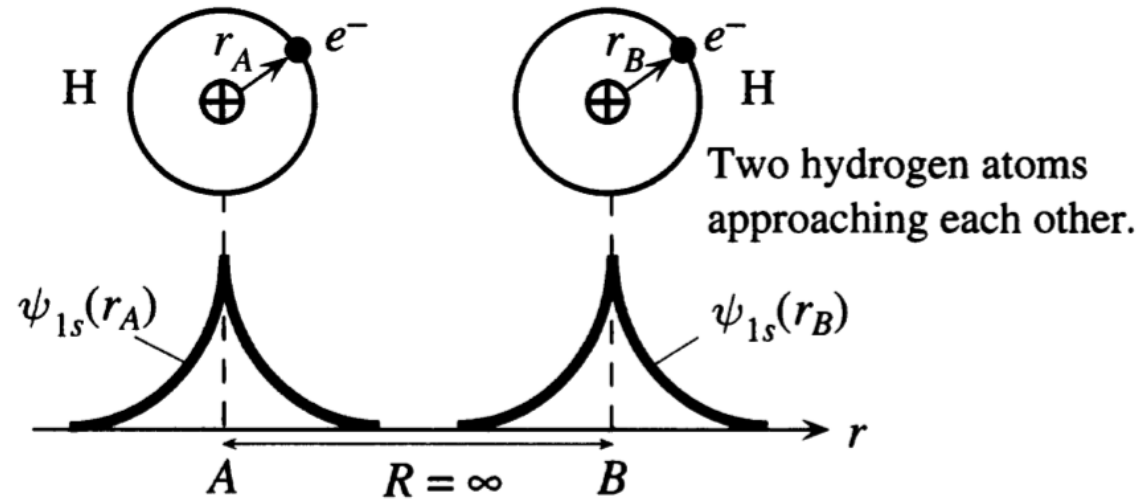


Band Theory of Solids



Let us bring two hydrogen atoms together!

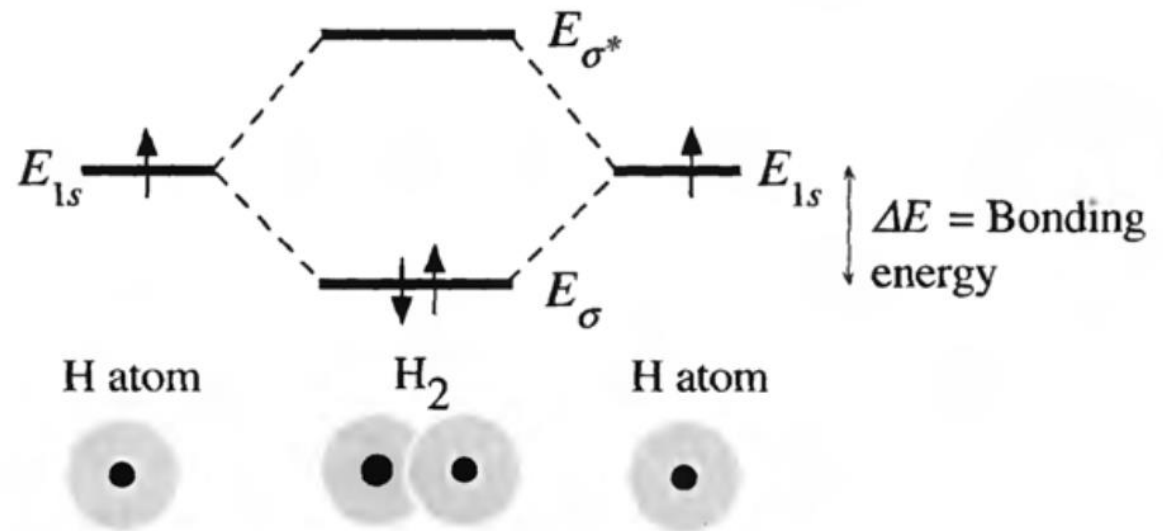
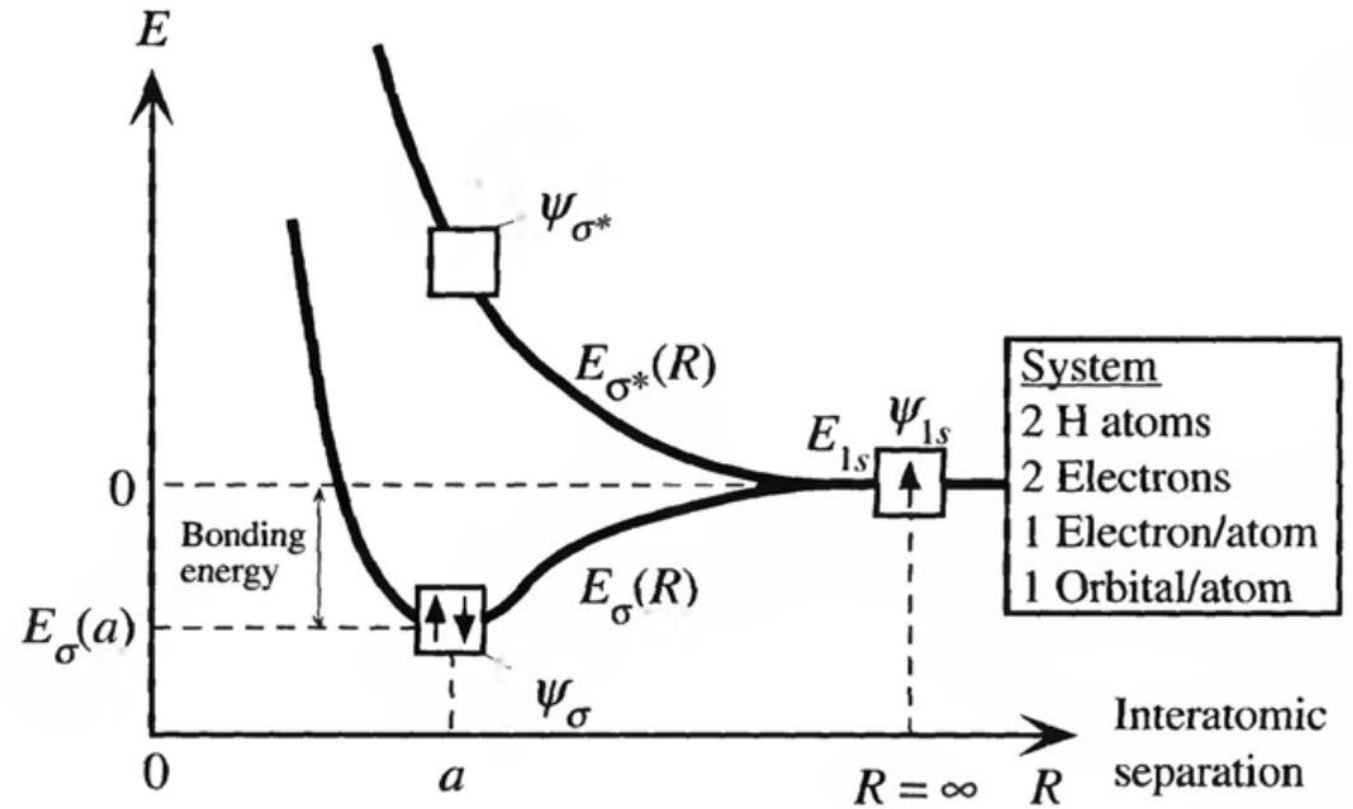
Each having a single electron with wavefunction $\psi_{n,l,m,s}(r_A)$ and $\psi_{n,l,m,s}(r_B)$

When we bring them together, The electrons interact via coulombic forces!

The interaction changes the electronic potentials, They also lead to newer energy states!

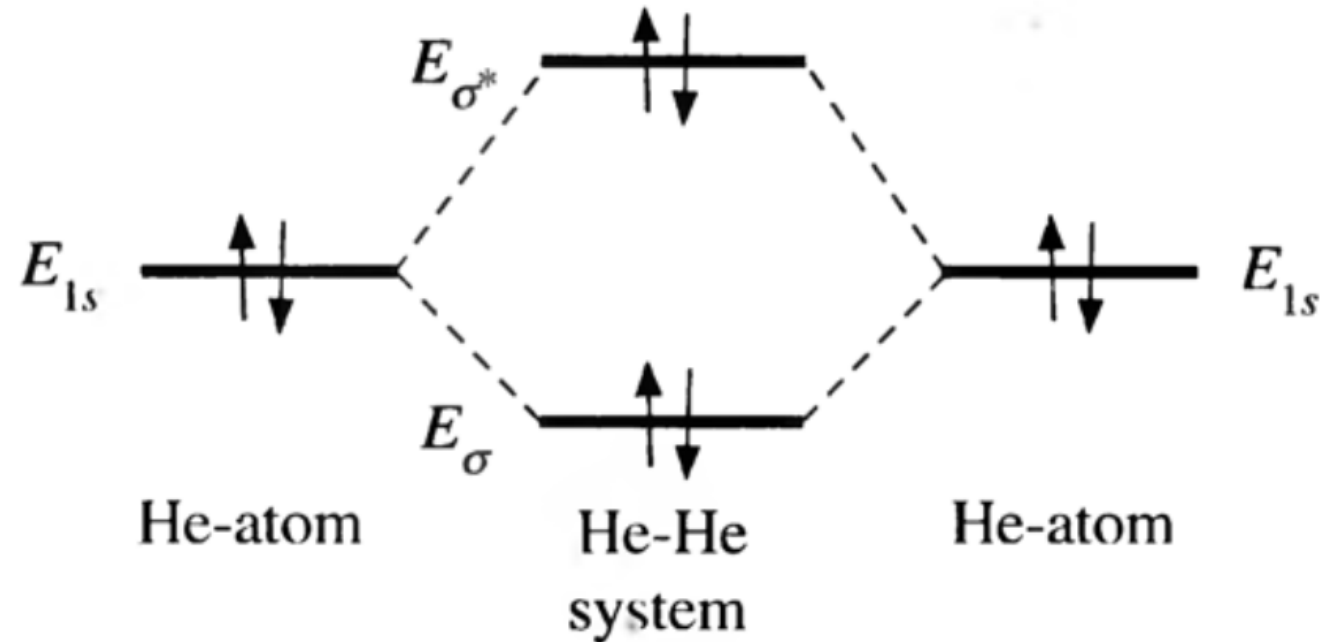
Two types of bonding

- Bonding states
 - Symmetric
 - No nodes
 - Lower energy than summation
- Anti-Bonding
 - Anti-symmetric
 - Nodes
 - Higher total energy than summation!



Case of He

- Each atom has paired electrons
- Both bonding and anti-bonding needs to be filled!
- Pairing has overall higher energy than isolated atoms!



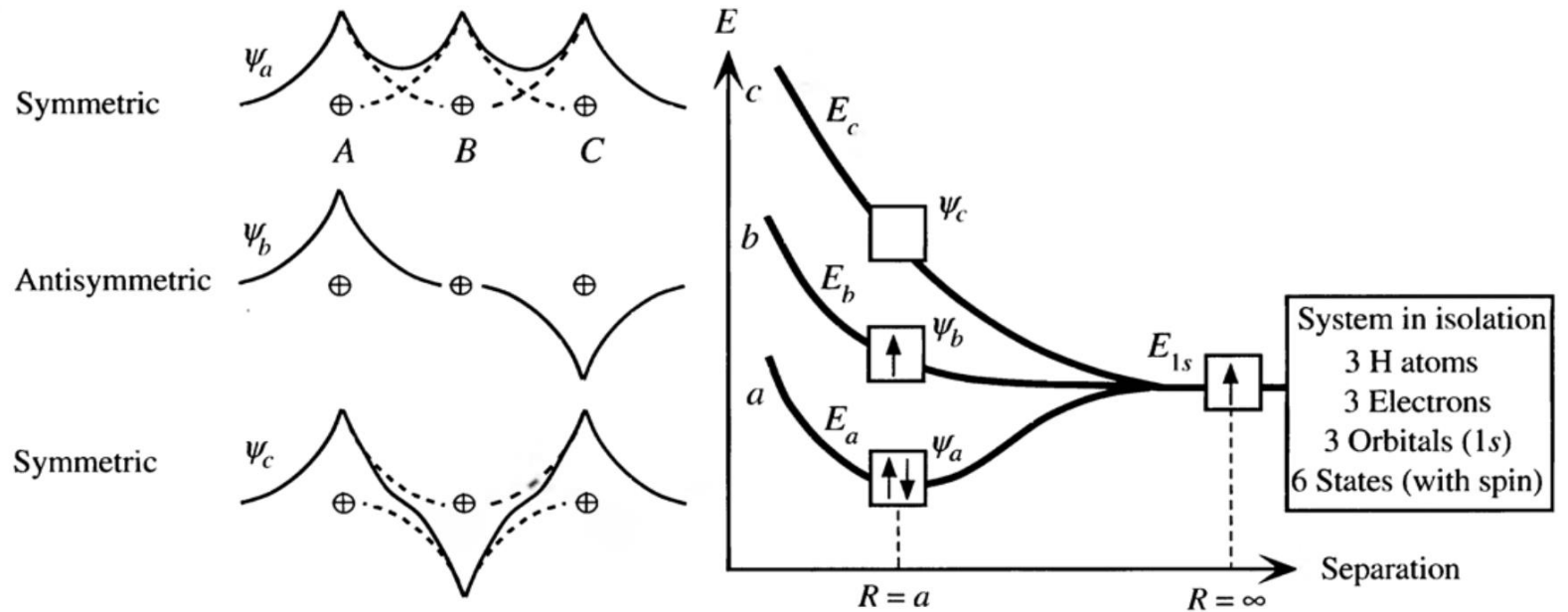
What happens if we bring 3 Hydrogen atoms

$$\psi_a = \psi_{1s}(A) + \psi_{1s}(B) + \psi_{1s}(C)$$

$$\psi_b = \psi_{1s}(A) - \psi_{1s}(C)$$

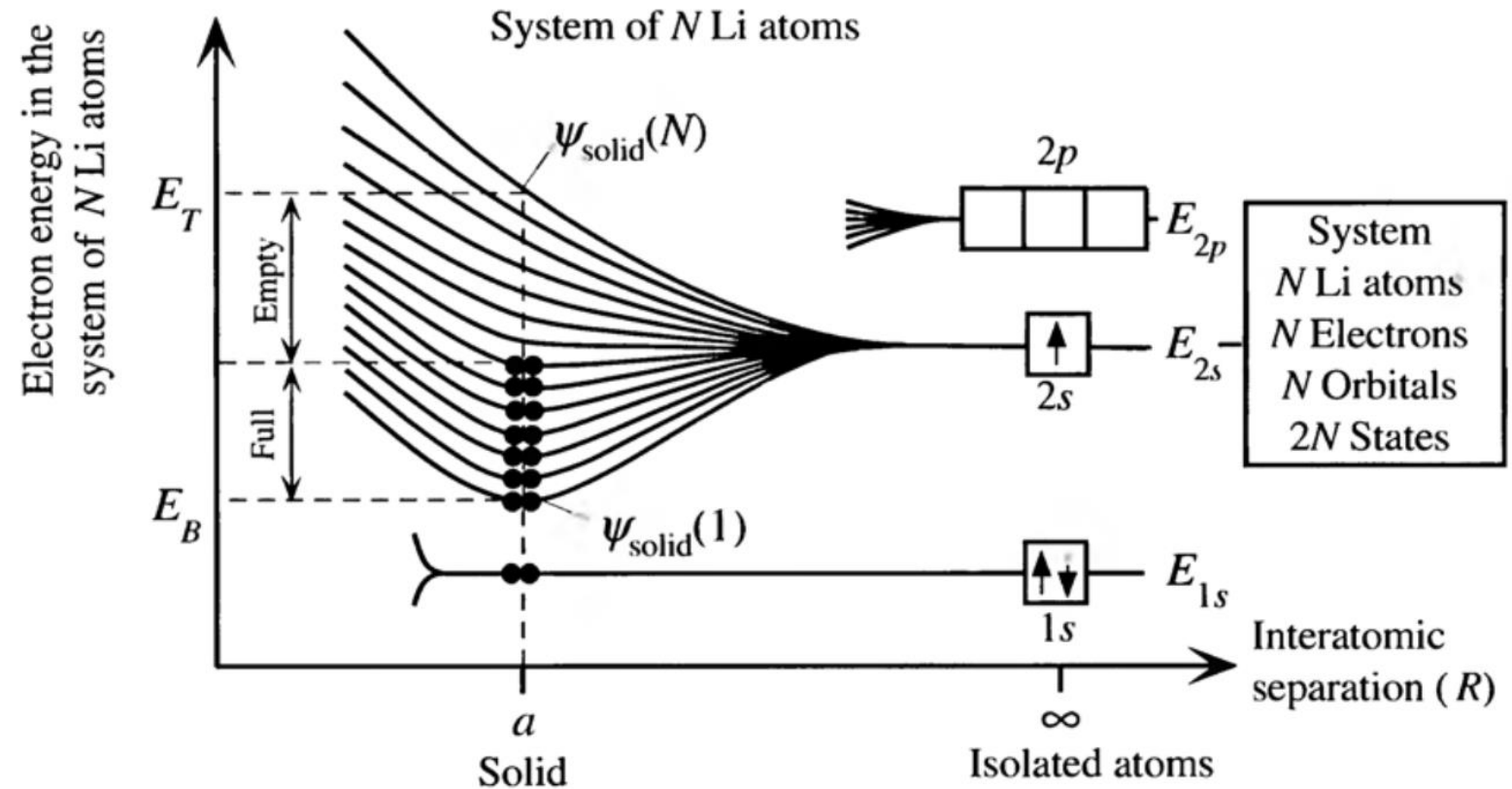
$$\psi_c = \psi_{1s}(A) - \psi_{1s}(B) + \psi_{1s}(C)$$

Adding a node to the wavefunction will increase its energy level.

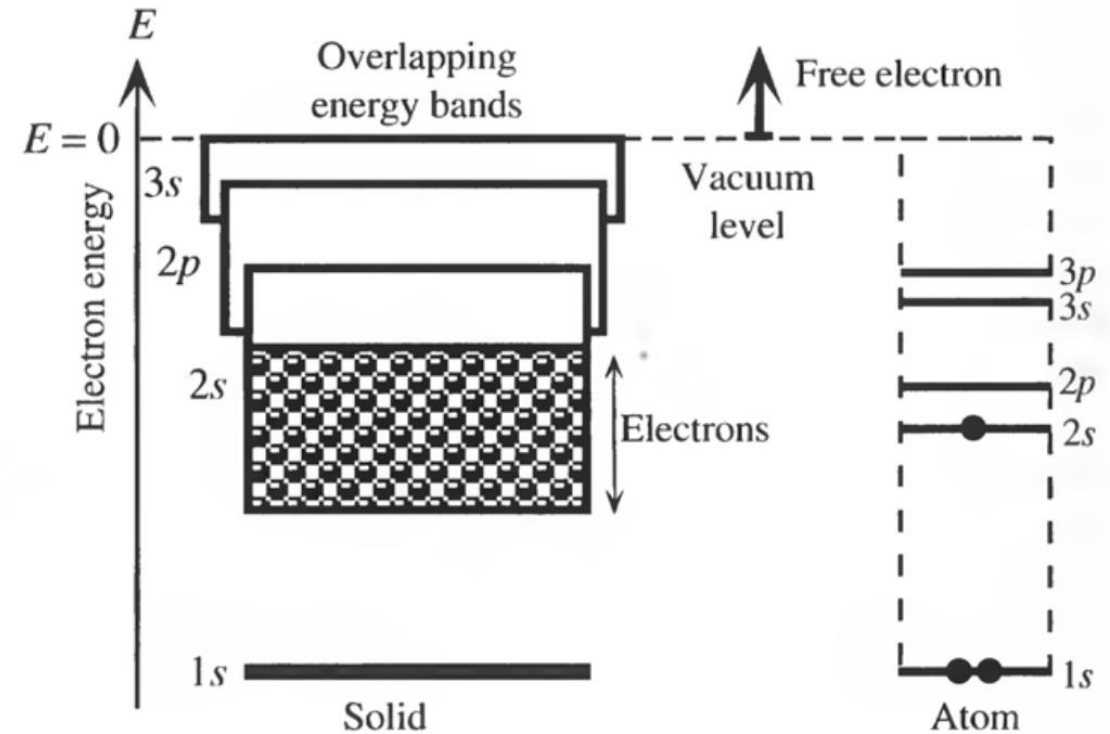
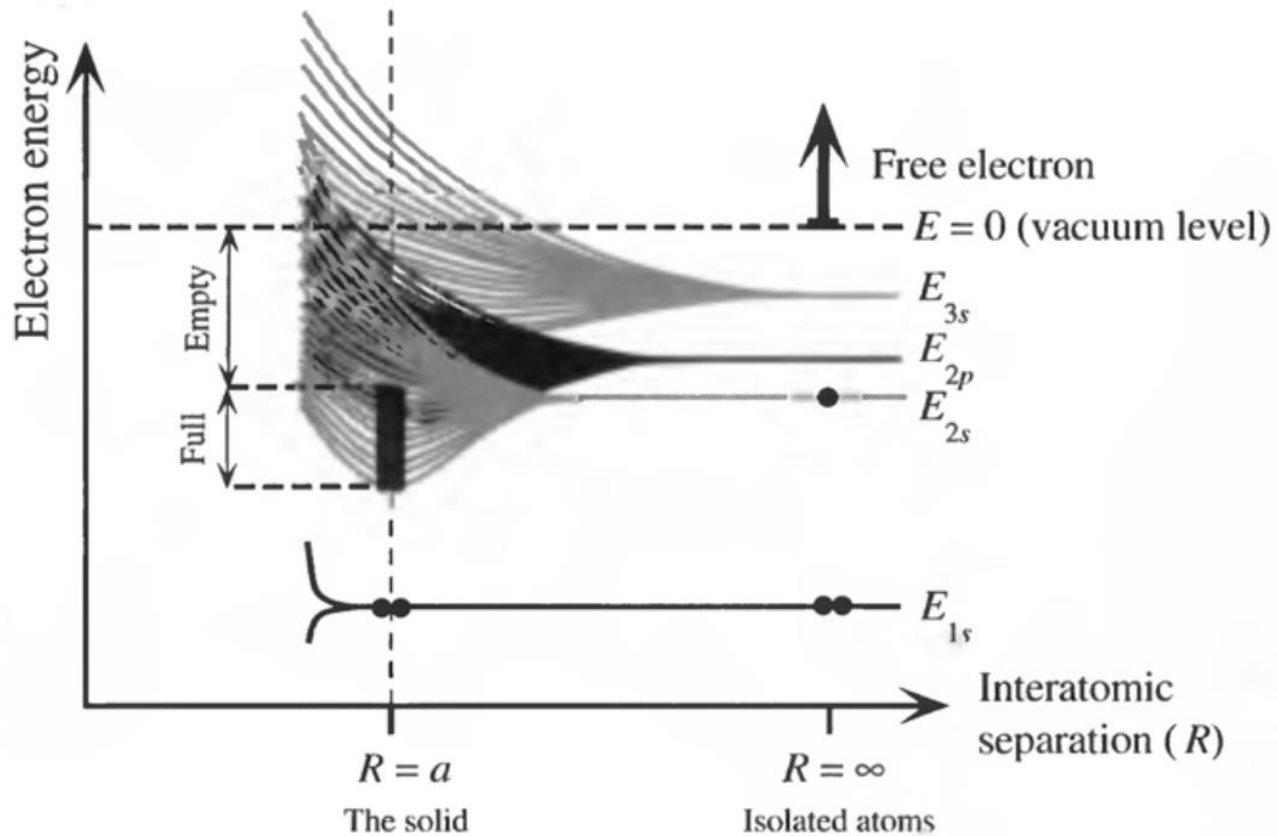


N- atoms of Lithium

- 1s electrons behave like He
 - They start splitting, but at a smaller inter-atomic distance.
- Before that distance is reached, 2S electrons interact.
 - They behave like 1S of hydrogen
 - N 2S states are seen whose separation depends on the interatomic distance.
- A stable Li solid is formed, if the last filled state has a summed energy lesser than the individual summation!

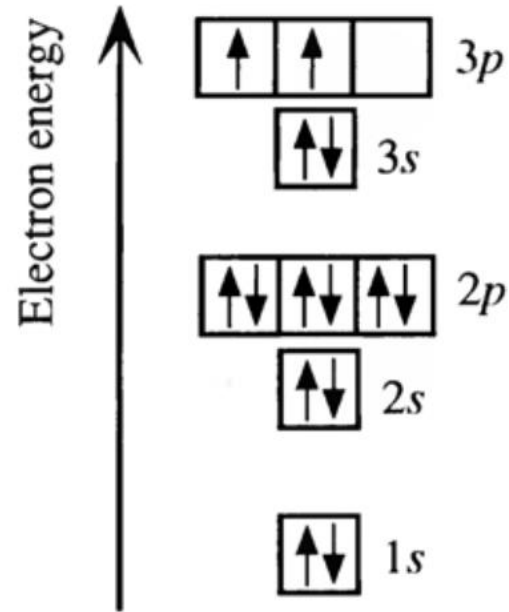


Energy bands in a metal

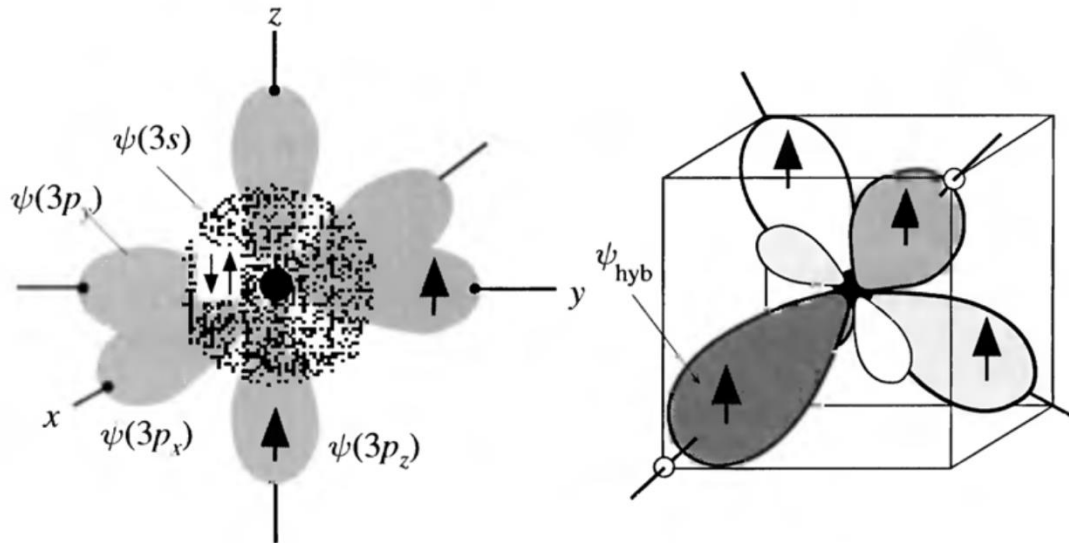


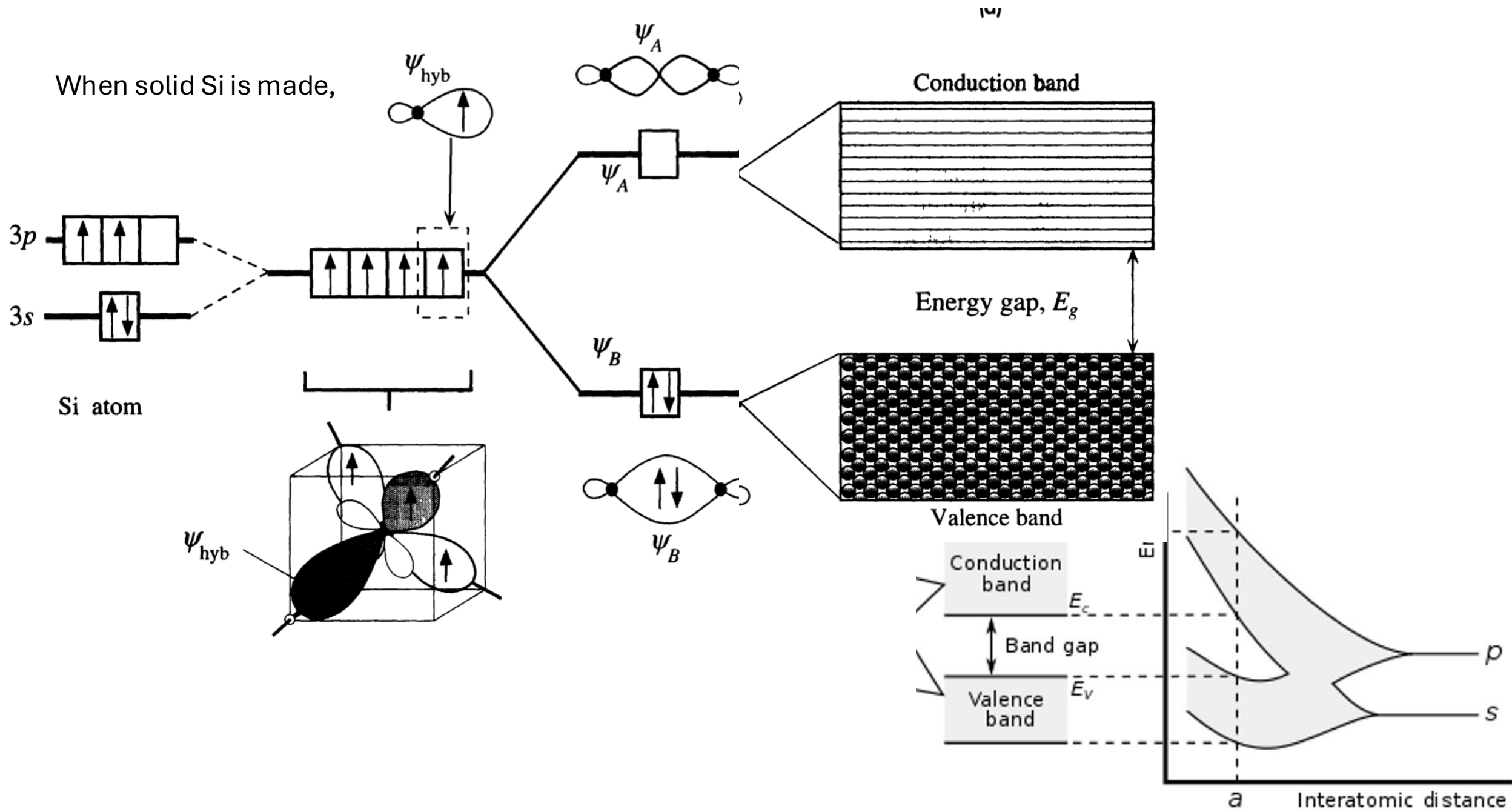
- All the valence electrons in the metal are delocalized.
- Last occupied energy level at 0K – Fermi Level

A Semiconductor



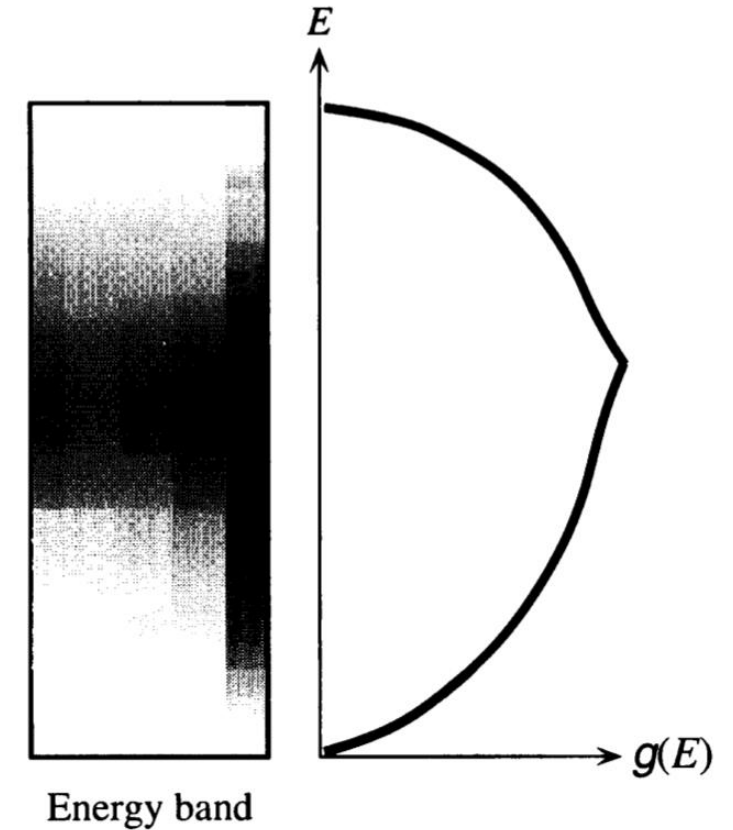
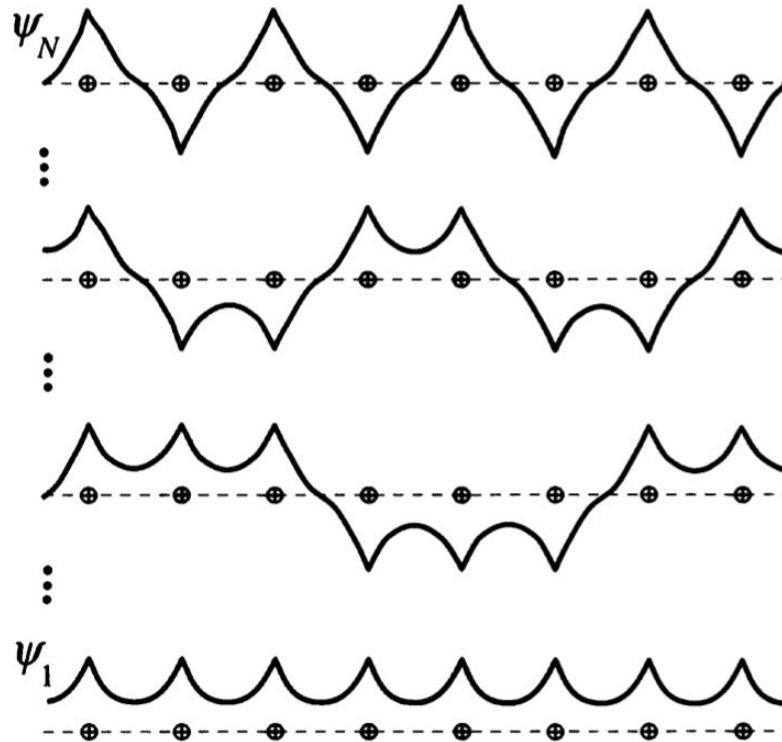
- Let us take the example of Si
- 3S is occupied. Only 3P is in valence!.
- However, 3S and 3P hybridize.
 - 3P states and 3S state combine to form 4 SP³ states.



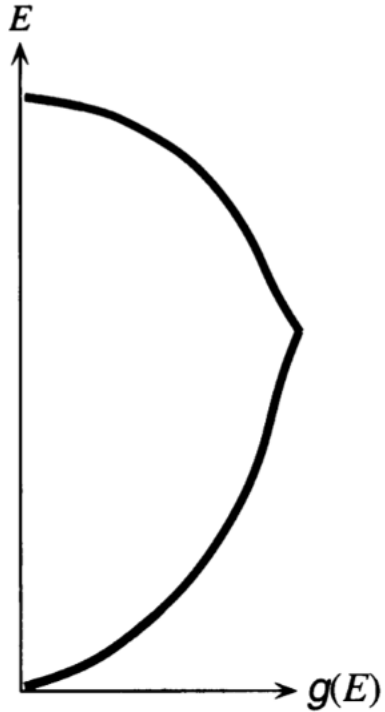


Density of states in a band

- Lowest energy is the symmetric function.
- Highest energy is also a symmetric function.
- These extremum wavefunctions can be obtained by fewer combinations.
- The density of states (possible energy levels) is non-uniform in a band

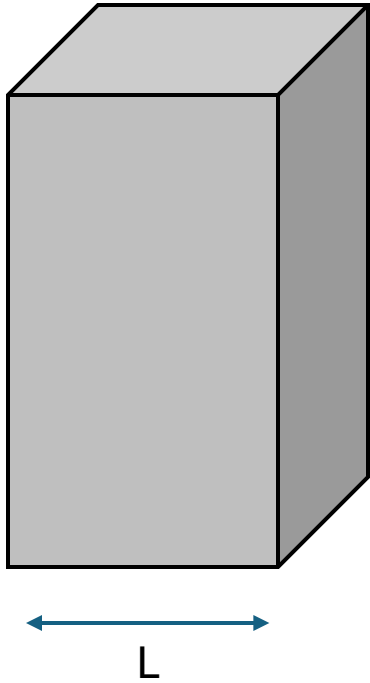


So how many states are there ?



- Total states $\int g(E) dE$
- Density of states $D(E) = \frac{1}{V} \frac{dg(E)}{dE}$

Density of states $D(E)$ at any energy E is the total number of states per energy per unit volume per



Imagine a cubic sample of side L

From our previous calculations, the allowed 'k' values in this sample is quantized!

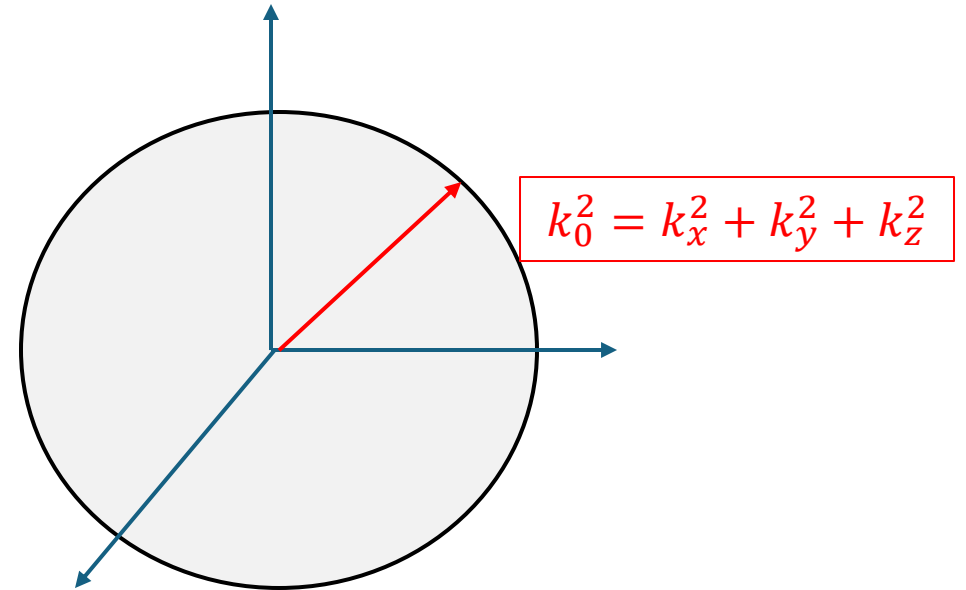
$$k_x = \frac{n\pi}{L} \quad \text{Where } n = 0, 1, 2, 3, \dots$$

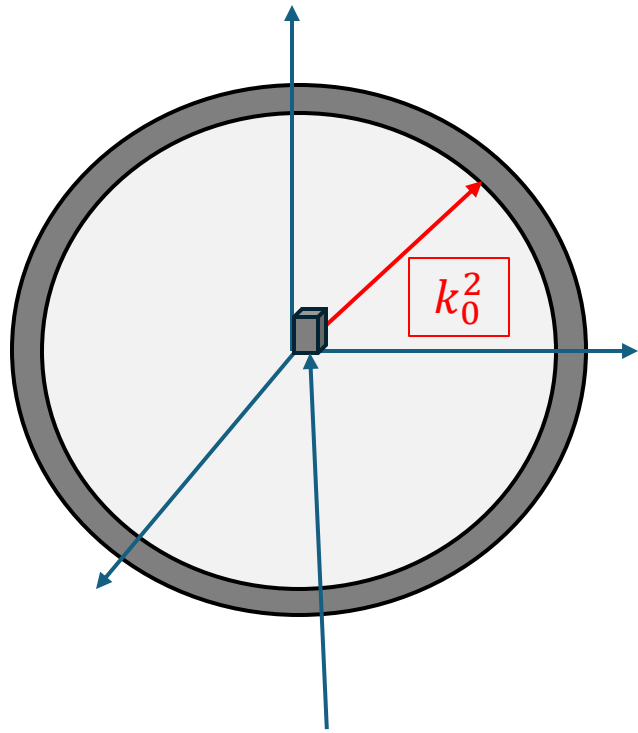
The energy values inside the box are:

$$E = \frac{\hbar^2 k^2}{2m}$$

Therefore for an electron at energy E_0 ,

The electron can have any 'k' value on the surface of the sphere with radius k_0





Smallest k-space volume = $\left(\frac{\pi}{L}\right)^3$

If we consider a sphere of radius k_0

The total available states inside this sphere is $N = \frac{\frac{4\pi k_0^3}{3}}{\left(\frac{\pi}{L}\right)^3}$

If we make a small change in $k_0 \rightarrow k_0 + dk$

The volume increment in k-space is $4\pi k_0^2 dk$

The number of states to the sphere: $dN = \frac{4\pi k_0^2 dk}{\left(\frac{\pi}{L}\right)^3}$

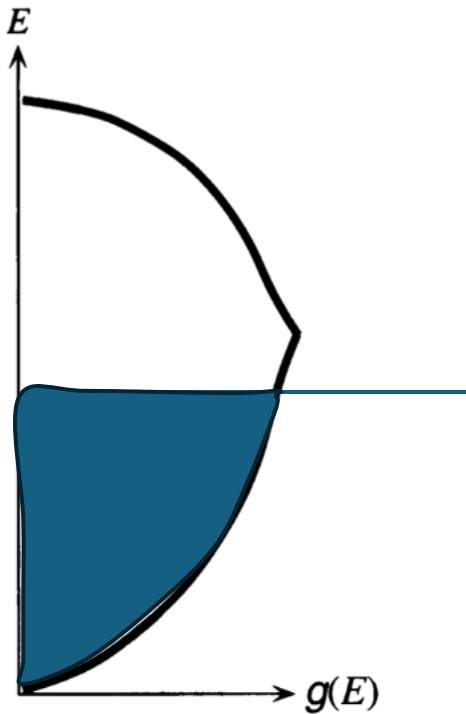
From the definition: $D(E) = \frac{1}{V} \frac{dN}{dE}$

$$D(E) = \frac{4k_0^2 dk}{\pi^2}$$

If we substitute $dE = \frac{\hbar^2 k_0 dk}{m}$

$$D(E) = \frac{1}{2\pi^2} \left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}} \sqrt{E}$$

Fermi Level

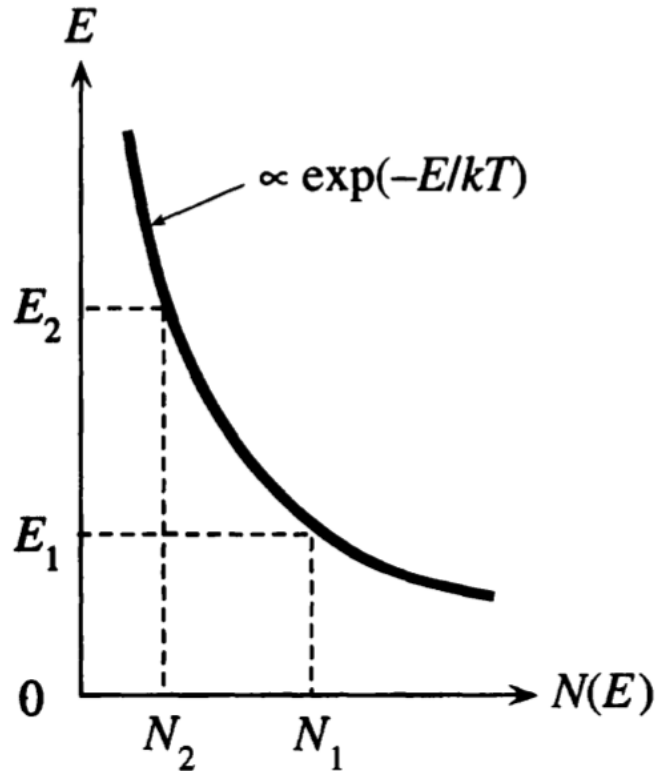


- At 0K, All the electrons of a system occupy lowest possible energy (following Pauli's exclusion)
- When all electrons are filled; The last occupied energy level is called as the Fermi level at 0K.

If there are in total N electrons at 0K

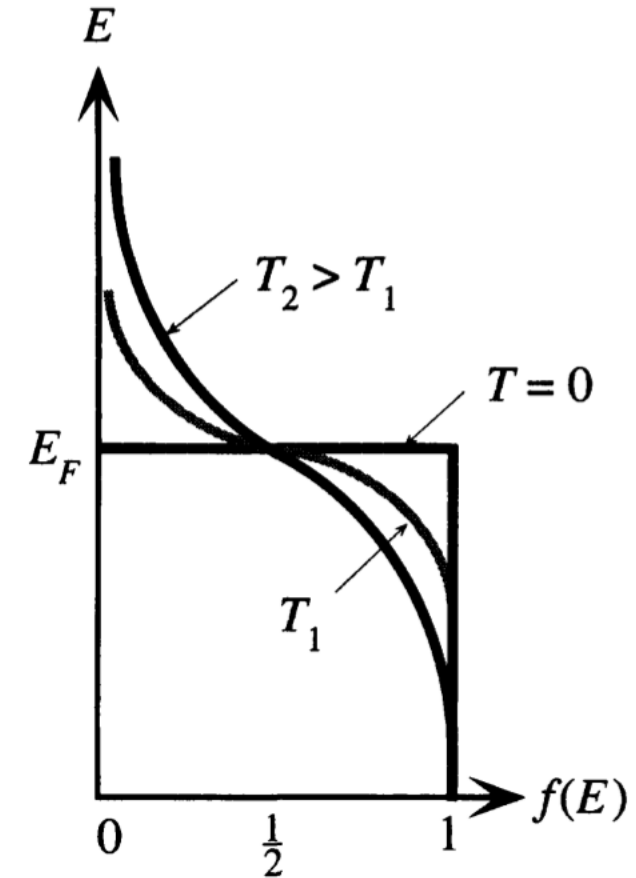
$$N = 2 \int_0^{E_F} D(E) dE$$

Occupational Probability



Classically, the number of particles with Energy E is proportional to $e^{-\frac{E}{kT}}$

Called Maxwell-Boltzmann statistics

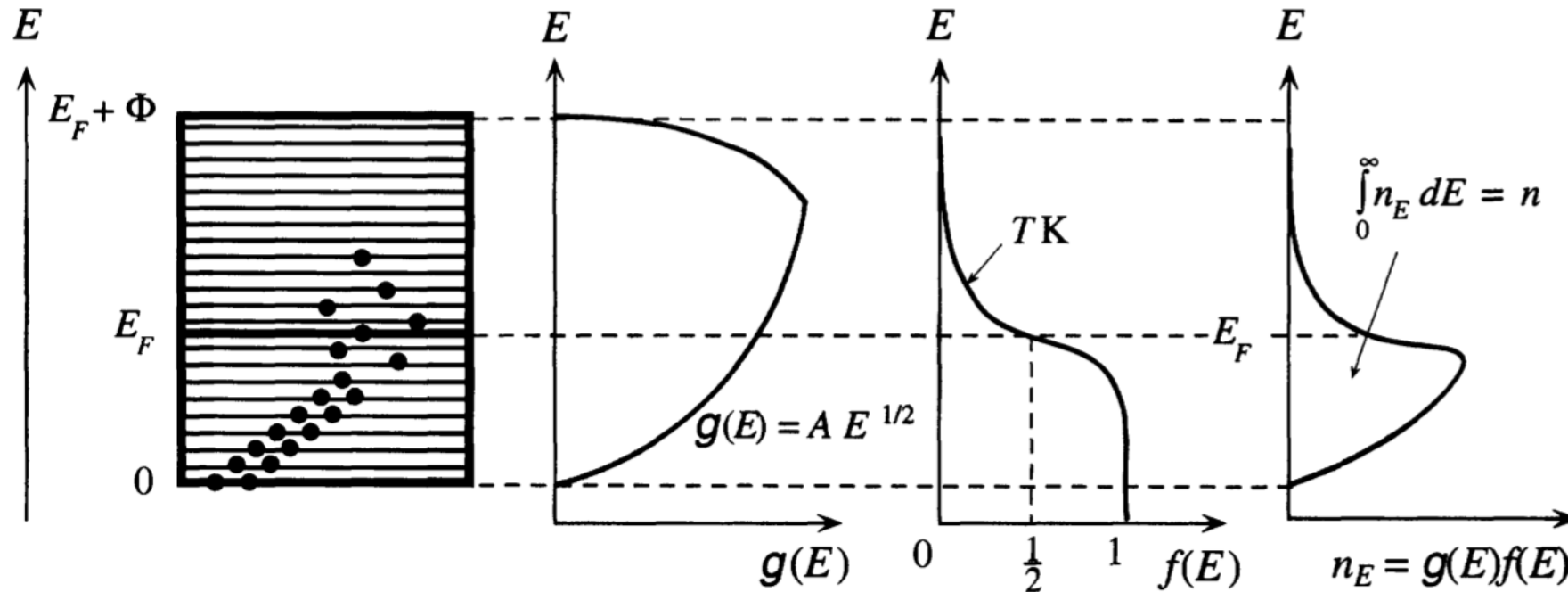


States of Fermions: Can only have occupancy 0 or 1

Probability that a state with energy E is filled

$$P(E) = \frac{1}{1 + e^{\frac{E - E_F}{kT}}}$$

At any non zero temperature

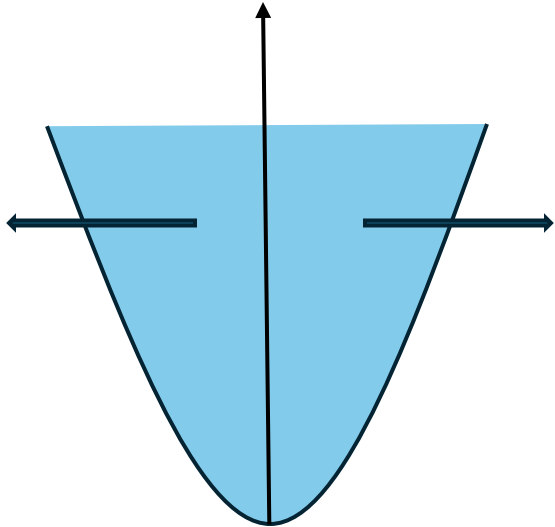


There is a non-zero probability of an electron to occupy energy levels higher than E_F

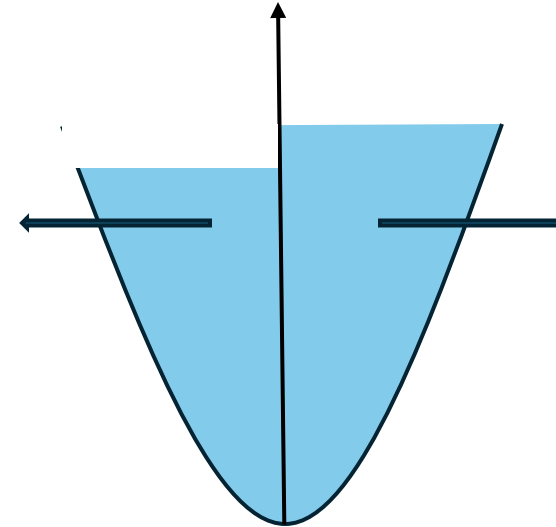
Quantum Conduction in metals

If a potential is applied across a metallic bar of length L

An electric field $E = \frac{V}{L}$ develops across its length



In the absence of an electric field, The total number of electrons moving in any random direction is cancelled by another electron moving in opposite direction



When an electric field is applied, there are more electrons on one side than the other.
Giving a net-electron flow along the applied direction

If $\mathcal{E}$ is the applied field

The additional momentum gained $\Delta P = \tau e\mathcal{E}$

An electron of energy $E = \frac{p^2}{2m}$ Without field

With the application of field $\Delta E = \frac{p}{m} \Delta P = \frac{p\tau e\mathcal{E}}{m}$

For a current obtained due to electrons with energy $\Delta E : J = N_e e V_x$

$N_e = G(E_f)\Delta E$ is the total number of electrons near the Fermi level
e – electronic charge

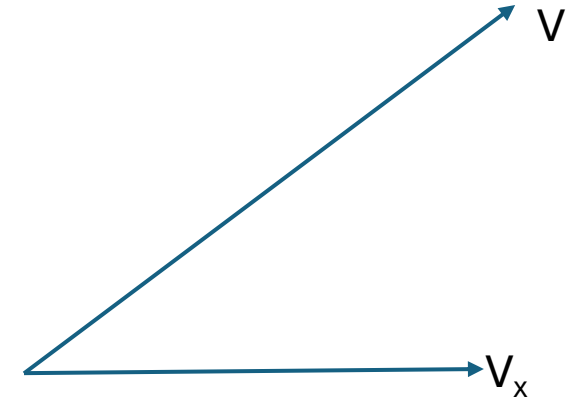
$V = \frac{p}{m}$ is the velocity of the electrons near the Fermi level

$$J = e[g(E_f)\Delta E]V_x = e[g(E_f)V\tau e\mathcal{E}]V = e^2V_x^2\tau g(E_f)\mathcal{E}$$

Quantum conductivity $\sigma = e^2 V_x^2 \tau g(E_f)$

However,

$$V^2 = V_x^2 + V_y^2 + V_z^2$$



If you have a symmetric device, $V_x = V_y = V_z$ giving $V^2 = 3V_x^2$

Therefore, the velocity along the x-direction $V_x^2 = \frac{V^2}{3}$

Quantum conductivity $\sigma = \frac{1}{3} e^2 V^2 \tau g(E_f)$