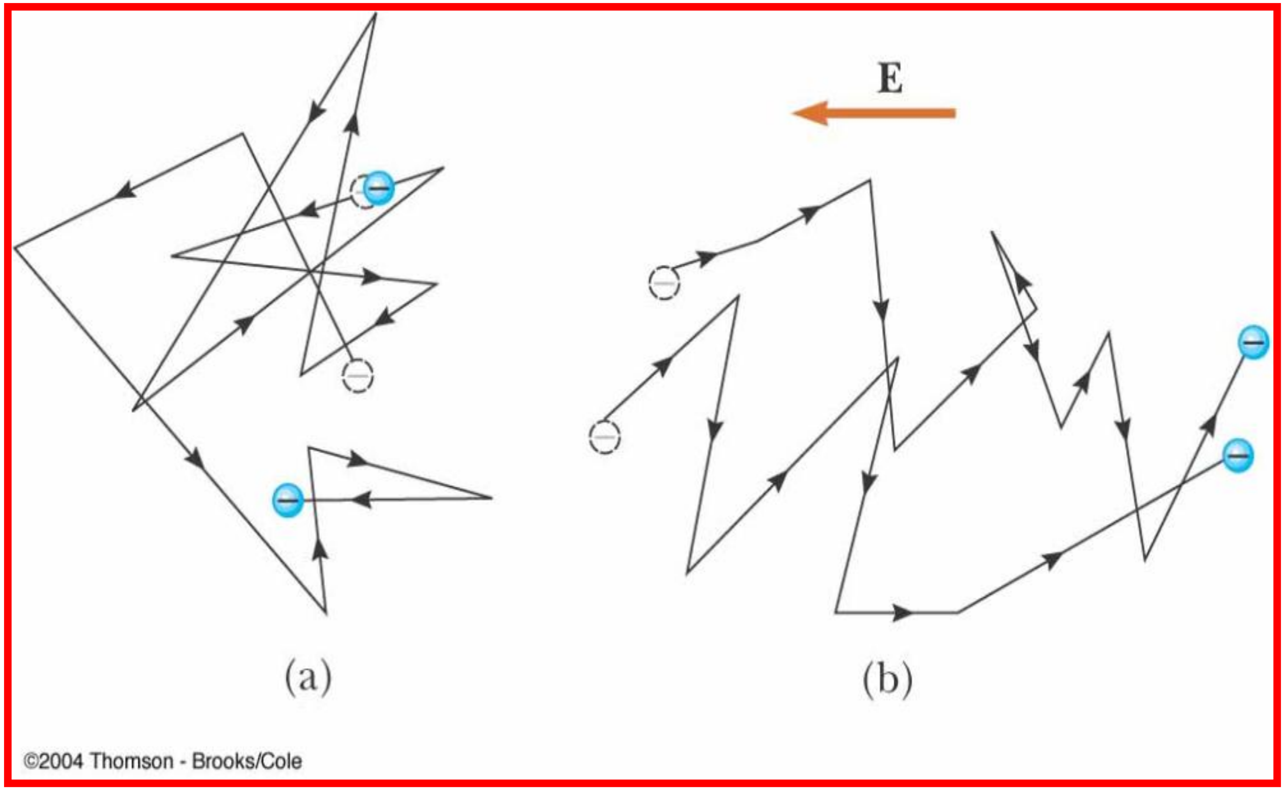
- Drift velocity, mobility, and electric field:

  : What scatters carriers?

$$\upsilon_d = \mu_e E$$

A : Disruptions in periodicity

  - defects
  - lattice vibrations
  - surfaces



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Effect of Temperature and Impurity on Electrical Resistivity of metals:

Two components of resistivity which are described below:

1.Resistivity ρ_{Ph} due to scattering of electrons by lattice vibrations (phonons) which increases with temperature. ρ_{Ph} is therefore temperature dependent. It is the resistivity exhibited by a pure specimen that is free of all defects, and hence called the **ideal resistivity.**

1. Resistivity ρ_i due to scattering of conduction electrons by the presence of impurities, and imperfections such as dislocation vacancies, and grain boundaries. This type of scattering is independent of temperature and contributes to resistivity even at the temperature $T = 0^0 K$. ρ_i is therefore called **residual resistivity.**

Since the two scattering mechanisms mentioned above act independently, the two resistivities are additive. If ρ is the total resistivity of the metal, then ρ is given by,

$$\rho = \rho_{Ph} + \rho_i$$

$$\rho = \frac{m}{ne^2\tau_{Ph}} + \frac{m}{ne^2\tau_i}$$

τ_i *is the mean collision time*

Failures of Classical Free Electron Theory

- **Specific heat:**

The molar specific heat of a gas at constant volume is,

$$C_v = \frac{3}{2}R.$$

the experimentally observed value of specific heat is far lower than expected value. Also, the theory predicts that the specific heat does not depend on temperature, whereas, it was found experimentally that the specific heat is proportional to temperature.

- **Temperature dependence of electrical conductivity:**

It has been experimentally observed that for metals, the electrical conductivity σ is inversely proportional to the temperature T. $i.e., \sigma_{\exp} \propto \frac{1}{T}$

$$According\ \ to\, Classical\, Theory\ \ \sigma \propto \frac{1}{\sqrt{T}}.$$

Failures of Classical Free Electron Theory

As per the classical free electron theory, the electrical conductivity σ is given by,

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

where, *n* is the electron concentration.

$$\therefore \sigma \propto n.$$

For some of the examples predicts that the classical free electron theory does not hold good.

Quantum Free Electron theory of metals

- For Identical particles, that can be distinguished from one another Maxwell-Boltzman Statistics.(Classical Theory)
- In classical picture, all the valence electrons were considered to contribute to the conduction process.
- In quantum free electron theory, the quantization of electron energy levels and the applicability of Pauli's exclusion principle have been incorporated.
- Drawing similarities between electrons in metal and electron inside a potential well of infinite depth, the energy values permitted for the electrons are given by the relation,

$$E_n = \frac{h^2 n^2}{8ml^2}$$

The distribution function for Fermions is known as Fermi-Dirac distribution or " Fermi Factor" and represent the probability of finding a Fermion in an energy state E at a given temperature T. This is given by

$$F_{FD}(E) = F(E) = \frac{1}{A\exp\left(\frac{E}{kT}\right)+1}$$

Quantum Free Electron theory of metals

3-D Cubic Infinite Potential Well

- **1-D Well**

$$\psi_n(x) = \left(\frac{2}{L}\right)^{1/2} \sin\left(\frac{\pi x}{L} n\right)$$

$$E_n = \frac{\pi^2 \hbar^2}{2m L^2} n^2$$

- **3-D “Cubic” Well (with sides length *L*)**

$$\psi_{n_1 n_2 n_3}(x) = \left(\frac{2}{L}\right)^{3/2} \sin\left(\frac{\pi x}{L} n_1\right) \sin\left(\frac{\pi y}{L} n_2\right) \sin\left(\frac{\pi z}{L} n_3\right)$$

$$E_{n_1 n_2 n_3} = \frac{\pi^2 \hbar^2}{2mL^2}\left(n_1^{\;2} + n_2^{\;2} + n_3^{\;2}\right) = E_0 n^2$$

ENERGY BANDS IN SOLIDS

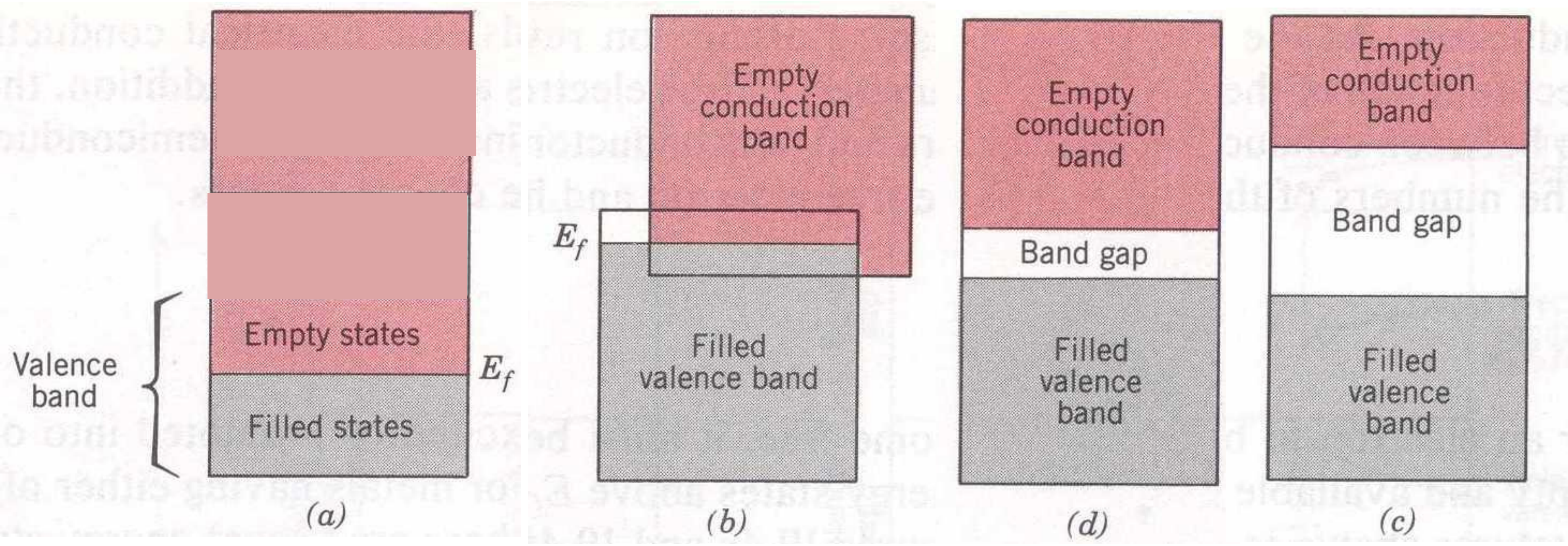
Bands in Metals, Semiconductors, & Insulators

Metals:
e.g., Cu

Metals:
e.g., Mg

Semiconductor
e.g., Si

Insulators:
e.g., Al_2O_3



$E_g < 2eV$ $\quad$ $E_g > 2eV$

Density of States

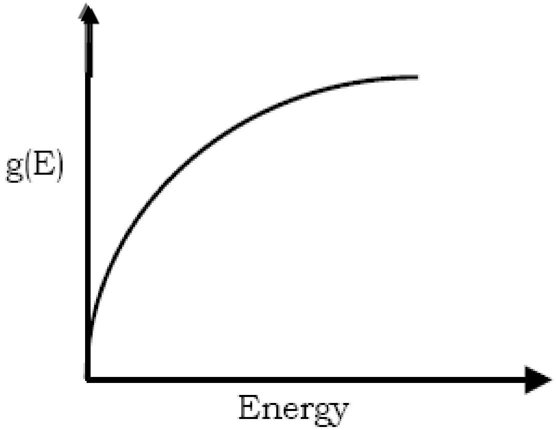
The exact dependence of density of energy levels on the energy is realized through a function denoted as *g(E)* which is known as density of states function.

It is the number of allowed energy levels/unit energy interval in the band associated with the material of unit volume. In an energy band, as *E* changes *g (E)* also changes.

The number of energy levels in the range *E* and *(E + dE)* is obtained by evaluating the product of *g(E)* and *dE.*

$$g(E)dE = \left[\frac{8\sqrt{2}\pi m^{3/2}}{h^3}\right] E^{1/2} dE.$$

A plot of *g(E)* versus *E*



Evaluation of density of states for the electrons in a 3-dimensional solid of unit volume:

We have the equation for the allowed energy for the particle in one dimensional potential well as,

$$E = \frac{n^2 h^2}{8ma^2}$$

where, *n* = 1,2,3,……

h, is the Planck's constant

m, is the mass of the Particle, and

a, is the length over which the particle is free to move in one dimension.

We consider the free electrons in a metal as particles in a 3-dimensional potential well.

$$E = \frac{h^2}{8ma^2}\left(n_x{}^2 + n_y{}^2 + n_z{}^2\right),$$

where, n_x, n_y, n_z are positive integers greater than zero, and, *m* is the mass of the electron.

Let, $\frac{h^2}{8ma^2} = E_0,$ (which is a constant),

And,

$$R^2 = \left(n_x{}^2 + n_y{}^2 + n_z{}^2\right), \quad \therefore E = E_0 R^2.$$

Evaluation of density of states for the electrons in a 3-dimensional solid of unit volume:

The number of allowed energy values up to a maximum energy E= No. of points in the octant of radius R,

= Volume of the octant of sphere of radius R X number of points/unit volume.

If we consider a small energy range between *E & (E + dE)*, then,

The number of allowed energy values in an energy range between E and (E + dE) = No. of points in the space between two octant Shells of radii R and (R +dR) = (Volume of space between two octant shells of radii R and R + dR) X (number of points/unit volume)

$$=\left(\frac{1}{8}\times 4\pi R^2 dR\right)(1)=\frac{1}{2}\pi R^2 dR$$

$\therefore$ The number of allowed energy states in the energy range E and $(E + dE)$

$$=2\times\frac{1}{2}\pi R^2 dR=\pi R^2 dR.$$

Let *g(E)* be the number of energy states/unit energy range. Then the number of energy states in the energy range *E*, and *(E + dE)* is *g (E) dE.*

$$\therefore\ g(E)\,dE=\pi\,R^2\,dR$$

Evaluation of density of states for the electrons in a 3-dimensional solid of unit volume:

$$g(E)dE = \left[\frac{8\sqrt{2}\pi m^{3/2} a^{3}}{h^{3}}\right] E^{1/2} dE.$$

In the above equation, a^3 represents the volume of the solid. If we consider the solid to be of unit volume (*i.e.*, a^3=1), then,

where, is a constant

$$g(E)dE = \left[\frac{8\sqrt{2}\pi m^{3/2}}{h^{3}}\right] E^{1/2} dE.$$

$$= CE^{1/2} dE,$$

$$C = \left[\frac{8\sqrt{2}\pi m^{3/2}}{h^{3}}\right],$$

Is the number of states in an energy range *E* and *(E+dE)* for the electrons in a 3-dimensional solid of unit volume.

Carrier Concentration in Metals- Fermi Energy

Fermi energy and Fermi level as follows. The energy corresponding ton the highest occupied level at zero degree absolute is called the Fermi energy, and the energy level is referred to as the Fermi level. The Fermi energy is denoted as E_F.

Fermi energy: energy at which the probability of occupancy is ***50%***

Metals - small energy difference between the Fermi energy (E_f) and excited state

Conduction electron

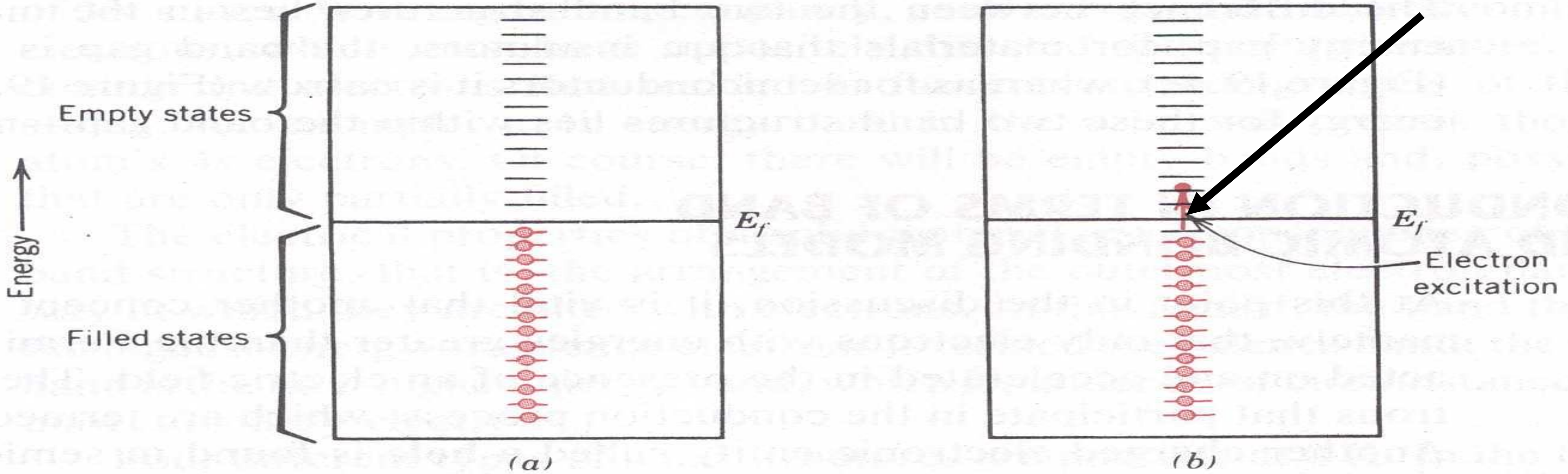
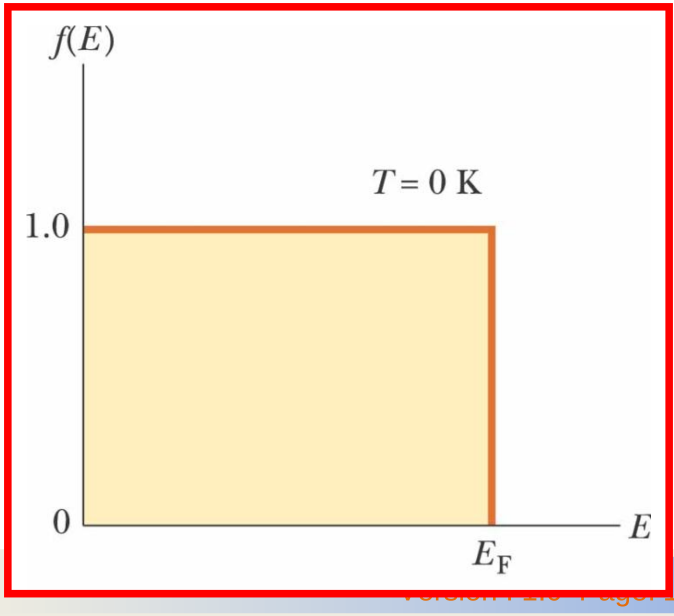


Figure 19.5 For a metal, occupancy of electron states (*a*) before and (*b*) after an electron excitation.

Fermi-Dirac Distribution Function

- **We introduce the probability distribution function, *F*(*E*), which describes the probability that a state with energy *E* is occupied**
- **For electrons this function is the** *Fermi-Dirac Distribution Function*
  - **At $T = 0$**

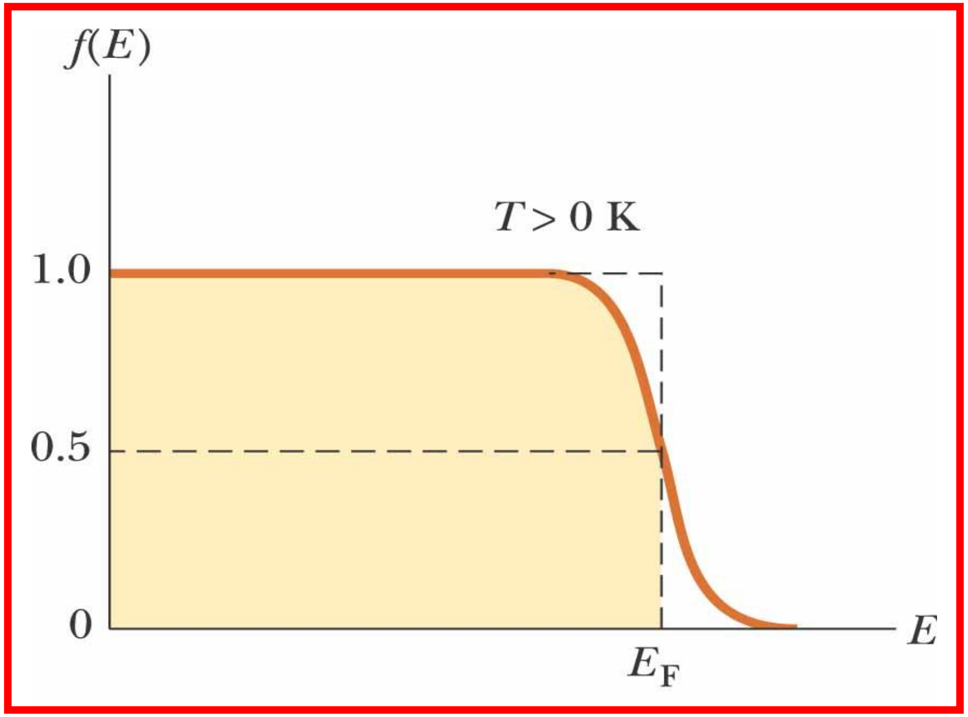
$$f(E) = \begin{cases} 0, \text{for } E > E_F \\ 1, \text{for } E < E_F \end{cases}$$



Fermi-Dirac Distribution Function

- At $T > 0$ K

$$f(E) = \frac{1}{e^{(E - E_F)/k_B T} + 1}$$



Free electron Models

Classical Model:

- **Metal is an array of positive ions with electrons that are free to roam through the ionic array**
  - Electrons are treated as an ideal neutral gas, and their total energy depends on the temperature and applied field
  - In the absence of an electrical field, electrons move with randomly distributed thermal velocities
  - When an electric field is applied, electrons acquire a net drift velocity in the direction opposite to the field

Quantum Mechanical Model:

- **Electrons are in a potential well with infinite barriers: They do not leave metal, but free to roam inside**
  - Energies that electrons can have are discrete (quantized) and well defined, so the assumption about electron thermal velocity is wrong
  - Electrons occupy energy levels according to Pauli's exclusion principle
  - Electrons acquire additional energy when electric field is applied

Consequences for Metal Theories

- **At $T = 0$ K**

$$\boxed{E_F(0) = \frac{\hbar^2}{2m_e}\left(3n_e\pi^2\right)^{2/3}}$$

  - – n_e is the electron density, i.e. the number of electrons per unit volume of metal

- **Calculations show that**

$$\boxed{E_F(0) \sim 5 - 10\,\mathrm{eV}}$$

- **Thermal energy at room temperature:**

$$k_B T \sim 0.025 \text{ eV} \;\Rightarrow\; k_B T \ll E_F(0)$$

Consequences for Metal Theories

- **Only electrons occupying levels close to the Fermi Energy will participate in the conduction, since only these electrons can be excited into the higher energy states by the electric field**
- **From QM point of view, energy supplied by the electric field excites electrons into higher lying energy levels**
- **We can consider that "conducting" electrons move in real space with the speed corresponding to the Fermi Energy**

Temperature Dependence of Metals Resistivity

Let's introduce the Fermi velocity:

$$E_F = \frac{1}{2} m v_F^2, \; v_F = \sqrt{\frac{2E_F}{m_e}}$$

Then:

$$\frac{1}{\rho} = \sigma = \frac{q^2 n_e \tau}{m}$$

$$\tau = \frac{l}{v_F}$$

⇒

$$\sigma = \frac{q^2 n_e l}{m v_F}$$

$$\rho = \frac{m v_F}{q^2 n_e l}$$

Conductivity of Metals

There is still a problem, since according to our definition of the free mean path, the conductivity is temperature independent

$$\boxed{\sigma = \frac{q^2 n l}{m v_F}}$$

QM resolves the problem:

Electrons inside the metal have de Broglie wavelength:

$$\boxed{\lambda_F = \frac{h}{p_F} = \frac{h}{\sqrt{2m_e E_F}} \sim 3-5\,\mathring{A}}$$

But wave in a crystal lattice undergoes Bragg scattering when the condition, $2d\sin\theta = n\lambda$, is satisfied. If $\lambda > 2d$, Bragg scattering cannot occur at any angle. In copper, $\lambda_F = 4.65\ A$, while, $d = 2.09\ A$. So Bragg scattering cannot occur.

Conductivity of Metals

Thus, the scattering mechanism is not collisions of electrons with ions, but rather scattering of electron wave from deviations in the crystal that may arise from imperfections in the lattice or vibrations of the ions in the lattice

In a high quality metal the latter mechanism dominates

When the atoms vibrate the lattice is no longer ideal and presents an effective cross sectional area for scattering of $\pi r^{2,}$ where r is the amplitude of vibration.

The electron mean free path l is inversely proportional to the scattering cross section

$$l = \frac{1}{\pi r^2}$$

But the energy of a vibrating atom, $E \sim r^2 \sim kT$

So $l \sim 1/T$

Hence

$$\sigma = \frac{e^2 n l}{m v_F} \sim \frac{1}{T}$$