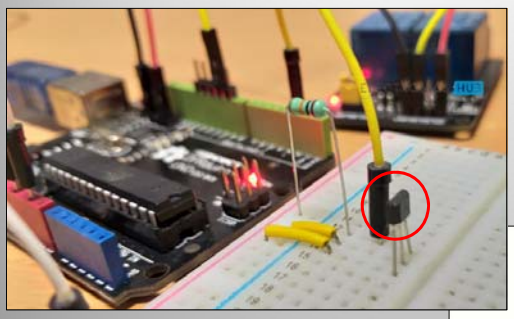
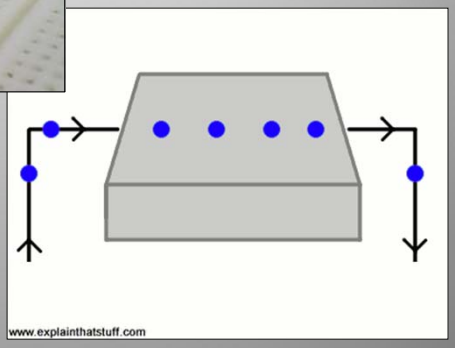
Dr. Gregory W. Clark
Manchester University

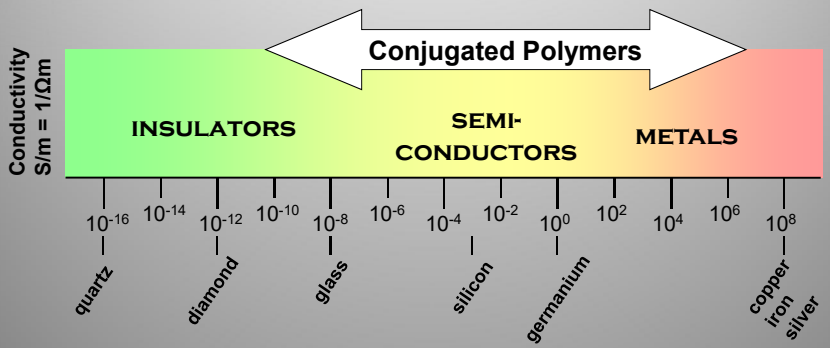




PHYS432
Materials Physics

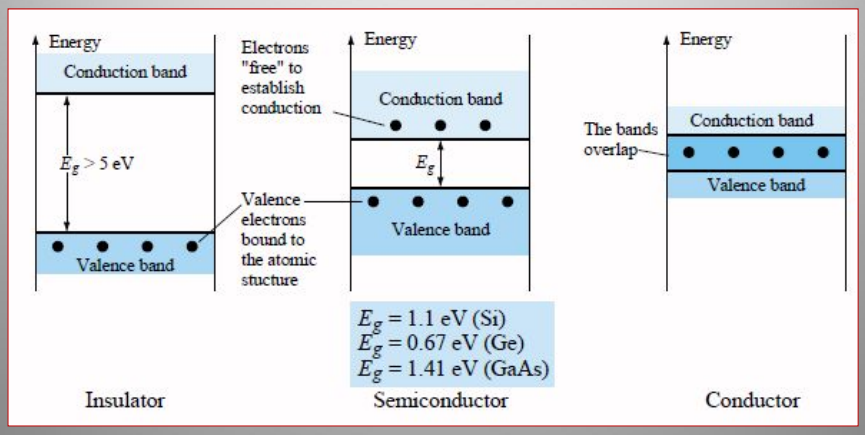
Electrical conductivity

- Wide range of values!
- Early attempts to model:
  - Drude: free electron gas
  - Sommerfeld: quantum free electron gas



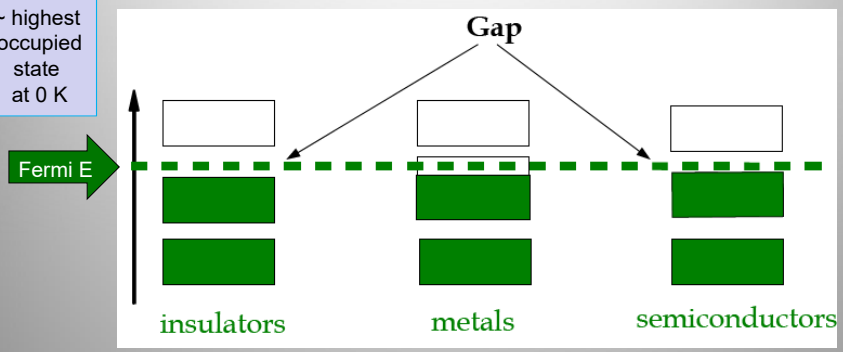
Electrical conductivity

- Modern models: much more complicated!
- **Band theory** is an important model



ENERGY BANDS IN SOLIDS

Fermi E: ~ highest occupied state at 0 K



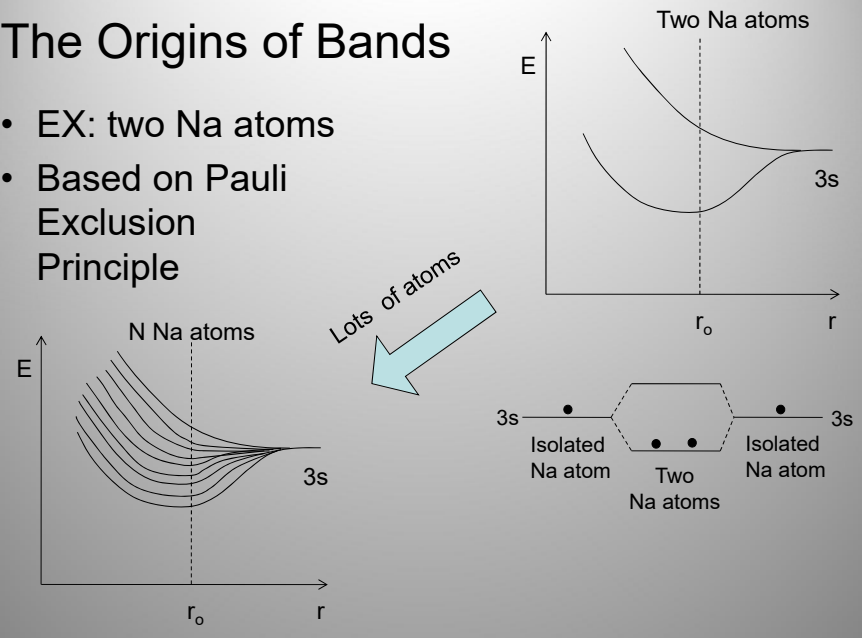
Fermi energy lies in the gap; gap is relatively large (~10 eV); e- cannot be excited to higher states

Fermi energy lies in band of accessible states!

Fermi energy lies in the gap; gap is relatively small (~1 eV); some e- can be thermally excited to higher states

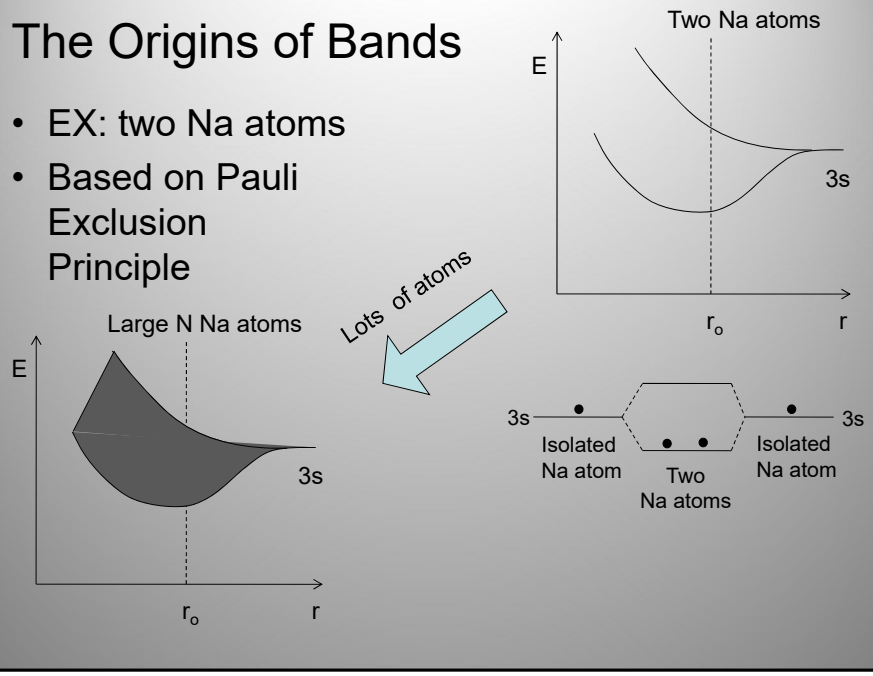
The Origins of Bands

- EX: two Na atoms
- Based on Pauli Exclusion Principle

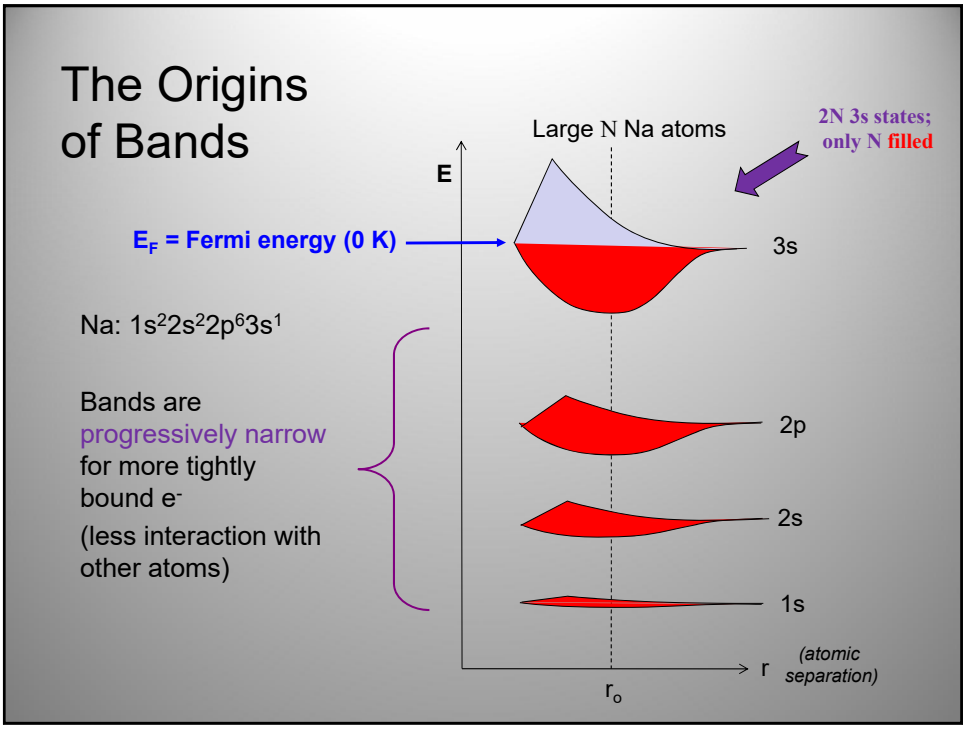


The Origins of Bands

- EX: two Na atoms
- Based on Pauli Exclusion Principle



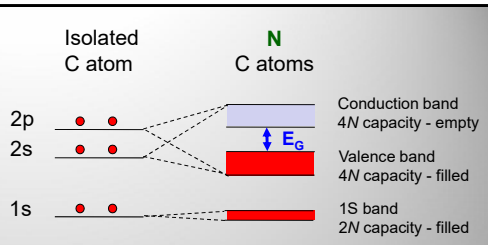
The Origins of Bands



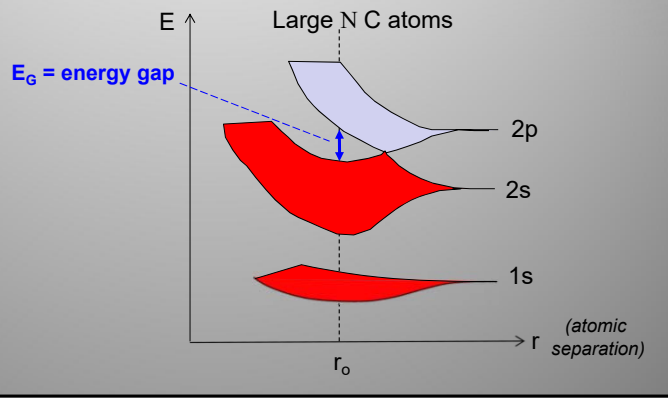
Na: $1s^2 2s^2 2p^6 3s^1$

Bands are progressively narrow for more tightly bound e⁻ (less interaction with other atoms)

The Origins of Bands: C (diamond)

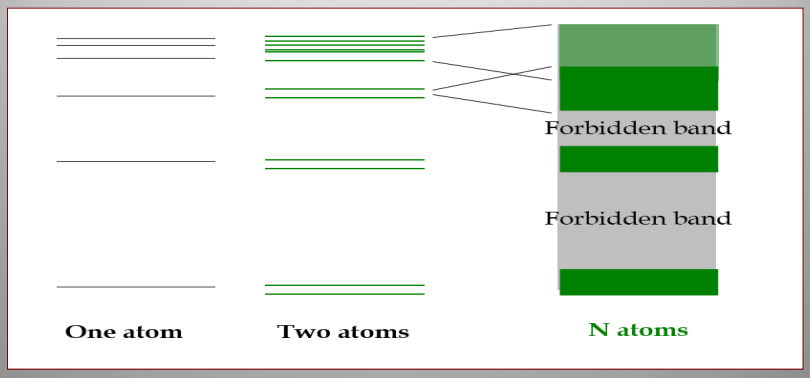


C: $1s^2 2s^2 2p^2$

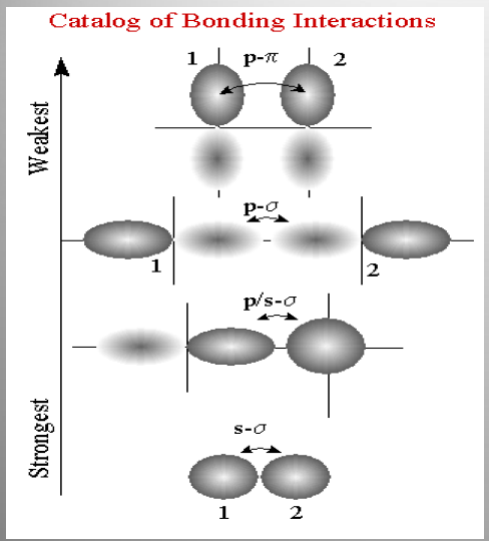


E Bands: Another view

- Pauli exclusion principle holds: no two e- in same state.



LCOA – Language of Chemists



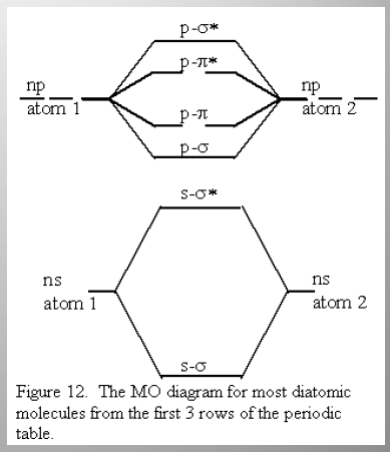
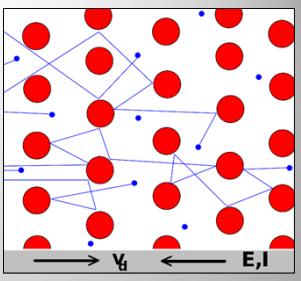


Figure 12. The MO diagram for most diatomic molecules from the first 3 rows of the periodic table.

voh.chem.ucla.edu/vohtar/winter00/20A/lec6.html

Drude model: free electron gas



- only free *e*- contribute to conduction

$$n = \text{conduction e- density} = \frac{p_a Z_V}{V}$$

where p_a = # e-/unit cell, Z_V = # valence e-/atom
and V = volume of unit cell

- estimate (random) velocities of *e*-:

$$\frac{1}{2} m v_t^2 = \frac{3}{2} k_B T \quad (v_t = \text{thermal velocity})$$

[v_t ~ 10^5 m/s @ RT]

- in an applied electric field:

$$\vec{v}_d = -\frac{e\tau}{m}\vec{E} \quad (v_d = \text{drift velocity})$$

[v_d ~ 0.02 m/s @ E ~ 10 V/m]

here, τ = relaxation time $= \sqrt{\lambda^2/(3k_B T)}$, λ = mean free path

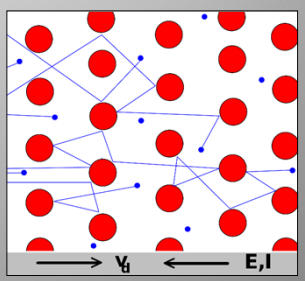
Drude model: free electron gas

- so the conductivity can be written as

$$\sigma = n\left(\frac{e\tau}{m}\right)e = n\,\mu_e\,e, \text{ where } \mu = \text{electron mobility}$$

- σ measures ease with which e- move through material
- correctly predicts

$$\vec{J} = \sigma\vec{E} \quad \text{(Ohm's law)}$$



Drude model successes

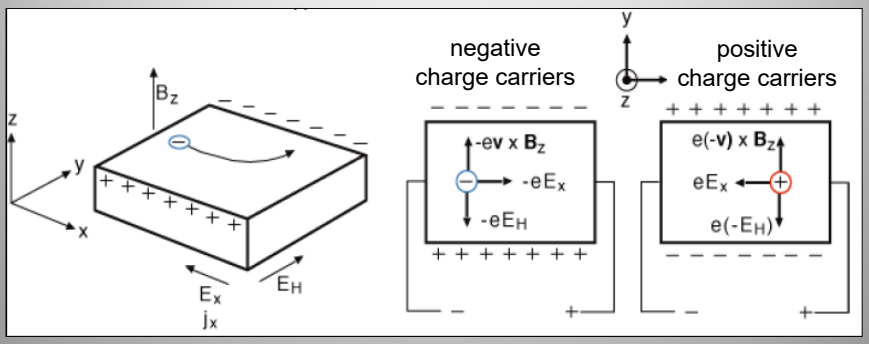
The Drude model contained some very extreme simplifications: electrons treated as classical, ideal gas. The Drude Model was quite successful at explaining a number of observed phenomena of metals:

First Ohm's law prediction!
Electrical conductivity, σ
Classical Hall effect
Plasma frequency
Thermal conductivity, κ
Wiedemann-Franz Law: $\kappa/\sigma \sim T$

Source: Kings College

Classical Hall Effect (Hall, 1879)

Effect of magnetic field on the current in a conductor



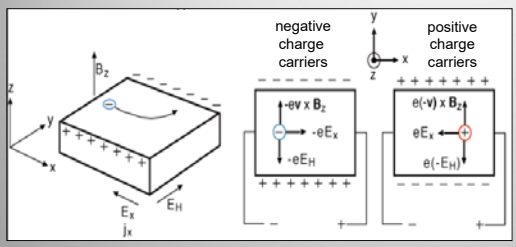
Hall: magnetic field B_z deflects current (charges) resulting in E_H that is perpendicular to both the B-field and current.

$$E_H = R_H J_x B_z$$

See section 4-4 of Stokes

Source: Kings College

Classical Hall Effect (Hall, 1879)



$$E_H = R_H J_x B_z$$

The Lorentz force magnetic force is compensated by the Hall electric force:

$$-eE_H = -evB_z$$

$$\frac{eE_H}{evB_z} = \frac{neE_H}{nevB_z} = \frac{neE_H}{-J_x B_z} = \frac{E_H}{R_H J_x B_z}$$

Measuring the Hall coefficient provides direct experimental access to charge densities!

where $R_H = -\frac{1}{en}$

Recall that $J = - n e v$

Source: Kings College

Drude model failures

Hall effect: no T or B_z dependence of R_H and does not allow for positive values:

Metal	1/(neR$_H$)
Drude	-1
Na	-1.2
K	-1.1
Ag	-1.3
Al	+0.3

No temperature dependence of electrical conductivity

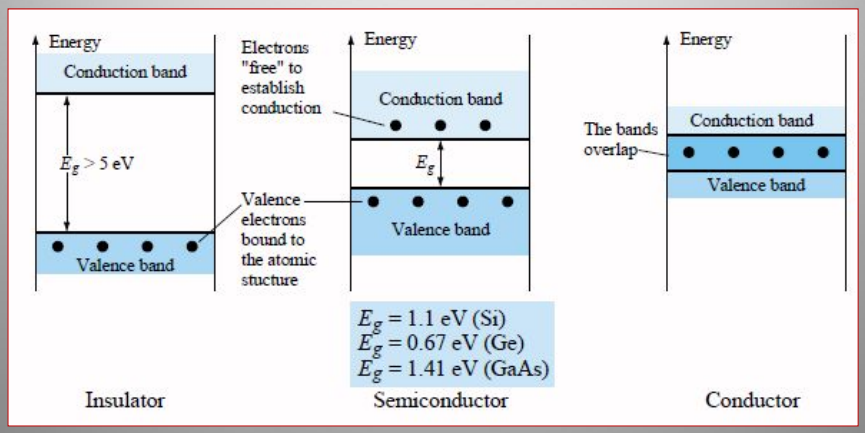
No explanation for varying number of conduction e-

No room for band structure

Low T specific heat behavior incorrect

Electrical conductivity

- Modern models: much more complicated!
- Band theory is an important model



Sommerfeld Theory

The application of quantum mechanics to statistical mechanics led to modification of Drude's theory to a more apt theory for the many-fermion system.

Source: Kings College

Sommerfeld Theory

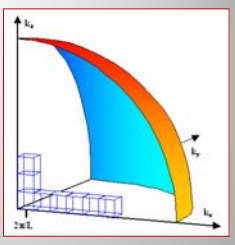
The application of quantum mechanics to statistical mechanics led to modification of Drude's theory to a more apt theory for the many-fermion system.

Fermi-Dirac distribution approaches Maxwell-Boltzmann distribution at large T; most striking differences occur in the vicinity of absolute zero.

Room temperature still low enough for Sommerfeld model to achieve better predictions; most improvements related to thermodynamic phenomena.

Source: Kings College

Quantum Free Electron Gas: Density of available states



- Start with the simple cubic lattice!
- Some definitions:

$$V = L^3 = \text{volume of unit cell in real space}$$

$$V_G = \left(\frac{2\pi}{L}\right)^3 = \text{cubic "volume" of unit cell in k-space}$$

$$D_G = \left(\frac{L}{2\pi}\right)^3 = \frac{V}{(2\pi)^3} = \text{density of lattice points in k-space}$$

- Each value of *k* is a different state, but e- can have 2 spin states, so

$$g_k(\vec{k}) = \text{density of e- states in k-space} = 2D_G = 2\left(\frac{L}{2\pi}\right)^3$$

Quantum Free Electron Gas: Density of available states

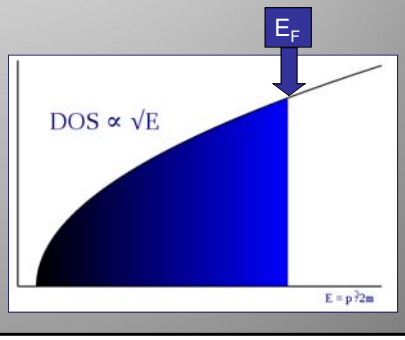
	E_F(eV)
Na	3.22
Cu	7.00
Ag	5.46
Al	11.58

- For electrons in a SC solid of lattice parameter L, the density of states as a function of energy

$$g(E) = (V / 2\pi^2)(2m / \hbar^2)^{3/2} E^{1/2}$$

- The *Pauli Exclusion Principle* requires that we "fill up" this distribution starting at the lowest E
- Energy of the highest state at T=0 is the Fermi energy, E_F:

$$E_F = (\hbar^2 / 2m)(3\pi^2 N / V)^{2/3}$$
$$= (\hbar^2 / 2m)(3\pi^2 n)^{2/3}$$



What about T > 0?

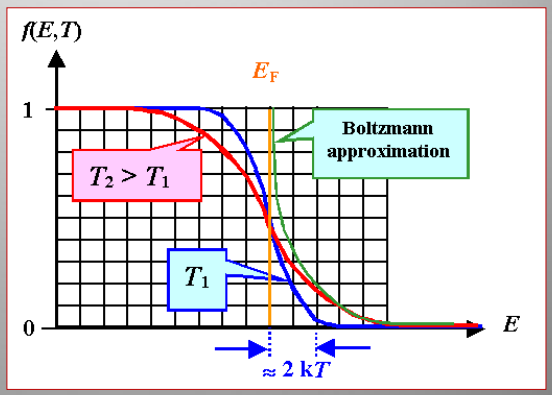
- Fermi-Dirac distribution function:

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

where E_F is the Fermi energy and k_B is the Boltzman constant

At T = 0,

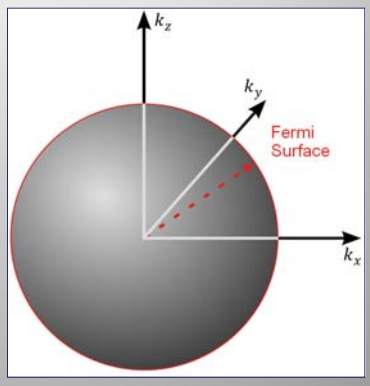
$$f(E) = \begin{cases} 1, & E < E_F \\ 0, & E > E_F \end{cases}$$



Fermi Surface

- In 3 dimensions, we can define a sphere in k-space of radius

$$k_F = \sqrt{\frac{2mE_F}{\hbar^2}}$$



- Electrons having values of k on the surface of this sphere are at the Fermi energy (T = 0)

$$E_F = \frac{4\hbar^2\pi^2}{2mL^2}(n_x^2 + n_y^2 + n_z^2)$$

$$\vec{k} = n_x\frac{2\pi}{L}\hat{i} + n_y\frac{2\pi}{L}\hat{j} + n_z\frac{2\pi}{L}\hat{k}$$

So, the density of *occupied* states is then

$$DOS = f(E)\,g(E)$$

- The total number of conduction electrons is given by

$$N = \int_0^\infty f(E)\,g(E)\,dE$$

* Note that the Fermi energy is a function of temperature; must be chosen to satisfy this integral.