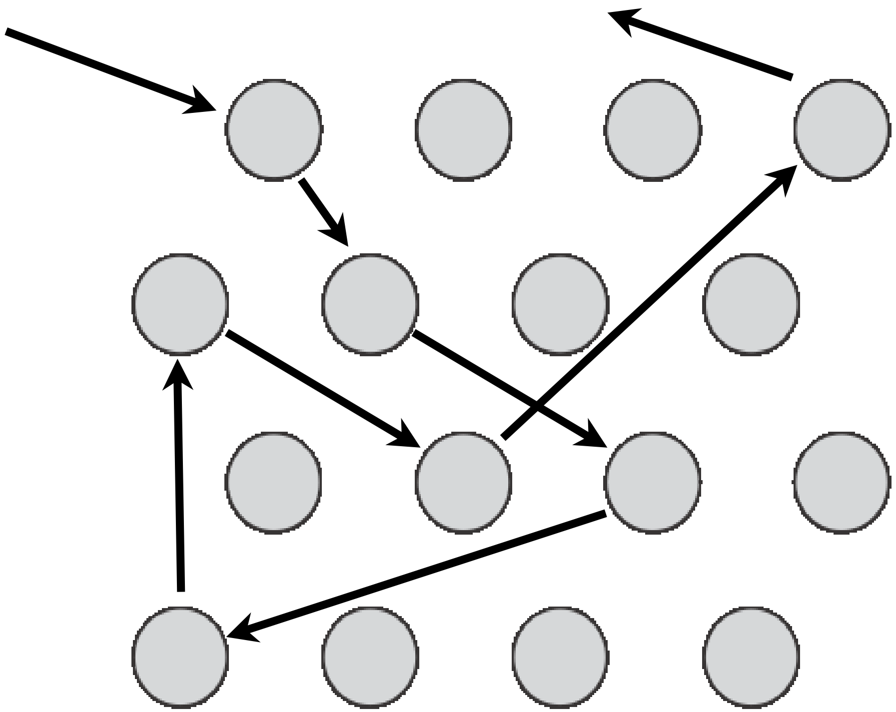
METALS-Drude's classical theory

- Theory by Paul Drude in 1900, only three years after the electron was discovered.
- Drude treated the (free) electrons as a **classical ideal gas** but the electrons should collide with the stationary ions, not with each other.



average speed

$$\frac{1}{2}mv_t^2 = \frac{3}{2}k_BT$$

$$v_t = \sqrt{\frac{3k_BT}{m}}$$

so at room temp.

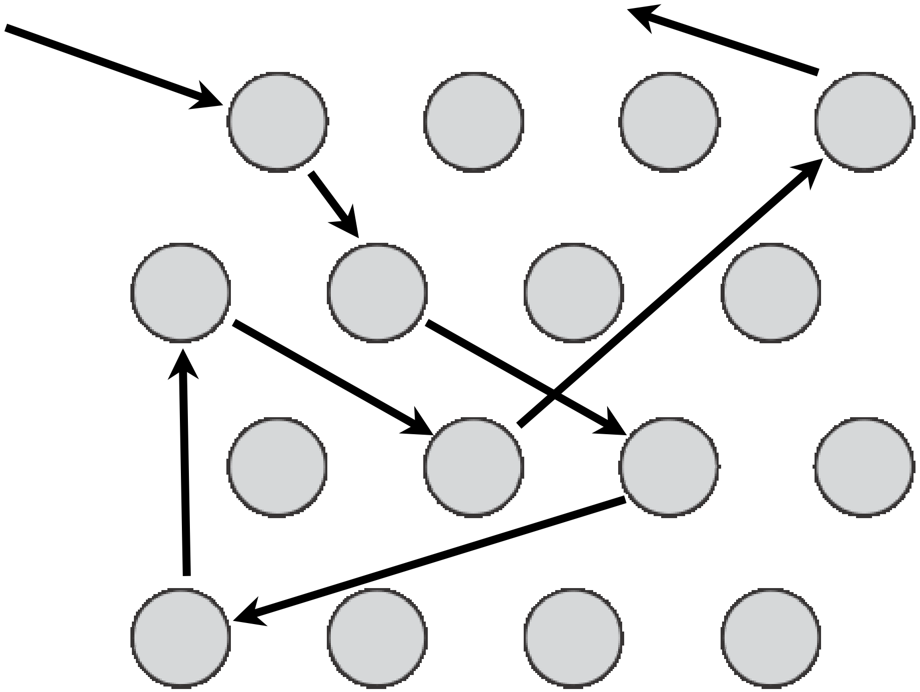
$$v_t \approx 10^5 \mathrm{ms}^{-1}$$

Drude's classical theory

relaxation time τ

scattering probability per unit time $1/\tau$

mean free path $\lambda = \tau v_t$



$$v_t \approx 10^5 \mathrm{ms}^{-1}$$

$$\lambda \approx 1\mathrm{nm}$$

$$\tau \approx 1 \times 10^{-14} \mathrm{~s}$$

classical ideal gas

Drude theory: electrical conductivity

Ohm's law

$$j = \frac{ne^2\tau}{m_e}E$$

$$j = \sigma E = \frac{E}{\rho}$$

and we can define the conductivity

$$\sigma = \frac{ne^2\tau}{m_e} = n\mu e$$

and the resistivity

$$\rho = \frac{m_e}{ne^2\tau} = \frac{1}{n\mu e}$$

and the mobility

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

classical ideal gas

Validity of Ohm's law

- Valid for metals.
- Valid for homogeneous semiconductors

Failures of the Drude model: heat capacity

consider the classical energy for one mole of solid in a heat bath: each degree of freedom contributes with $\frac{1}{2}k_B T$

- Experimentally, one finds a value of about $3N_\mathrm{A}k_\mathrm{B}$ at room temperature, independent of the number of valence electrons (rule of Dulong and Petit), as if the electrons do not contribute at all !!!!

Description by DOS - electron continuum
Only state close to so called Fermi energy contribute

5

Description by DOS- electron continuum

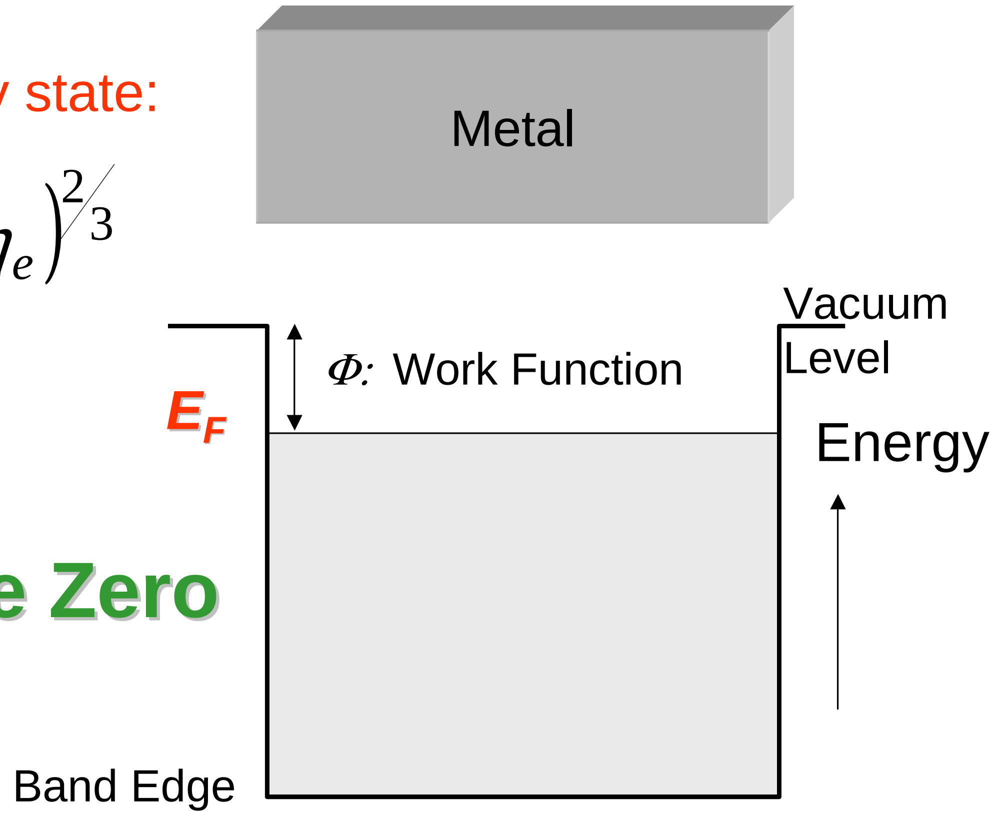
Fermi Energy – highest occupied energy state:

$$E_F = \frac{\hbar^2 k_F^2}{2m} = \frac{\hbar^2}{2m}\left(3\pi^2\eta_e\right)^{2/3}$$

Fermi Velocity: $v_F = \frac{\hbar}{m}\left(3\pi^2\eta_e\right)^{1/3}$

Fermi Temp: $T_F = \frac{E_F}{k_B}$

Absolute Zero



Element	Electron Density, η_e [10^{28} m^{-3}]	Fermi Energy E_F [eV]	Fermi Temperature T_F [10^4 K]	Fermi Wavelength λ_F [Å]	Fermi Velocity v_F [10^6 m/s]	Work Function Φ [eV]
Cu	8.47	7.00	8.16	4.65	1.57	4.44
Au	5.90	5.53	6.42	5.22	1.40	4.3
Fe	17.0	11.1	13.0	2.67	1.98	4.31
Al	18.1	11.7	13.6	3.59	2.03	4.25

Number and Energy Densities

classical ideal gas replaced by Electron Density of States- DOS

Number density: $$\eta_e = \frac{N}{V} = \int_0^{\infty} f(E) D_e(E) dE;$$

Energy density: $$\in_e = \frac{E_e}{V} = \int_0^{\infty} E f(E) D_e(E) dE$$

Density of States - Number of electron states available between energy *E* and *E+dE*

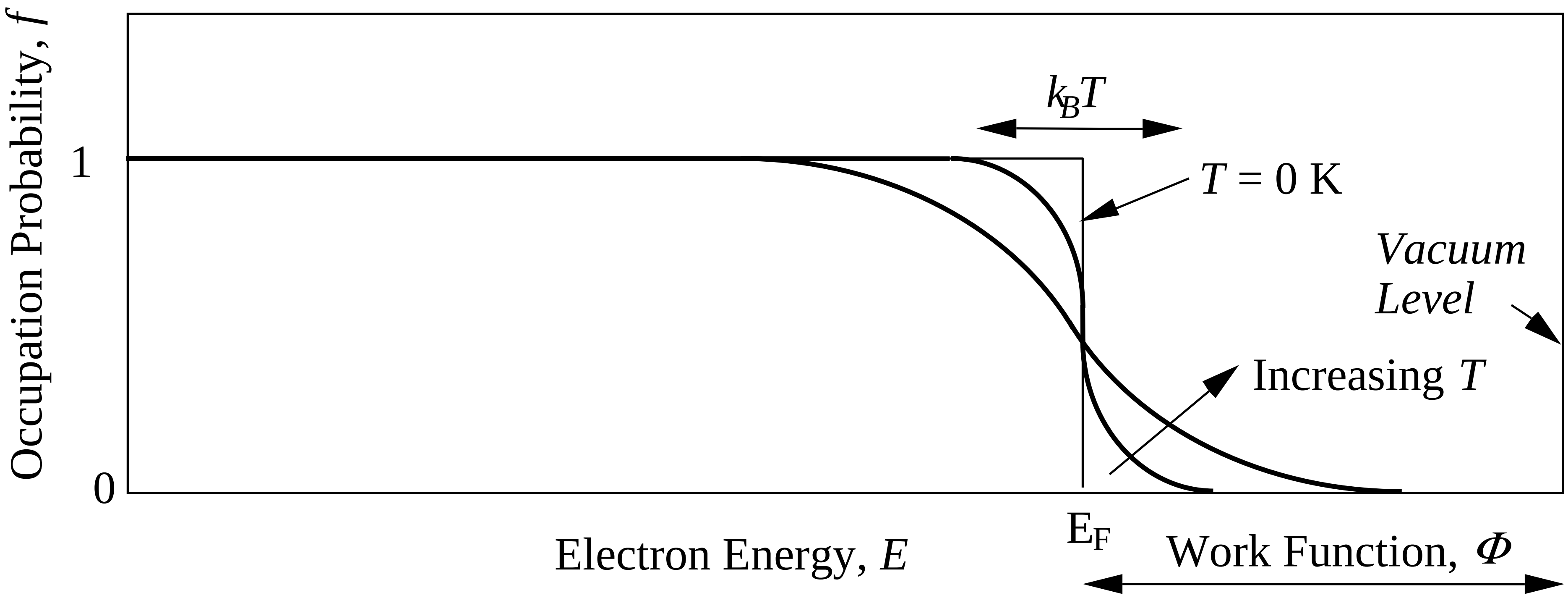
$$D_e(E) = \frac{m}{\hbar^2 \pi^2} \sqrt{\frac{2mE}{\hbar^2}}$$ in 3D

Effect of Temperature

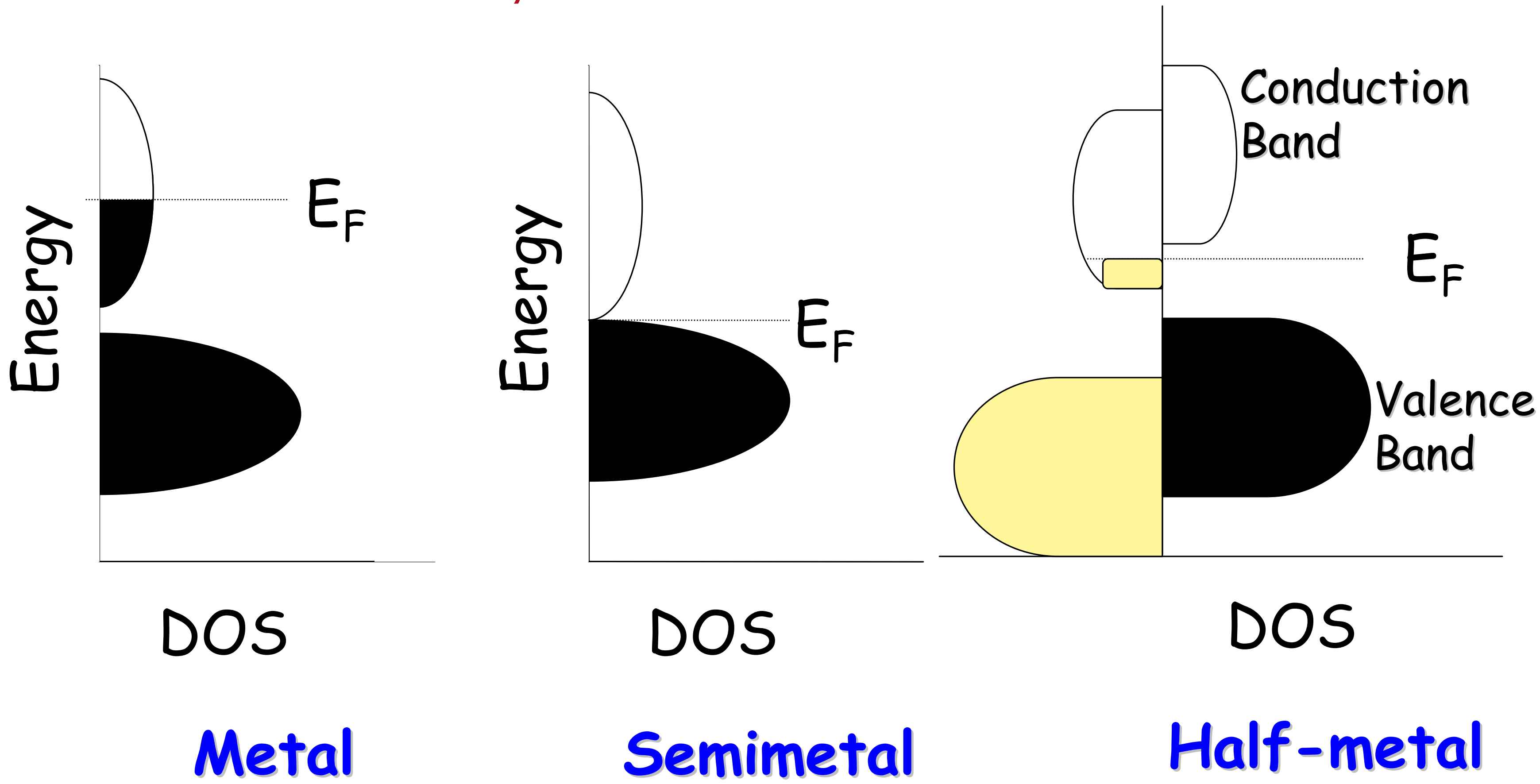
Fermi-Dirac equilibrium distribution

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

for the probability of electron occupation of energy level *E* at temperature *T*

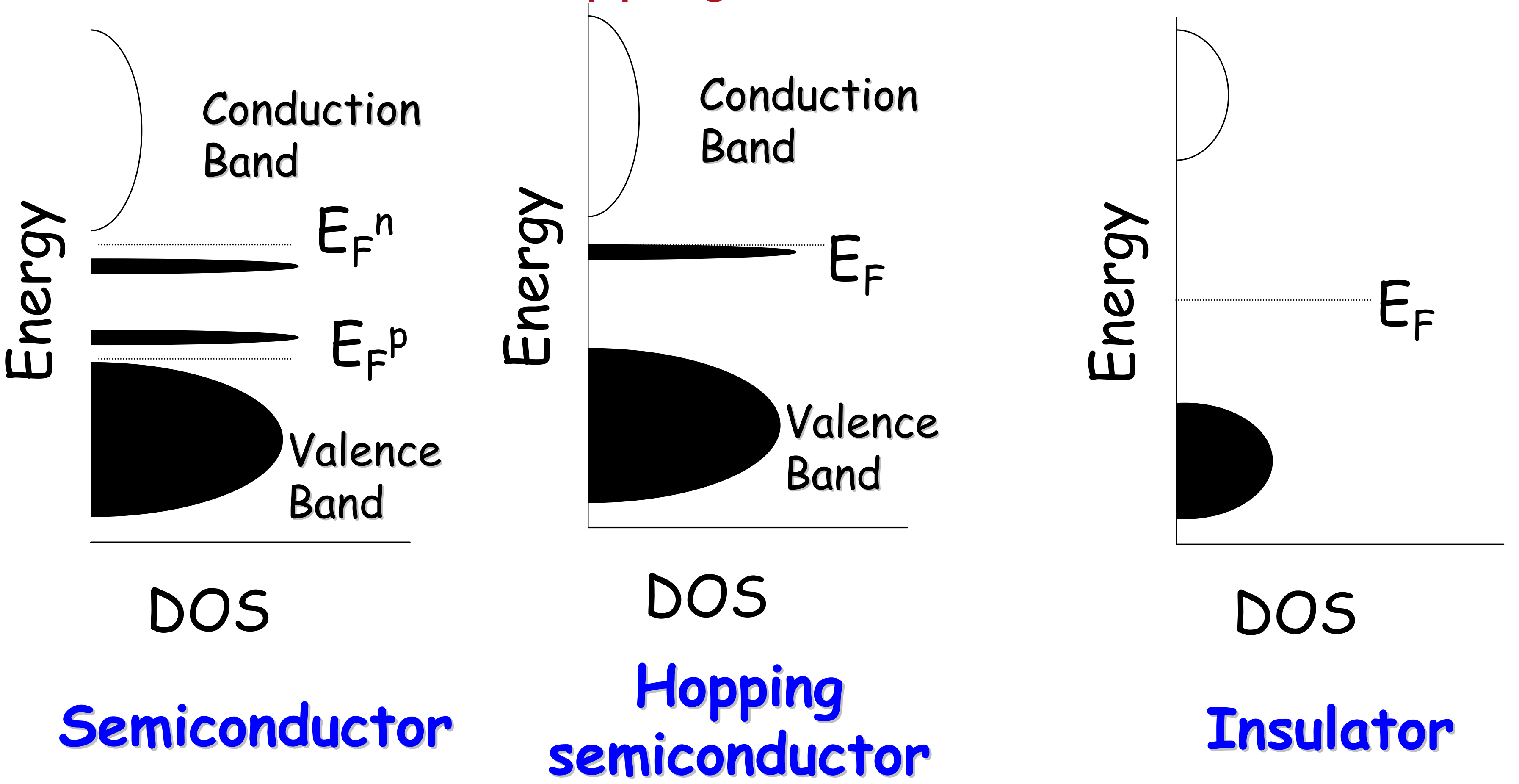


Metals, Semimetal & Half-metal



In a metal the Fermi level cuts through a band to produce a partially filled band. A semimetal results when the band gap goes to zero. A half metal results when there is only one spin (up or down) of charge carriers.

Semiconductors, Hopping conductors & Insulators



In a semiconductor/insulator there is an energy gap between the filled bands and the empty bands. The distinction between a semiconductor and an insulator is artificial, but as the gap becomes large the material usually becomes a poor conductor of electricity. A hopping semiconductor results when the Fermi level falls within narrow band, $W<k_BT$, polarons, impurities, disorder.

Electrical transport-Temperature Dependence-

$$\sigma = n e^2\tau / m^*$$

- **In Metals**
  - The carrier concentration, n, changes very slowly with temperature.
  - τ is inversely proportional to temperature ($\tau \propto 1/T$), due to scattering by lattice vibrations (phonons).
  - Therefore, a plot of σ vs. 1/T (or ρ vs. T) is essentially linear.
  - **Conductivity goes down as temperature increases**
- **In Semiconductors-**
  - The carrier concentration increases as temperature goes up, due to excitations across the band gap, E_g.
  - n is proportional to $\exp\{-E_g/2kT\}$.
  - τ is inversely proportional to temperature
  - The exponential dependence of n dominates, therefore, a plot of ln σ vs. 1/T is essentially linear.
  - **Conductivity increases as temperature increases**.

The Wiedemann-Franz law
link between thermal and electrical conductivity

$$\frac{\kappa}{\sigma} = constant$$

$$\frac{\kappa}{\sigma T} = L$$

- Wiedemann and Franz found in 1853 that the ratio of thermal and electrical conductivity for ALL METLALS is constant at a given temperature (for room temperature and above). Later it was found by L. Lorenz that this constant is proportional to the temperature.
- Let’s try to reproduce the linear behaviour and to calculate L here.

The Wiedemann Franz law

Thermal conductivity

$$\kappa = \frac{1}{3} v_t^2 \tau c_v$$

$$\sigma = \frac{ne^2\tau}{m_e}$$

Electrical conductivity

estimated thermal conductivity
(from a classical ideal gas)

$$\frac{\kappa}{\sigma} = \frac{3}{2}\frac{k_B^2}{e^2}T = LT.$$

the actual quantum mechanical result is

$$\frac{\kappa}{\sigma} = \frac{\pi^2}{3}\frac{k_B^2}{e^2}T = LT.$$

Comparison of the Lorenz number to experimental data

at 273 K

metal	10^{-8} Watt Ω K^{-2}
Ag	2.31
Au	2.35
Cd	2.42
Cu	2.23
Mo	2.61
Pb	2.47
Pt	2.51
Sn	2.52
W	3.04
Zn	2.31

$$\frac{\kappa}{\sigma} = \frac{\pi^2}{3}\frac{k_B^2}{e^2}T = LT$$

L = 2.45 10^{-8} Watt Ω K^{-2}

The electronic properties of metals, semimetals, half-metals, semiconductors and insulators