Physics of Electronics:

5. Electrons in Solids
Intro to Band Theory

July – December 2008

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- A simple model of a conductor.
- Electrons in a 3D box.
- Maximum number of possible energy states.
- Energy distribution of electrons in a metal.
- Fermi level in a metal.
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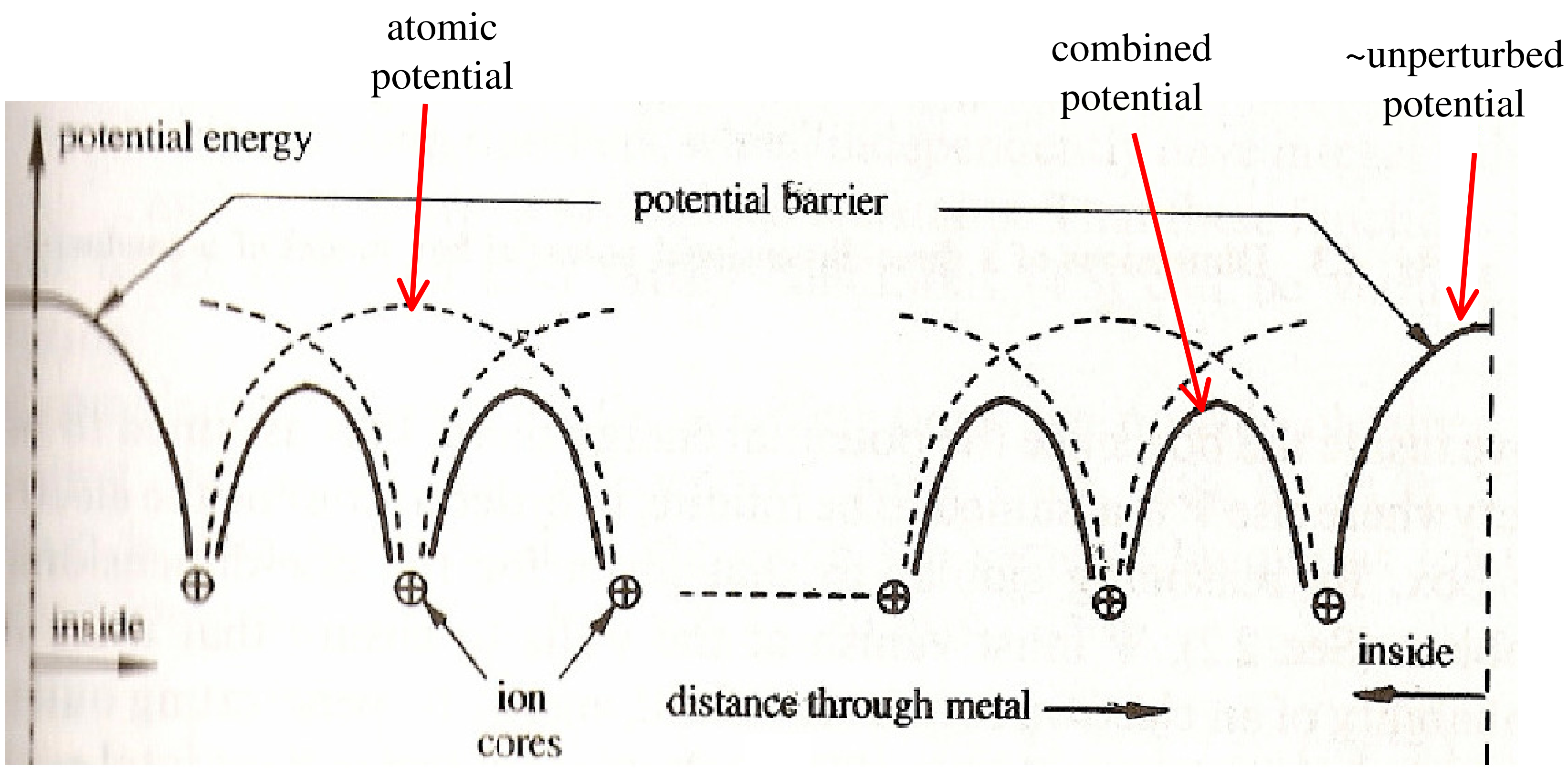
A Simple Model of a Conductor

- From one atom to a collection of atoms:



The potential barrier confines the electrons inside the faces of the conductor. Therefore we can model a conductor as unbound or free electrons confined to a potential box.

Electrons in a 3D box

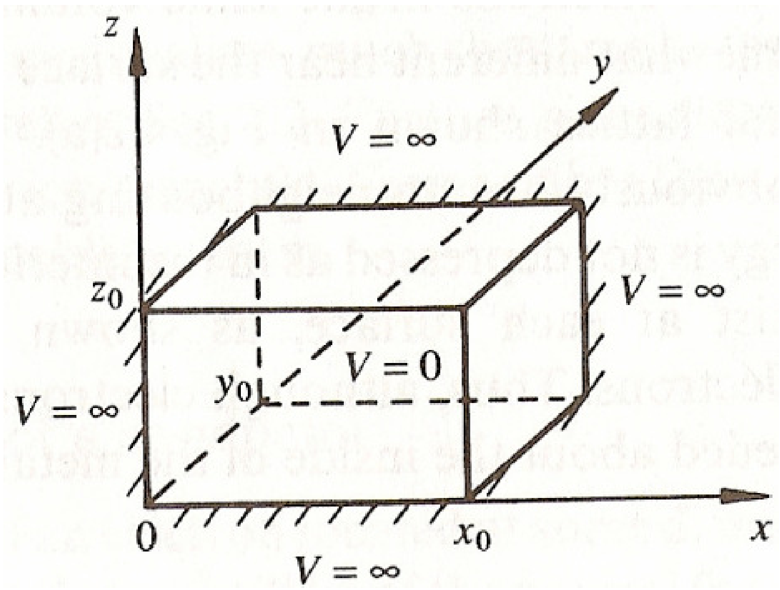
- Free electron model: V = 0 inside box & V = ∞ outside box
  - Solving the *t*-independent SE:

$$\Psi_{n_x n_y n_z} = \left(\frac{2}{x_0}\right)^{1/2} \sin\left(\frac{n_x \pi x}{x_0}\right) \left(\frac{2}{y_0}\right)^{1/2} \sin\left(\frac{n_y \pi y}{y_0}\right) \left(\frac{2}{z_0}\right)^{1/2} \sin\left(\frac{n_z \pi z}{z_0}\right)$$

For every triplet (n_x , n_y , n_z) there exists an allowed state.

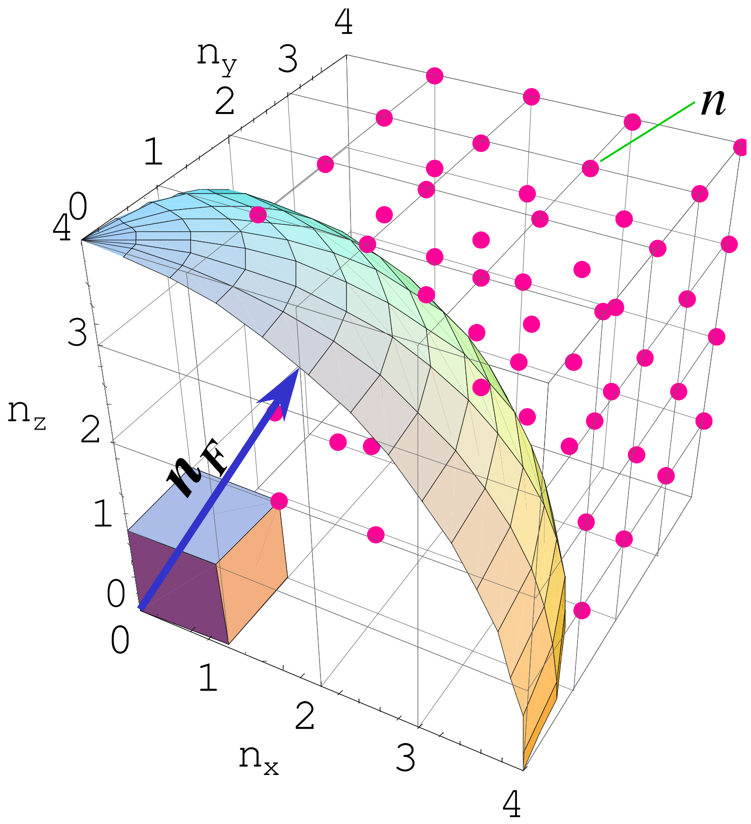
$$E = \frac{h^2}{8md^2} n^2$$

where $d = x_o = y_o = z_o$
$n^2 = n_x^2 + n_y^2 + n_z^2$



Maximum Number of States

- Given a (maximum) number n_F, how many allowed states are there?
  - Equivalently, how many triplets (n_x, n_y, n_z) are there such that $n_F \geq n = (n_x^2 + n_y^2 + n_z^2)^{1/2}$?



- The number of states such that $n \leq n_F$ corresponds to the volume generated by n_F:

$$\frac{1}{8}\left(\frac{4}{3}\pi n_F^3\right) = \pi n_F^3/6 \xrightarrow{\text{spin}} 2(\pi n_F^3/6) = \pi n_F^3/3$$

- $T = 0$: Number of electrons=Number states $n \leq n_F$

$$N d^3 = \pi n_F^3/3$$

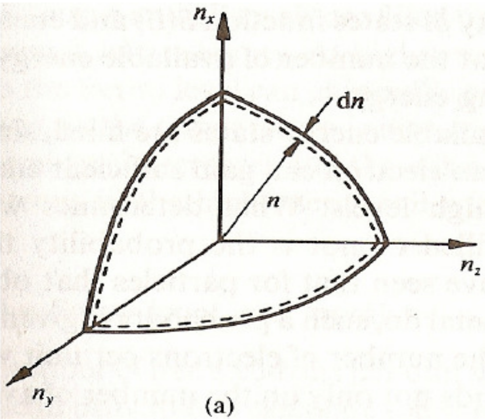
$$n_F = (3N/\pi)^{1/3} d$$

- The energy corresponding to n_F:

$$E_{F0} = \frac{h^2}{8m}\left(\frac{3N}{\pi}\right)^{2/3}$$

Energy Distribution of e- in a Metal

- What is the number of (available) states with energies in the range E and E+dE ?
  - N is large, we can consider that n varies continuously.



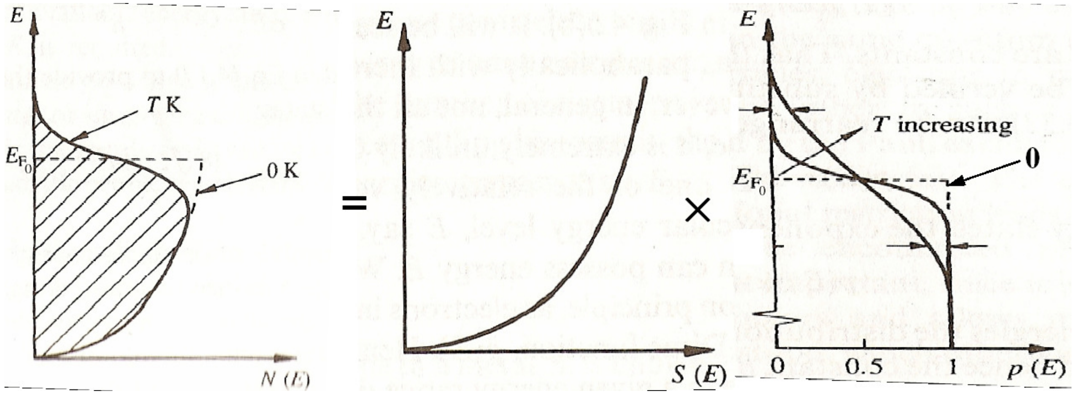
- Number of states in shell dn is equal to twice its volume:

$$2(4\pi n^2\,dn)/8 = \pi n^2\,dn$$

- Density of states, S(E), is defined such that $S(E)\,dE\,d^3 = \pi n^2\,dn$

$$\Rightarrow S(E) = \frac{\pi n^2}{d^3}\frac{dn}{dE} \Rightarrow S(E) = \frac{(8\sqrt{2})\pi m^{3/2}}{h^3}E^{1/2}$$

- $N(E)$, is defined such that: $\boldsymbol{N(E)dE = S(E)dE \times p(E)}$ $\Rightarrow$ $\boldsymbol{N(E) = S(E)\,p(E)}$



Fermi Level in a Metal

- From $N(E)$ the number of electrons in a metal is:

$$n=\int_0^\infty N(E)\,dE=\int_0^\infty S(E)p(E)\,dE=\frac{(8\sqrt{2})\pi m^{3/2}}{h^3}\int_0^\infty \frac{E^{1/2}\,dE}{1+\exp[(E-E_F)/kT]}$$

- At $T = 0$:

$$n=\frac{(8\sqrt{2})\pi m^{3/2}}{h^3}\int_0^{E_{F0}} E^{1/2}\,dE \Rightarrow E_{F0}=\frac{h^2}{8m}\left(\frac{3n}{\pi}\right)^{2/3}=3.65\times 10^{-19}\,n^{2/3}\text{ eV}$$

  - Note that in a gas the energy of the particles is 0.
  - In a metal the electrons have an energy up to E_{F0} (few eV's).

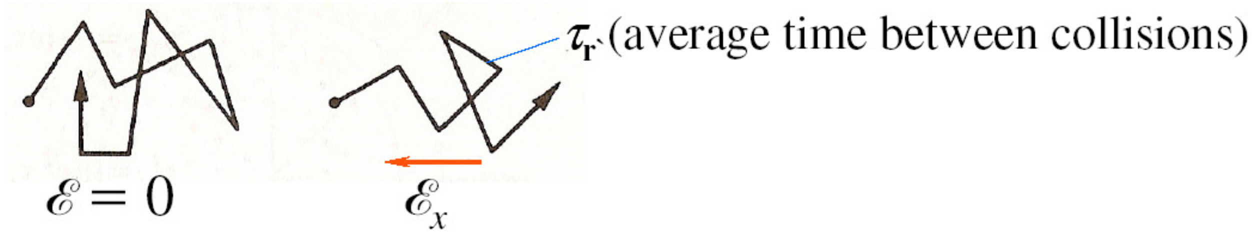
- At $T > 0$:

$$E_F \approx E_{F0}\left[1-\frac{\pi^2}{12}\left(\frac{kT}{E_{F0}}\right)^2\right]$$

  - At usual temperatures kT ~ meV E_F depends slowly on T.

Conduction Processes in a Metal

- Consider a (classical) free e^- moving in a metal.
  - There are collisions with the crystal structure:



  - Collisions are described by a friction term. Then, equation of motion of the electron in an external electrical field.

$$-e\,\mathscr{E}_x - f = m\,\ddot{x}$$

  - The friction is assumed to be proportional to $m\,\dot{x}/\tau_r$

$$\Rightarrow \quad -e\mathscr{E}_x = m\frac{\mathrm{d}}{\mathrm{d}t}(v_{Dx}) + \frac{m(v_{Dx})}{\tau_r}$$

$$\Rightarrow \quad v_{Dx} = \frac{-e\tau_r\mathscr{E}_x}{m}\left[1 - \exp(-t/\tau_r)\right]$$

Conduction Processes in a Metal

- Consider a (classical) free e^- moving in a metal.
  - Current density:

$$J = n\,q\,\dot{x} \quad \Rightarrow \quad J = n(-e)v_{Dx} = \frac{ne^2\tau_r\mathscr{E}_x}{m}[1-\exp(-t/\tau_r)]$$

  - At large times ($t >> \tau_r$) we have:

$$v_{Dx} = -(e\tau_r/m)\mathscr{E}_x = -\mu\,\mathscr{E}_x$$

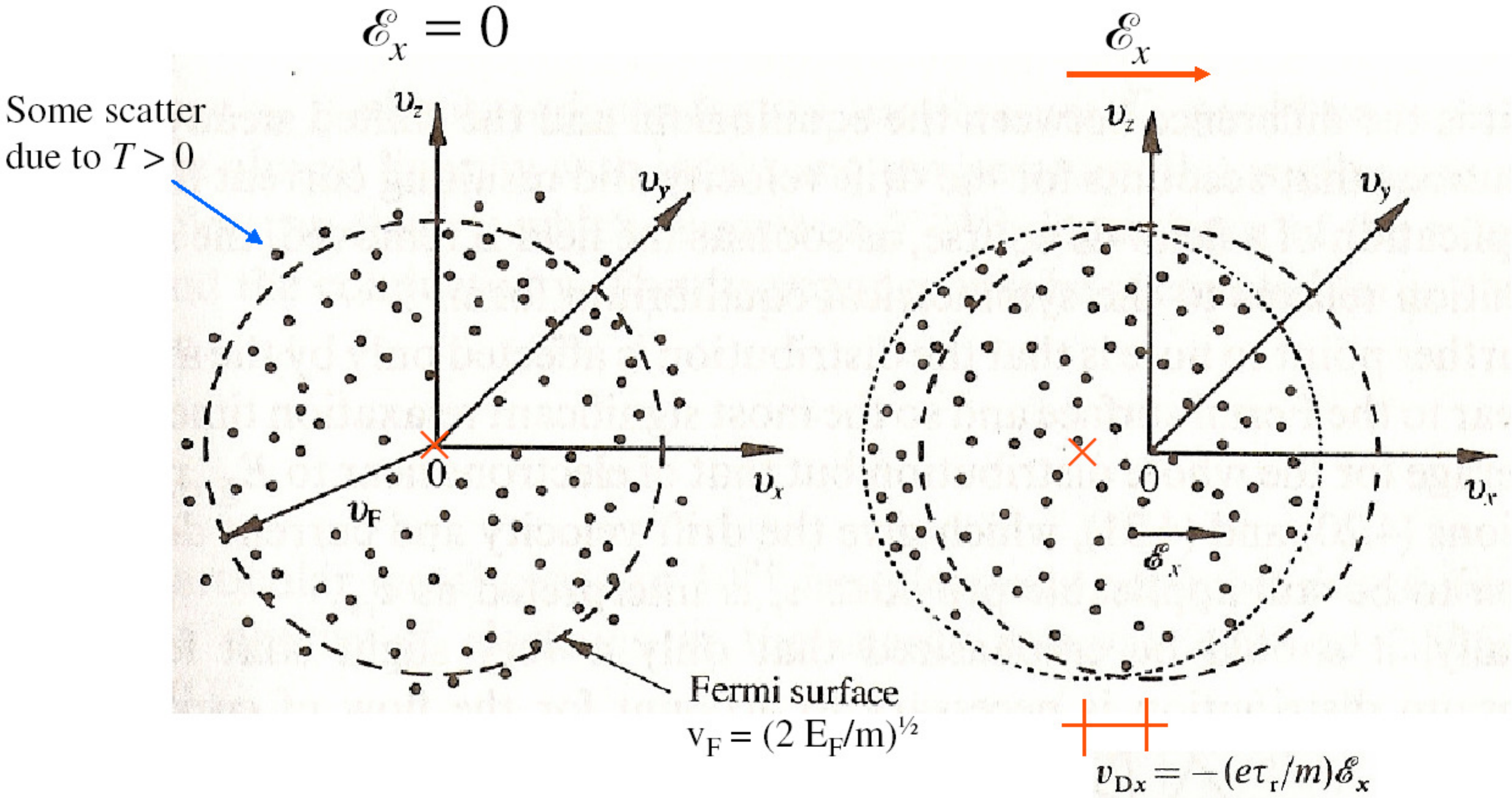
$$J_x = (ne^2\,\tau_r/m)\mathscr{E}_x = ne\mu\,\mathscr{E}_x$$

  - The last relation is Ohm's law with:

$$\sigma = ne\mu = ne^2\,\tau_r/m$$

Conduction Processes in a Metal

- Conduction and distribution of states:
  - Every available state is characterized by an energy E with which we can associate a velocity ($E = ½\, mv^2$) :



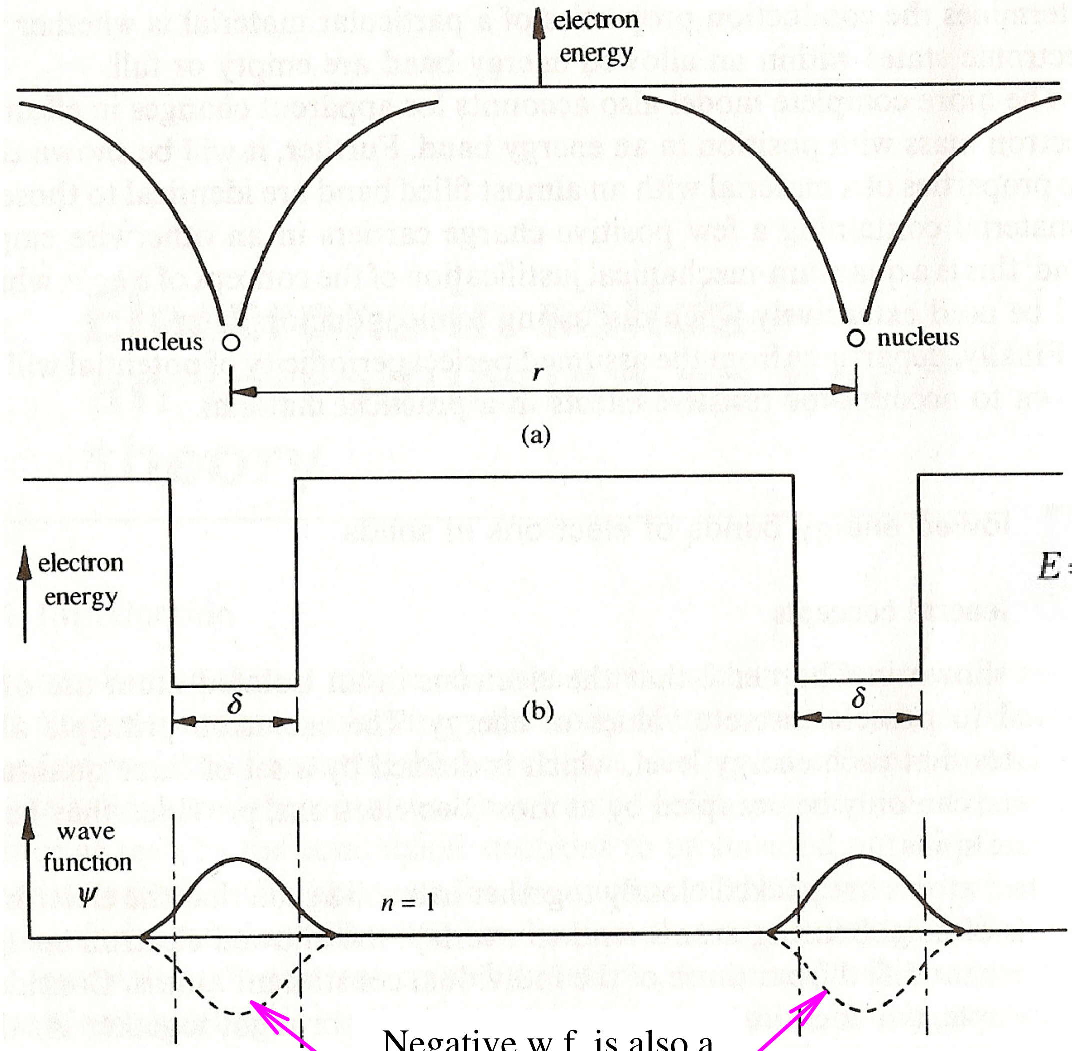
Allowed Energy Bands

- Energy splitting.

Two atoms separated a distance r.

Modeled by potential wells.

If r is large, w.f. are unperturbed.



$$E = \frac{\hbar^2 n^2 \pi^2}{2md^2} = \frac{n^2 h^2}{8md^2}$$

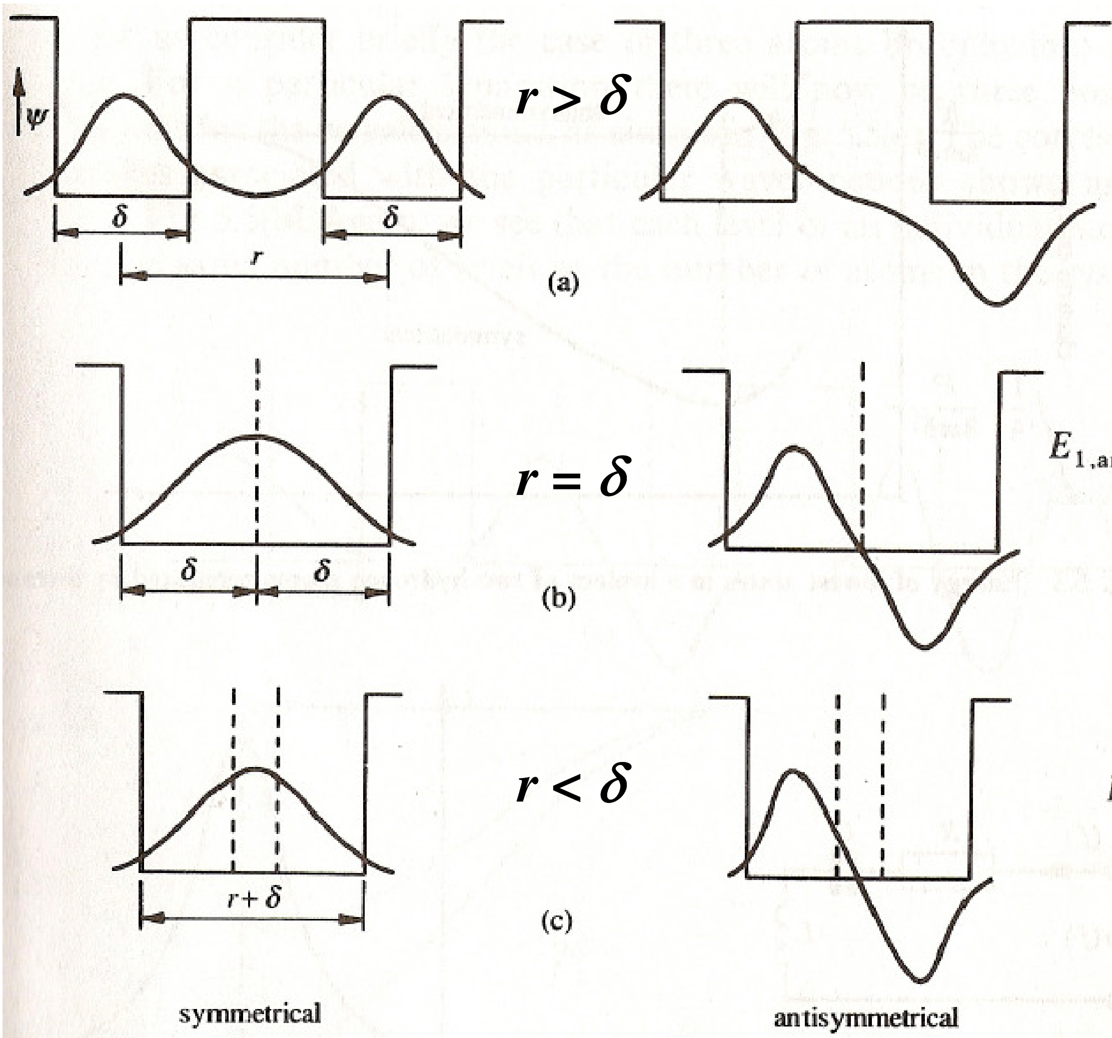
$$E_1 = h^2/(8m\delta^2)$$

Negative w.f. is also a possible solution

Allowed Energy Bands

- Energy splitting.

Two atoms separated a distance r are brought together.



$$E_{1,sym} = \frac{h^2}{8m(2\delta)^2} = \frac{1}{4}\,\frac{h^2}{8m\delta^2}$$

$$E_{1,antisym} = \frac{2^2 h^2}{8m(2\delta)^2} = \frac{h^2}{8m\delta^2}$$

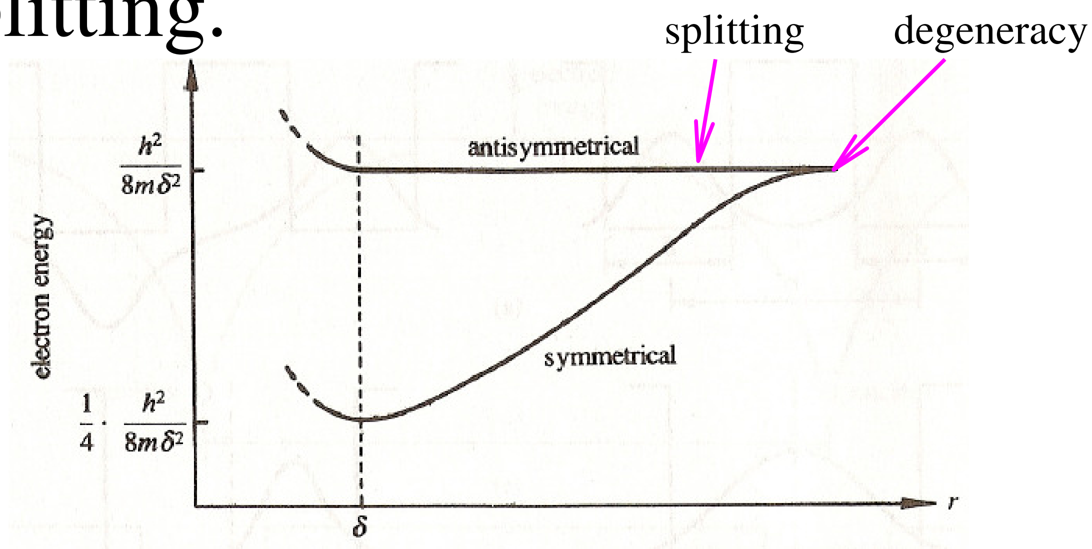
$$E_{1,sym} = \frac{h^2}{8m(r+\delta)^2}$$

$$E_{1,antisym} = \frac{4h^2}{8m(r+\delta)^2}$$

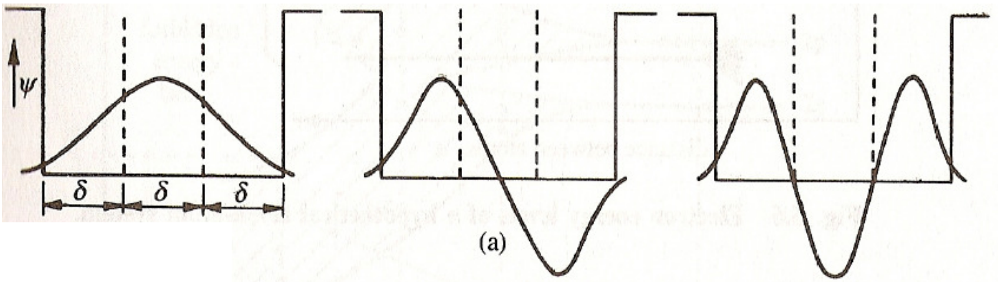
Allowed Energy Bands

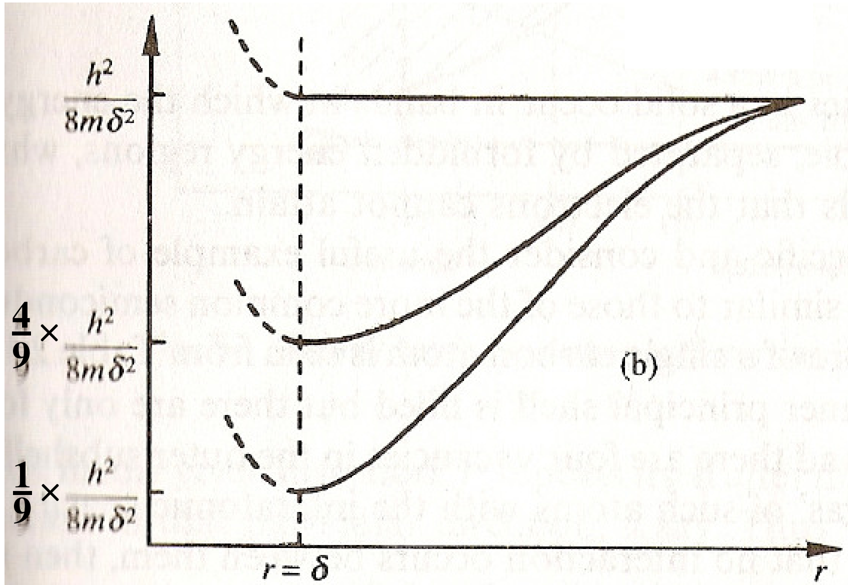
- Energy splitting.

Two atoms separated a distance r are brought together.



Three atoms separated a distance r are brought together.

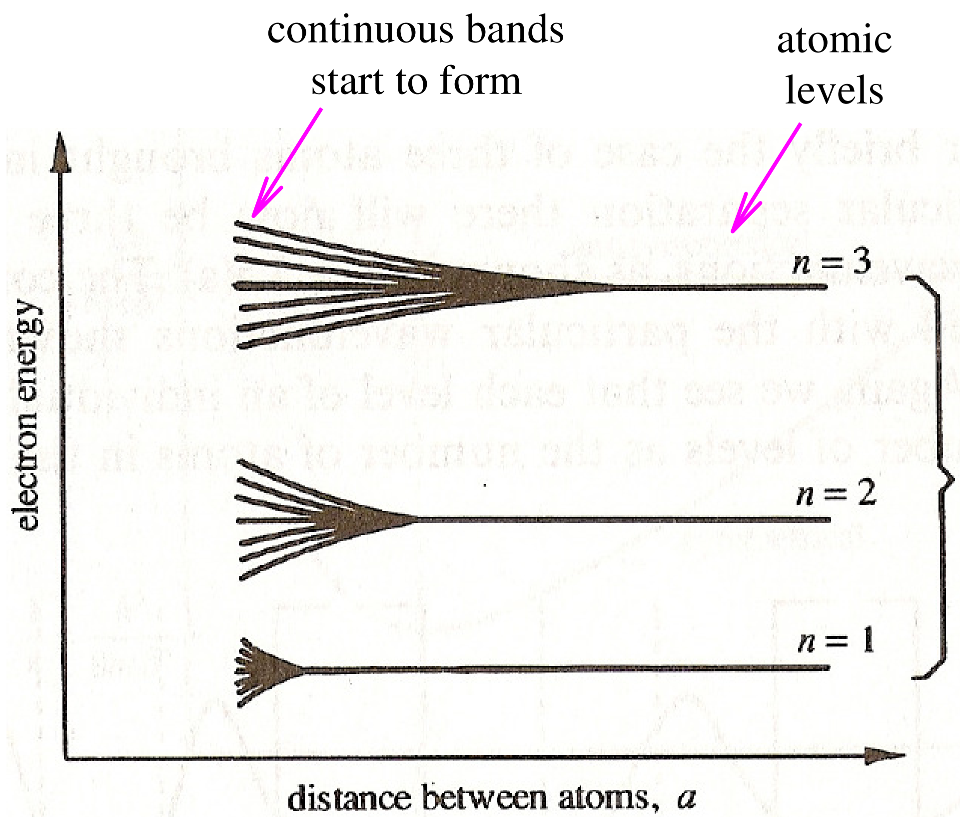




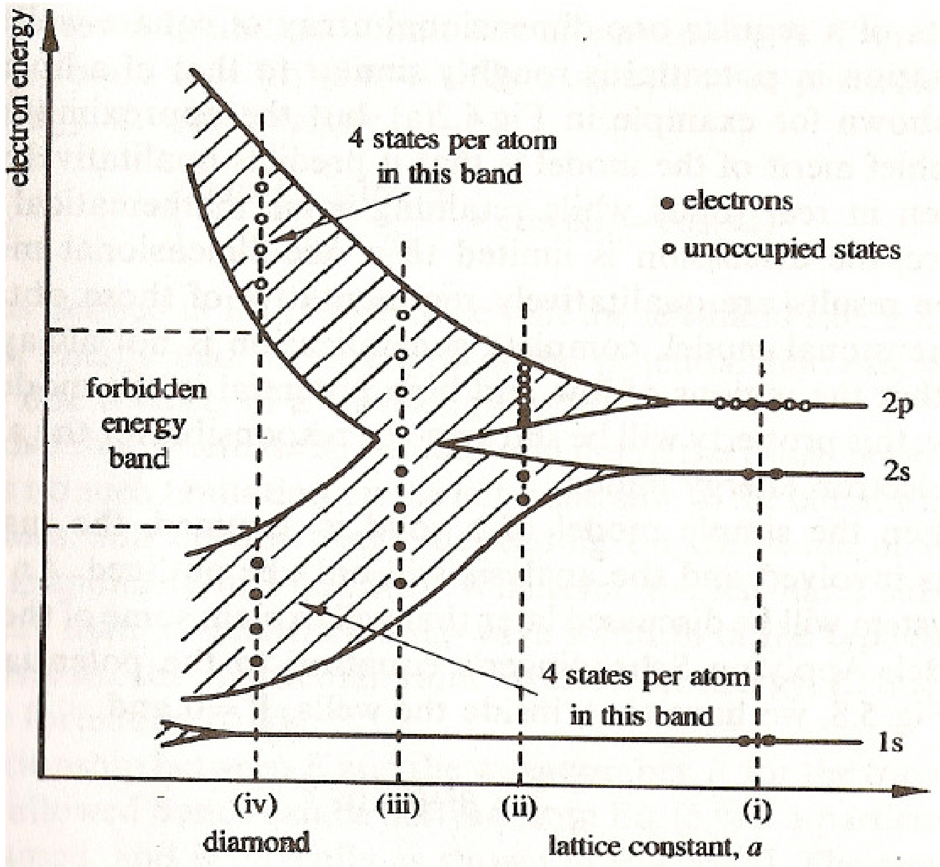
Allowed Energy Bands

- Energy splitting.

More atoms are brought together.

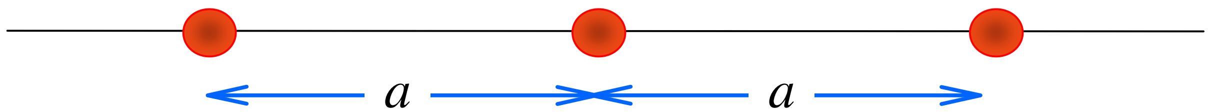


Example: Carbon.



Allowed Energy Bands

- Bloch's theorem.
  - Let's consider a 1D chain of N atoms of period a.



- The potential has the same periodicity: $V(x) = V(x+a) = V(x+2a) = \ldots$
- The w.f. has to have the same periodicity:

$$\psi(x + a) = C\psi(x)$$

- Further we consider that the chain forms a ring:

$$\psi(x + Na) = \psi(x) = C^N \psi(x)$$

$\Rightarrow$ $C^N = 1$ $\Rightarrow$ $C = \exp(i2\pi s/N)$; $s = 0, 1, 2, \ldots, N-1$.

- To satisfy the previous relations, the w.f. has to be of the form:

$\boxed{\psi(x) = u_k(x)e^{ikx}}$ with: $u_k(x) = u_k(x + a)$ & $k = 2\pi s/Na$

i.e. a plane wave modulated in space