Physics of Electronics:

4. Conduction in Metals
&
5. Energy Bands

July – December 2008

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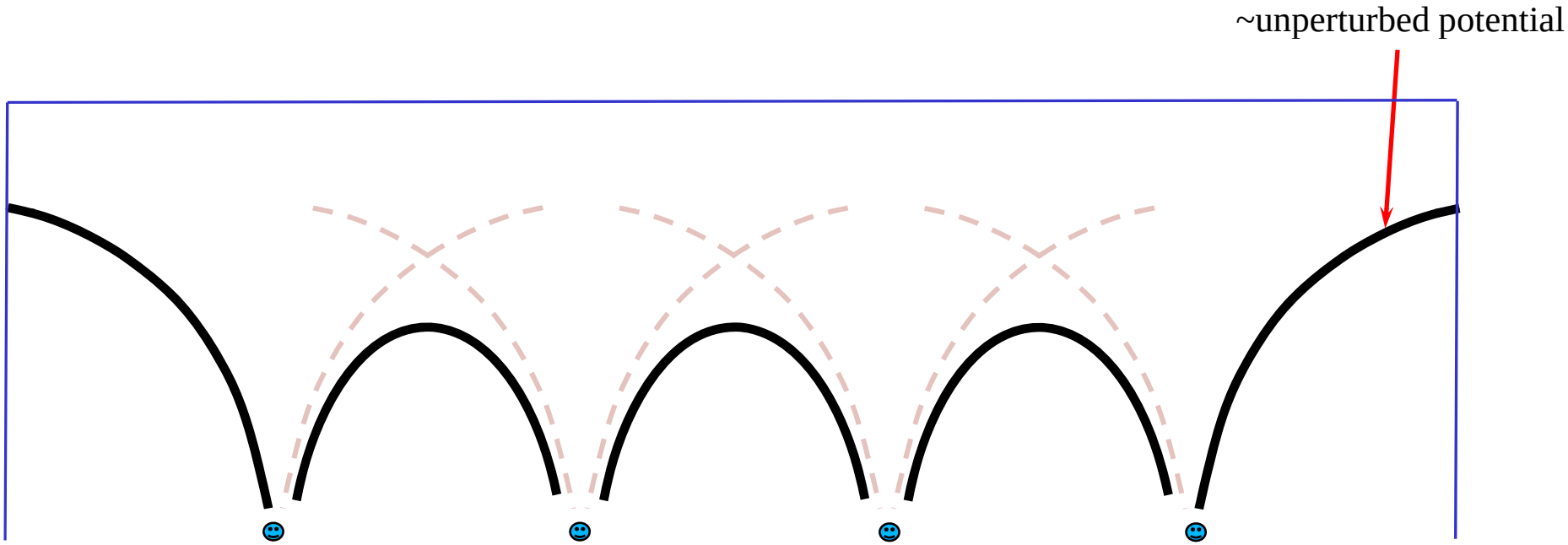
- A simple model of a conductor.
- Electrons in a 3D box.
- Maximum number of possible energy states.
- Energy distribution of electrons in a metal.
- Fermi level in a metal.
- Conduction processes in metals.
- Energy bands:
  - Energy splitting
  - Bloch's theorem

A Simple Model of a Conductor

- From one atom to a collection of atoms:

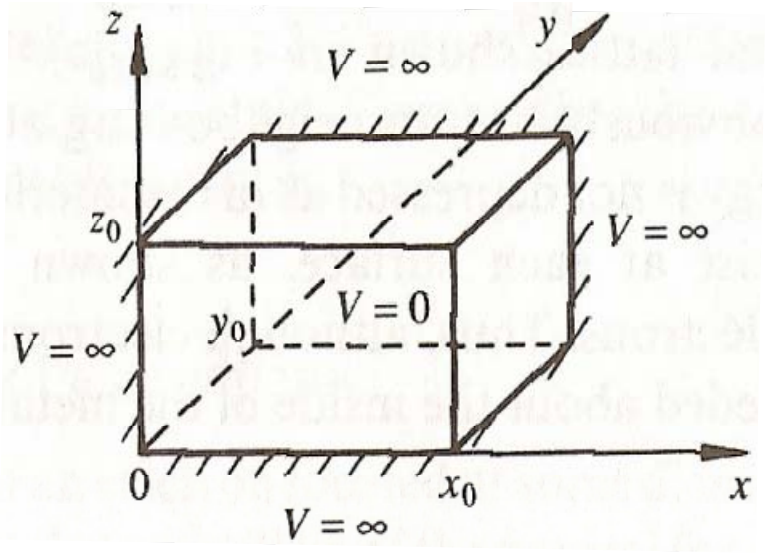


The potential barrier confines the electrons inside the faces of the conductor. Therefore we can model a conductor as unbound or free electrons confined to a potential box.

Electrons in a 3D box

- Free electron model: V = 0 inside box & V = ∞ outside box
  - Start from t-independent SE:

$$\nabla^2\Psi + \frac{2m}{\hbar^2}(E - V)\Psi = 0$$



$$\Rightarrow \quad \frac{\partial^2\Psi}{\partial x^2} + \frac{\partial^2\Psi}{\partial y^2} + \frac{\partial^2\Psi}{\partial z^2} + \frac{2m}{\hbar^2} E\Psi = 0$$

  - Solving, using continuity, and normalizing:

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

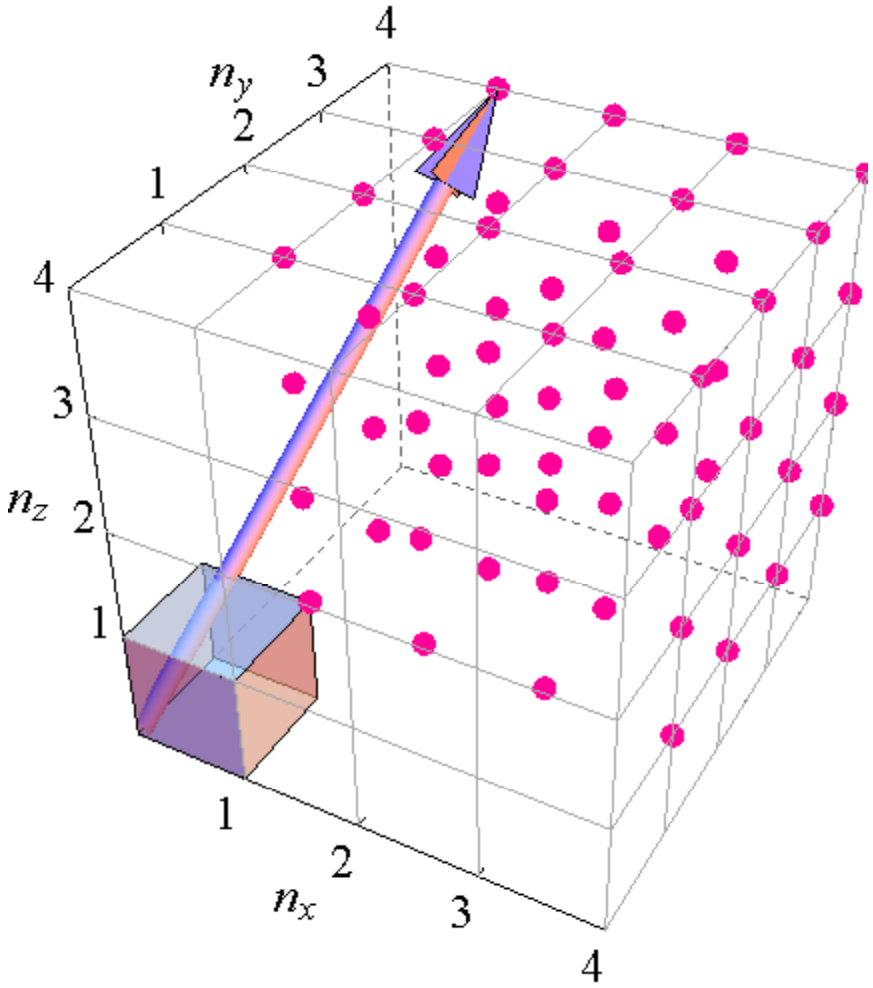
$$E = \frac{h^2}{8md^2} n^2$$

where: $d = x_o = y_o = z_o$

$n^2 = n_x^2 + n_y^2 + n_z^2$

Space of States

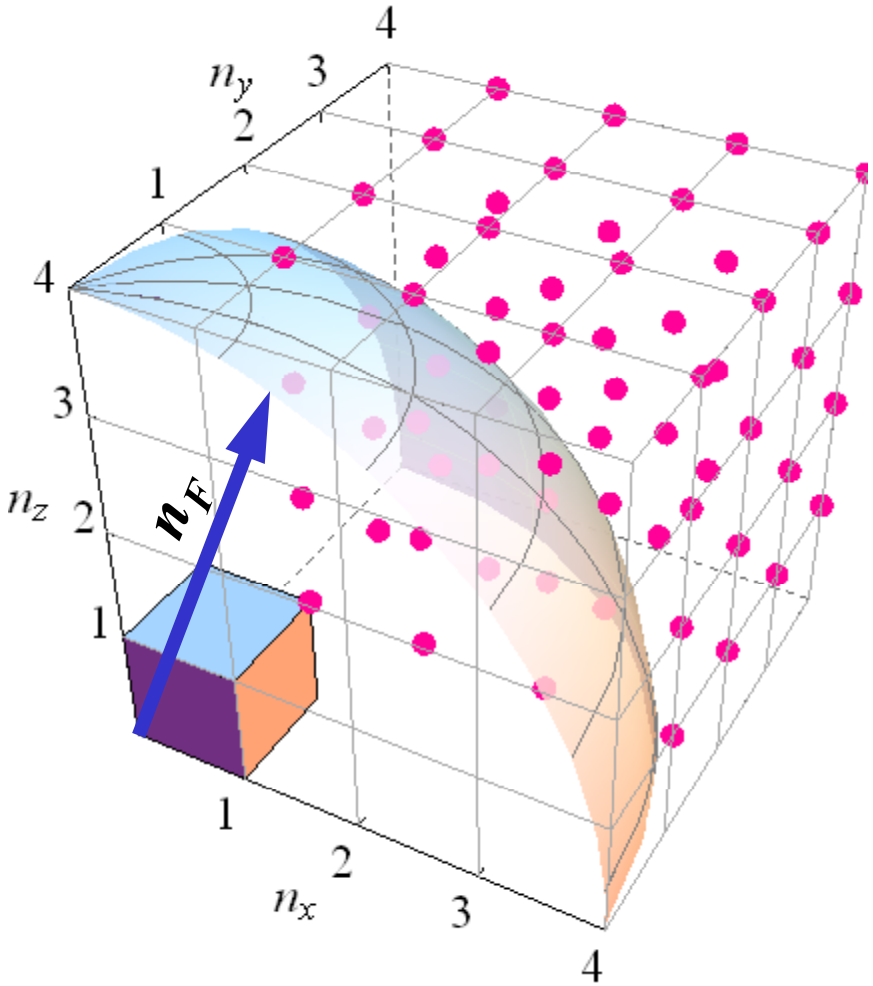
- We can represent every state as a point in a 3D space.



- In this representation, each point corresponds to one available state.
- To each unit of volume corresponds one available state.
- We will consider large number of points (continuum limit).

Maximum Number of States

- Given a (maximum) number n_F, how many Origin of states are there?



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

$$V_F = 2\pi n_F^3 / 6$$

- At 0 K we have:

Number of electrons = Number states $n \leq n_F$

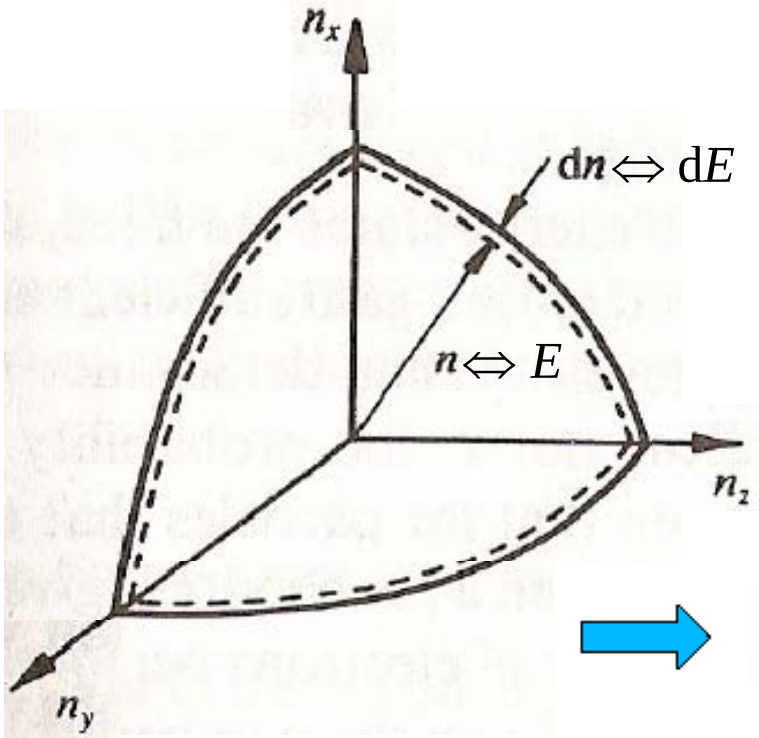
$$Nd^3 = \pi n_F^3 / 3$$

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

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

Energy Distribution of e- in a Metal

- What is the number of (available) states with energies in the range E and $E+\mathrm{d}E$?



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

$$2(4\pi n^2\,\mathrm{d}n)/8 = \pi n^2\,\mathrm{d}n$$

- Density of (available) states, S(E): S(E)dE gives the number of states with energies in the range E and $E+\mathrm{d}E$

$$S(E)\,\mathrm{d}E\,d^3 = \pi n^2\,\mathrm{d}n \quad\Rightarrow\quad S(E) = \frac{\pi n^2}{d^3}\frac{\mathrm{d}n}{\mathrm{d}E}$$

$$E = \frac{h^2}{8md^2}n^2 \quad\Rightarrow\quad \boxed{S(E) = \frac{(8\sqrt{2})\pi m^{3/2}}{h^3}E^{1/2}}$$

Energy Distribution of e- in a Metal

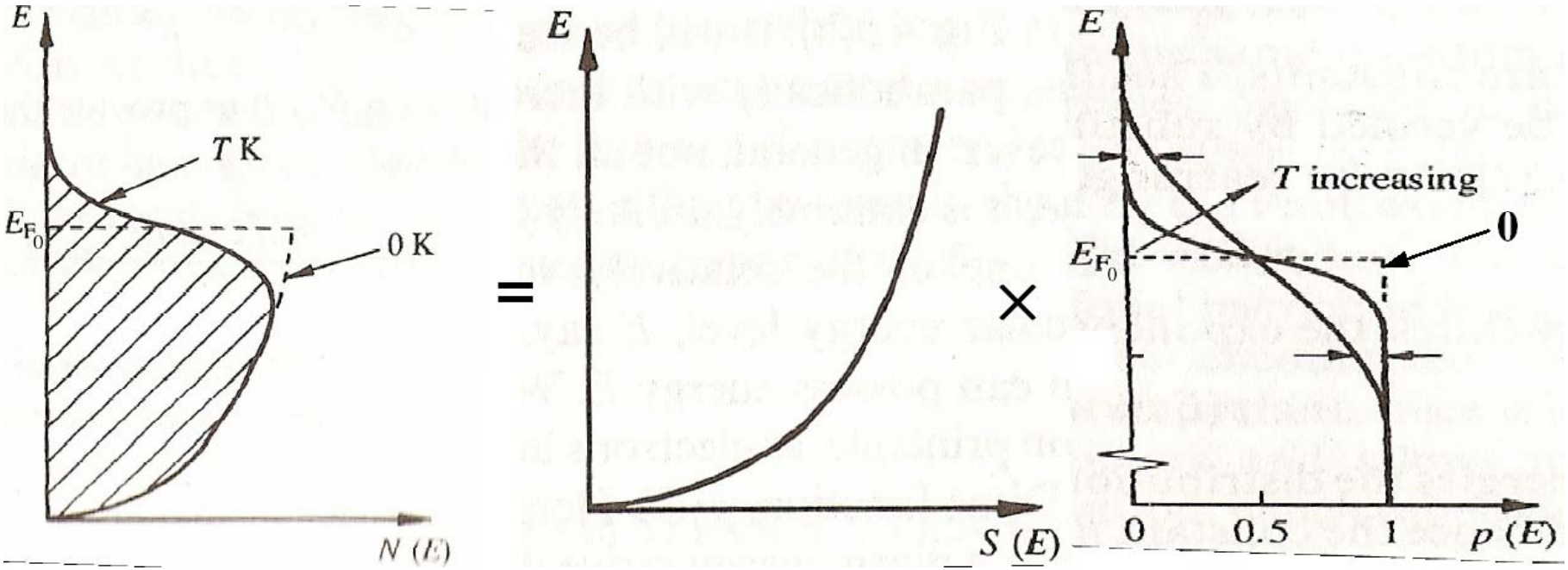
- What is the number of (available) states with energies in the range E and $E+\mathrm{d}E$?

$$N(E)\mathrm{d}E = S(E)\mathrm{d}E \times p(E)$$

number of e$^-$ = number of available states × probability of occupation

$$N(E) = S(E)\,p(E)$$

number of e$^-$ per unit volume and unit energy



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:

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

  - 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).

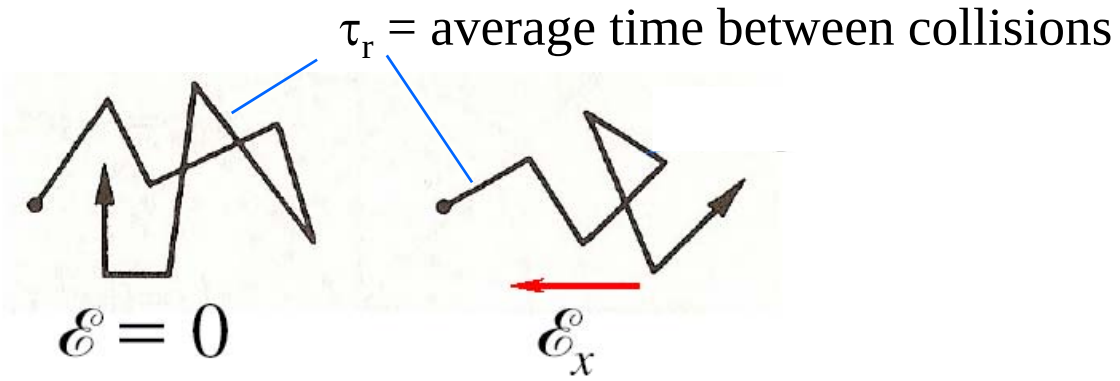
- At T > 0:

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

  - 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.
  - The equation of motion of the electron in an external electrical field is:

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

Conduction Processes in a Metal

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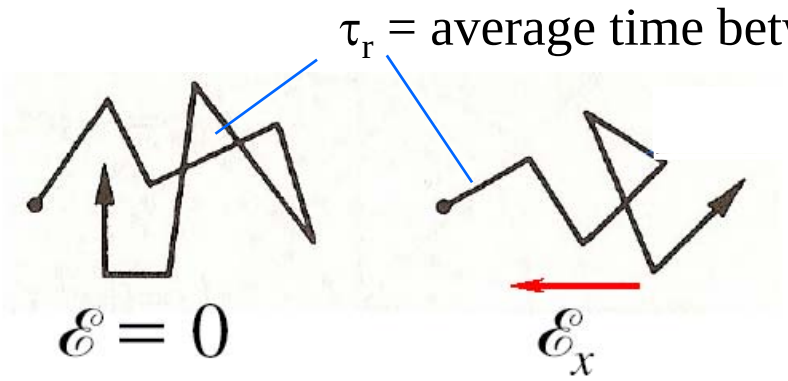


  - The friction is assumed to be proportional to $m\,\dot{x}/\tau_r$:

$$-e\mathscr{E}_x - \frac{m}{\tau_r}\dot{x} = m\ddot{x} \quad \Rightarrow \quad -e\mathscr{E}_x = m\frac{d}{dt}(v_{Dx}) + \frac{m(v_{Dx})}{\tau_r}$$

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

  - At large times ($t >> \tau_r$): $v_{Dx} = -(e\tau_r/m)\mathscr{E}_x = -\mu\mathscr{E}_x$

Conduction Processes in a Metal

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

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

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

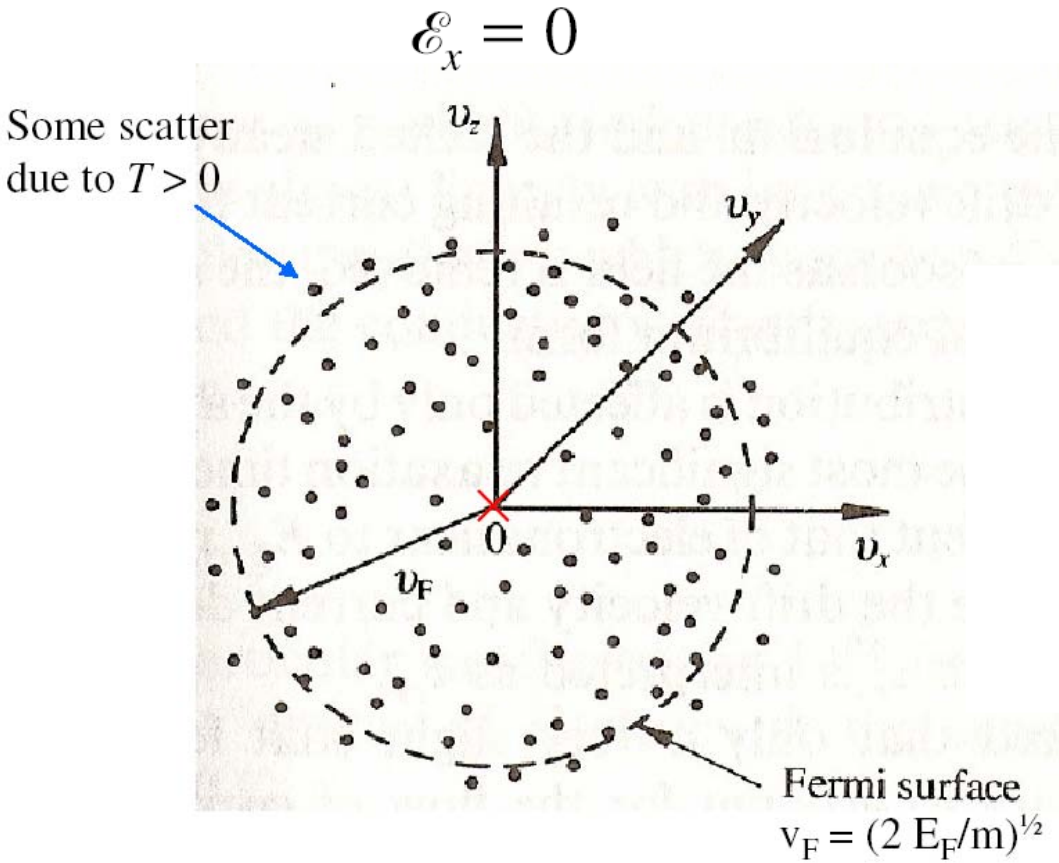
$$J_x = (ne^2\,\tau_r/m)\mathscr{E}_x = ne\mu\,\mathscr{E}_x$$

  - 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 ($E = \frac{1}{2} mv^2$) :



Conduction Processes in a Metal

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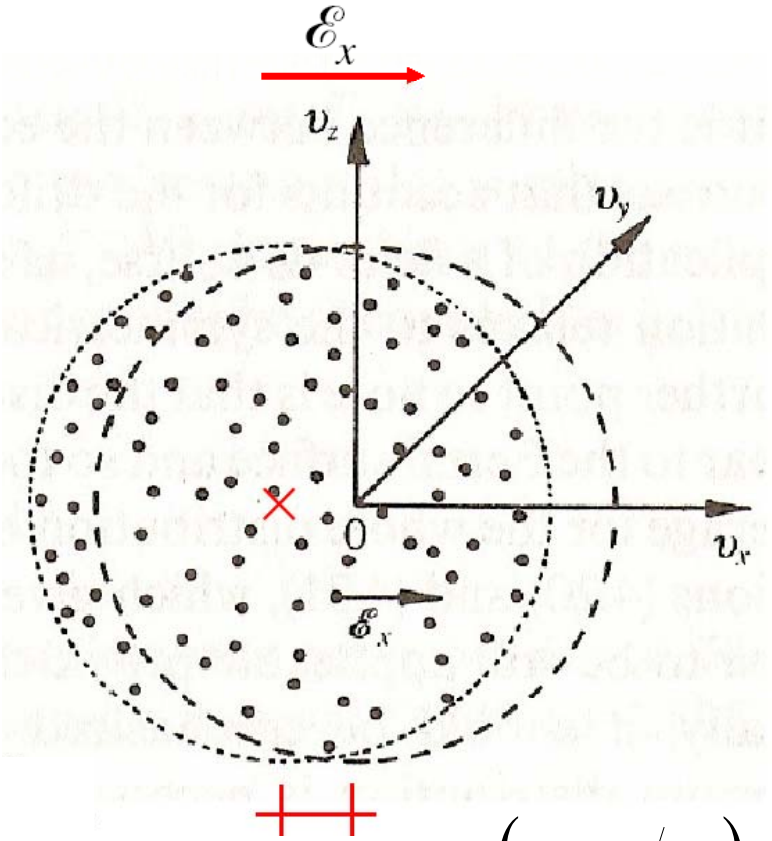


- Only the electrons close to the Fermi surface can move.

- Previous equations are valid but with:

$$\tau_r \equiv \tau_{rF}$$

$$v_{Dx} \equiv -\left(e\,\tau_{rF}/m\right)\mathscr{E}_x$$

Conduction Processes in a Metal

- Conduction and distribution of states:
  - What are the scattering centers?
  - Are they the nuclei?

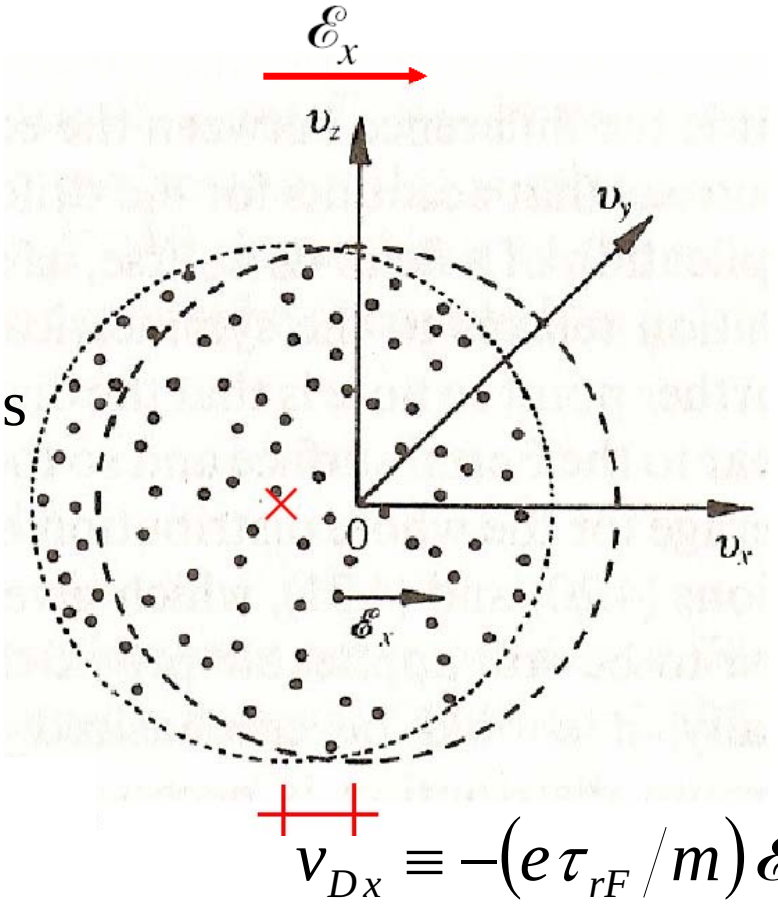
$$\bar{l}_F = v_F \tau_{rF} = (2E_F e/m)^{1/2} \tau_{rF}$$

For copper:

$$E_F \approx 7\text{eV}; \quad v_F \approx 10^6\ \text{m/s}; \quad \tau_{rF} \approx 10^{-14}\ \text{s}$$

$$\Rightarrow \quad \bar{l}_F \approx 10\text{nm}$$

Scattering centers cannot be nuclei!!!
(atomic distances are of the order of 0.1 nm)



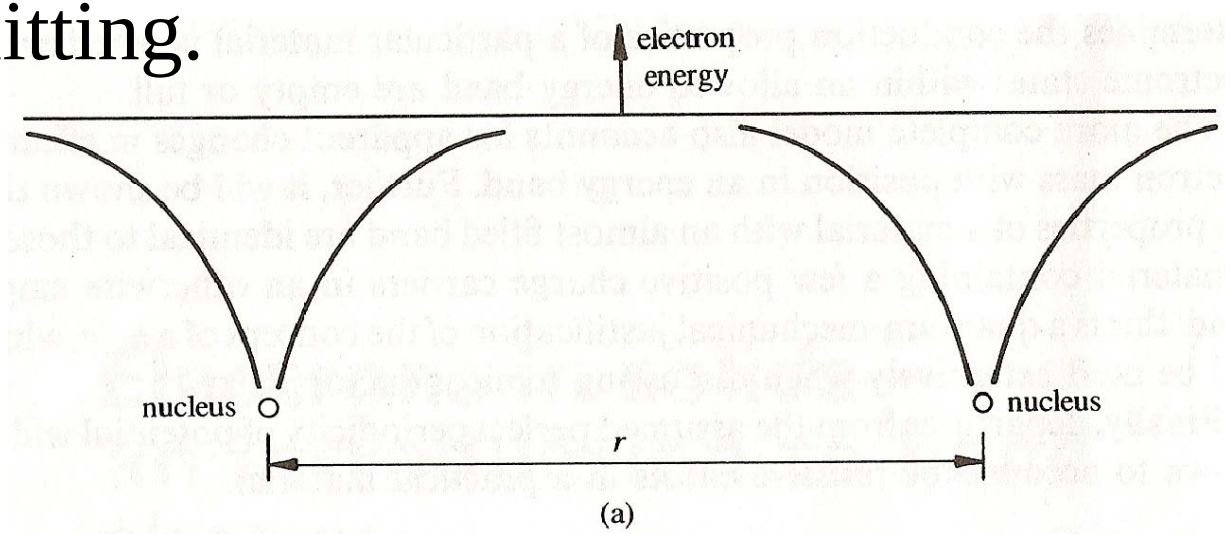
$$v_{Dx} \equiv -(e\tau_{rF}/m)\mathscr{E}_x$$

5. Energy Bands

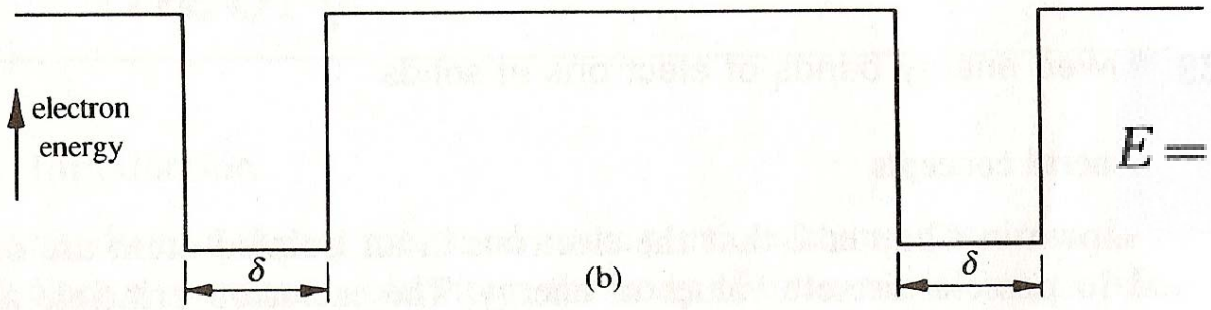
Origin of Energy Bands

- Energy splitting.

Two atoms separated a distance *r*.

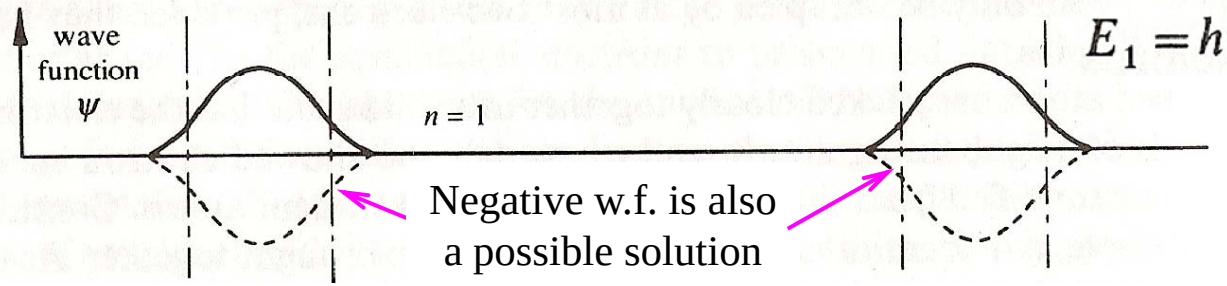


Modeled by potential wells.



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

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

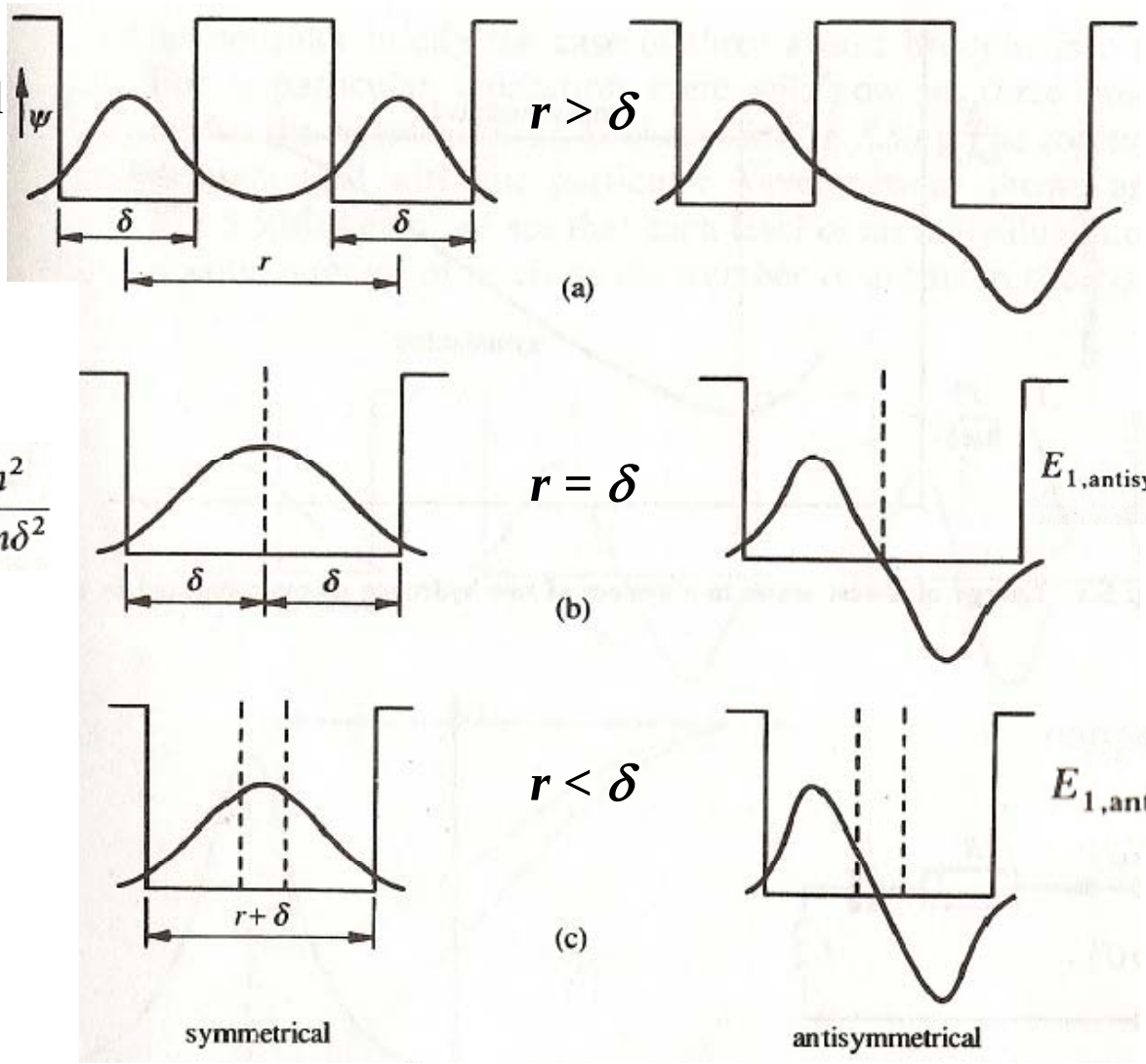


$$E_1 = h^2/(8m\delta^2)$$

Origin of Energy Bands

- Energy splitting.

Two atoms separated a distance r are brought together.



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

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

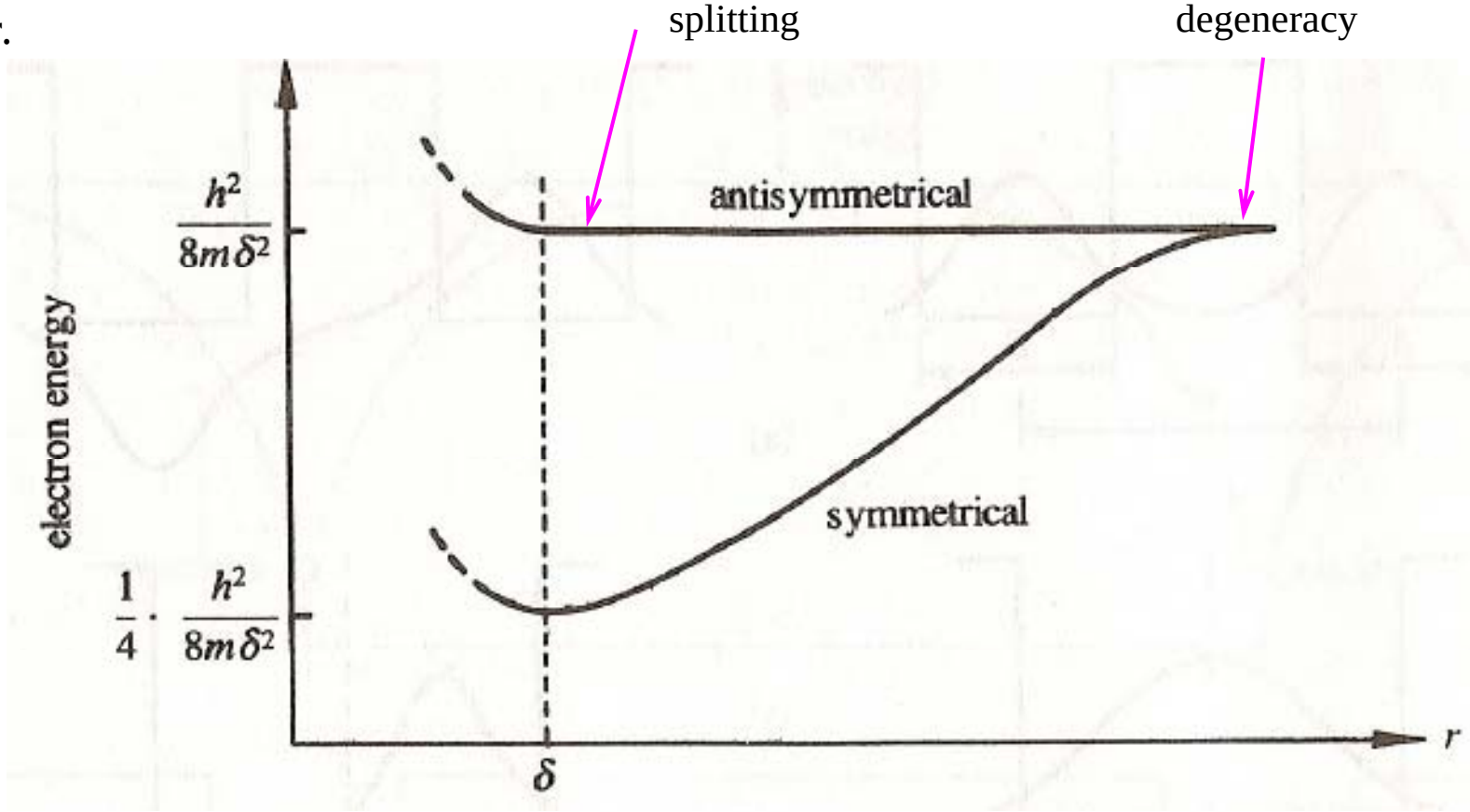
$$E_{1,\mathrm{sym}} = \frac{h^2}{8m(r+\delta)^2}$$

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

Origin of Energy Bands

- Energy splitting.

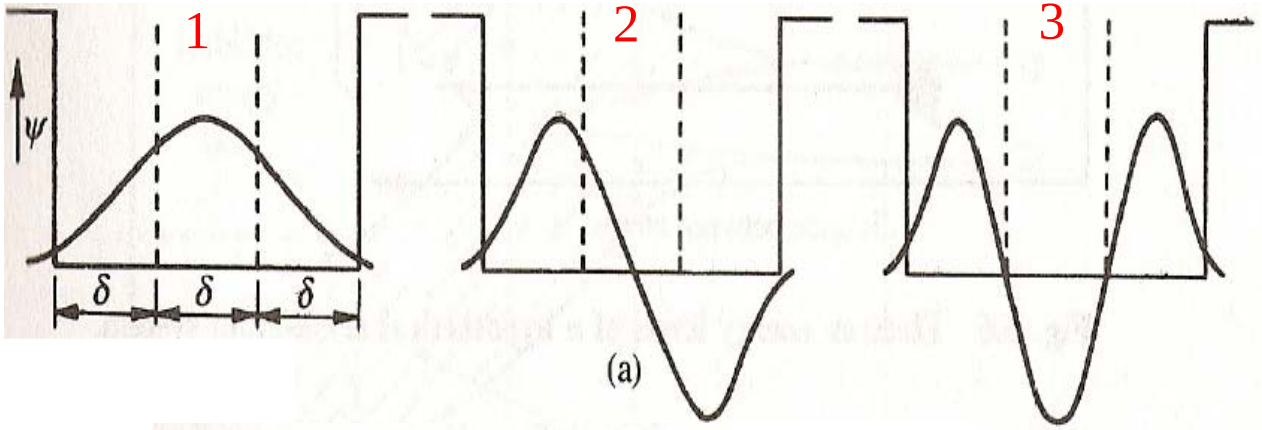
Two atoms separated a distance r are brought together.

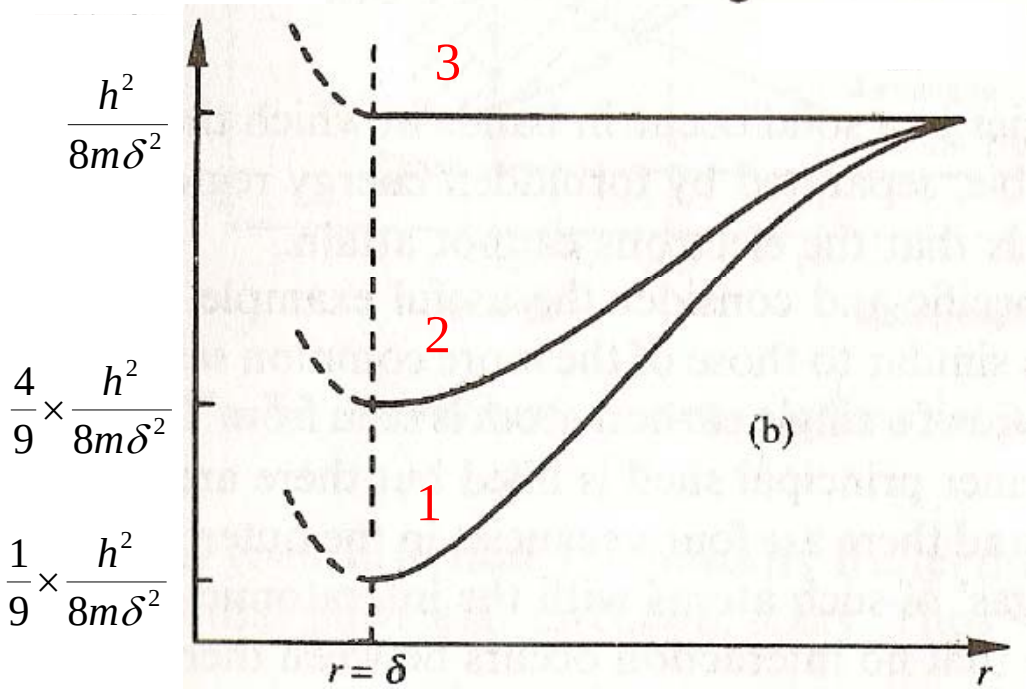


Origin of Energy Bands

- Energy splitting.

Three atoms separated a distance *r* are brought together.

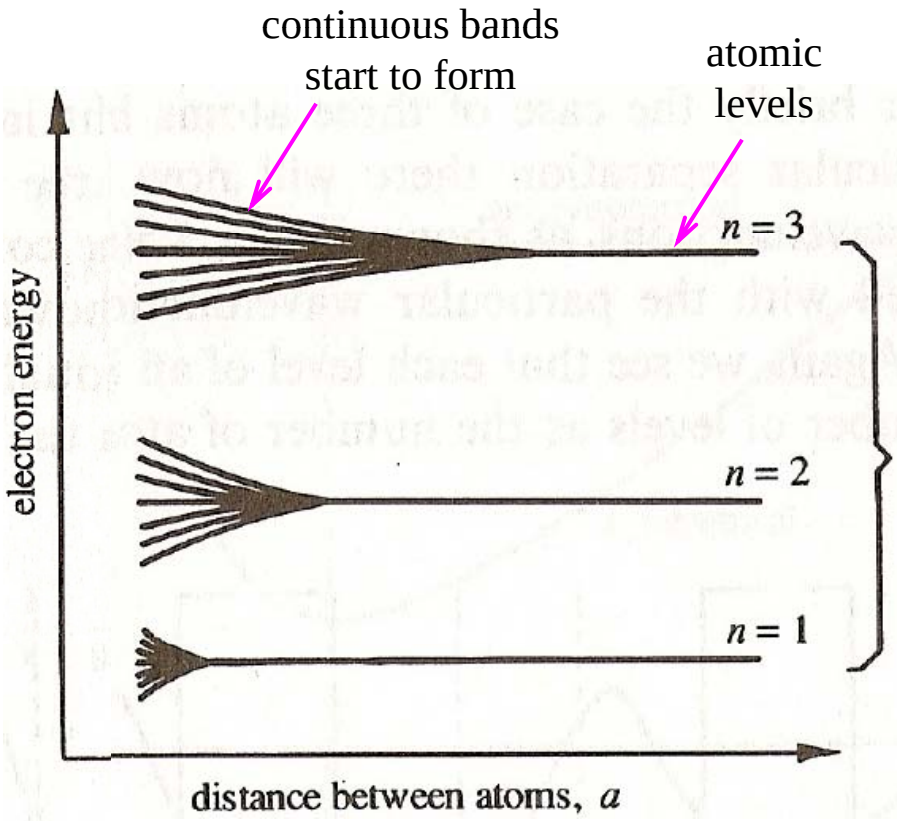




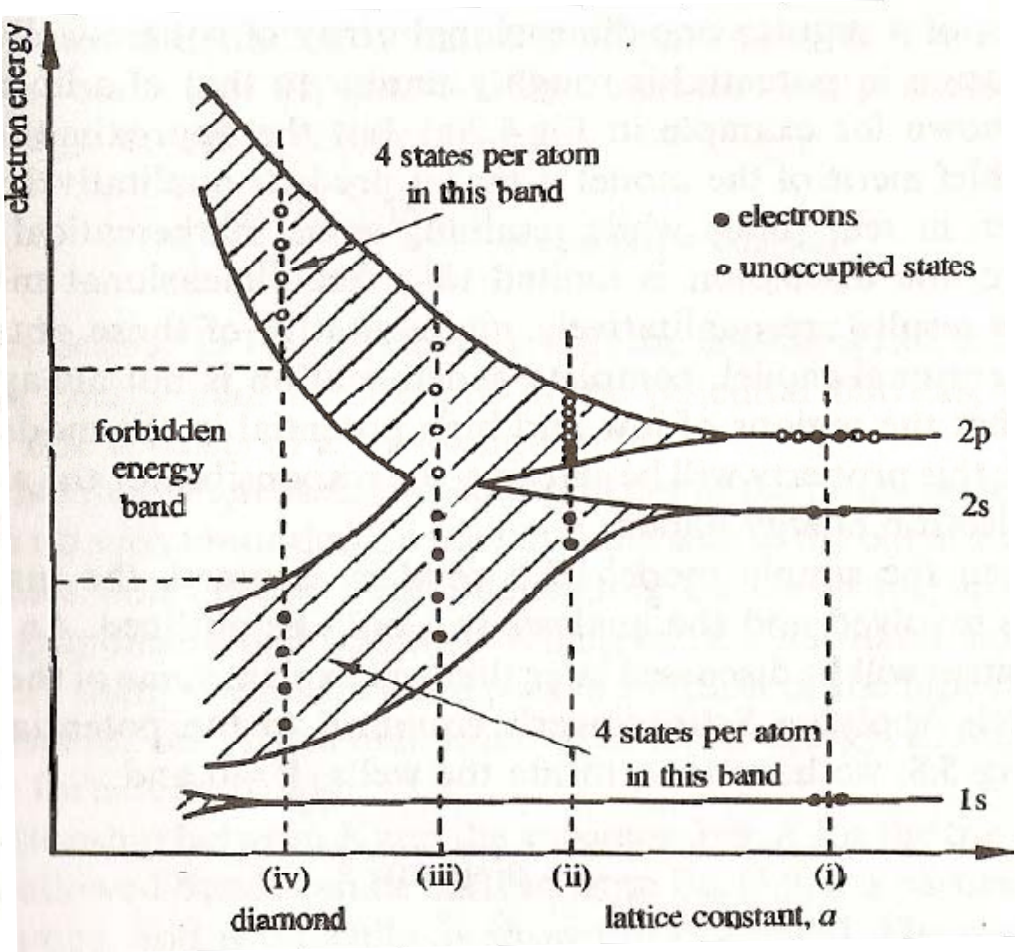
Origin of Energy Bands

- Energy splitting.

More atoms are brought together.

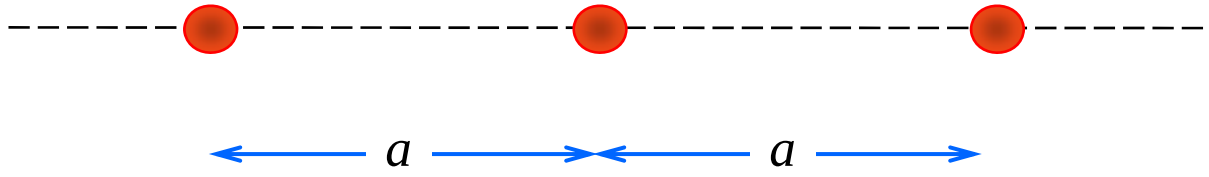


Example: Carbon.



Origin of Energy Bands

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



- The potential has the same periodicity:

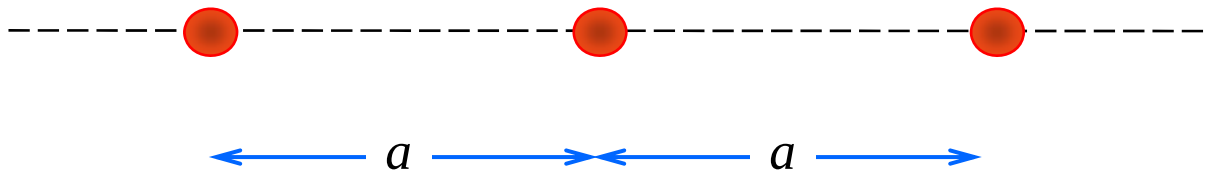
$$V(x) = V(x+a) = V(x+2a) = \ldots$$

- The w.f. has to have the same periodicity:

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

Origin of Energy Bands

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



- Further we consider that the chain forms a ring:

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

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

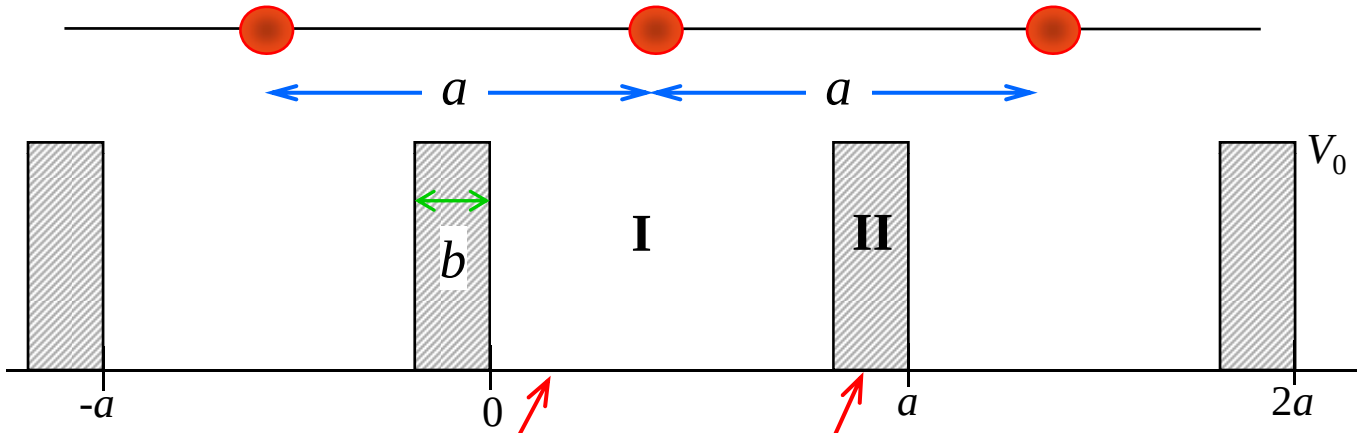
- To satisfy the periodicity and the value of C, the w.f. has to be:

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

i.e. a plane wave modulated in space

Allowed Energy Bands

- Kronig-Penney model.
  - Let's consider a 1D chain of *N* atoms of period *a*.



$$\frac{\partial^2\Psi}{\partial x^2}+\beta^2\Psi=0 \qquad \frac{\partial^2\Psi}{\partial x^2}-\alpha^2\Psi=0$$

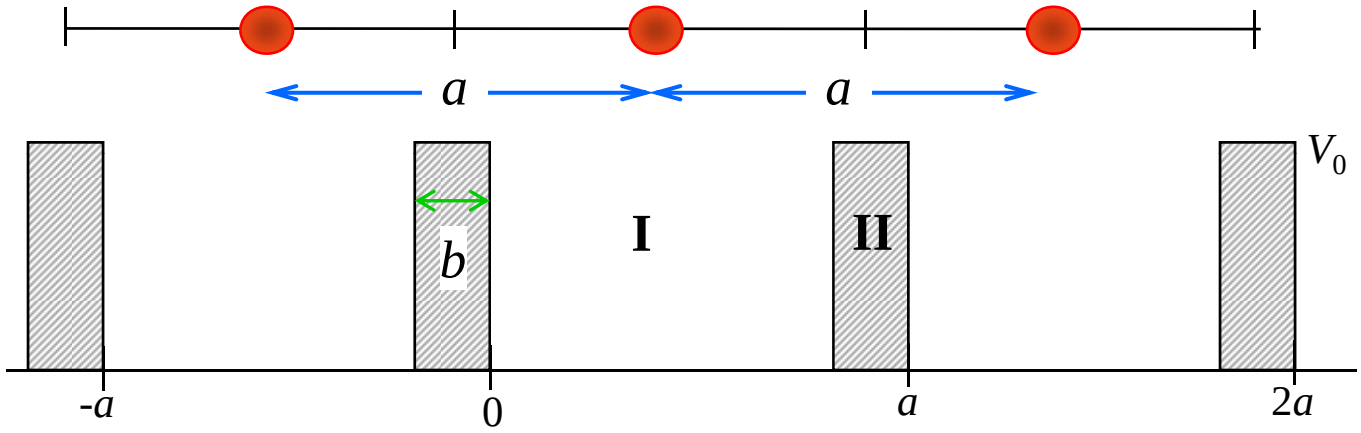
we are looking for bound states

$$\beta^2=2mE/\hbar^2 \qquad \alpha^2=2m(V_0-E)/\hbar^2$$

$$\Psi_I=Ae^{j\beta x}+Be^{-j\beta x} \qquad \Psi_{II}=C\exp(\alpha x)+D\exp(-\alpha x)$$

Allowed Energy Bands

- Kronig-Penney model.
  - Let's consider a 1D chain of N atoms of period a.



  - From continuity of ψ and $d\psi/dx$ at the boundaries:
    - At $x = 0$: $A + B = C + D \;;\; i\beta(A - B) = \alpha(C - D)$.
  - From Bloch's theorem, $\psi(x + a) = \psi(x)e^{ika}$:
    - At $x = -b$:

$$Ae^{i\beta(a-b)} + Be^{-i\beta(a-b)} = (Ce^{i\alpha(-b)} + De^{-i\alpha(-b)})\, e^{-ika}$$

$$i\beta[Ae^{i\beta(a-b)} - Be^{-i\beta(a-b)}] = \alpha[Ce^{i\alpha(-b)} - De^{-i\alpha(-b)}]\, e^{-ika}$$

Allowed Energy Bands

- Kronig-Penney model.
  - The previous system of 4 equations have a solution only if its determinant is equal to zero giving:

$$[(\alpha^2 - \beta^2)/2\alpha\beta]\sinh \alpha b \sin \beta(a-b) + \cosh \alpha b \cos \beta(a-b) = \cos ka$$

NOTE: The solution of this equation gives the values of the allowed E

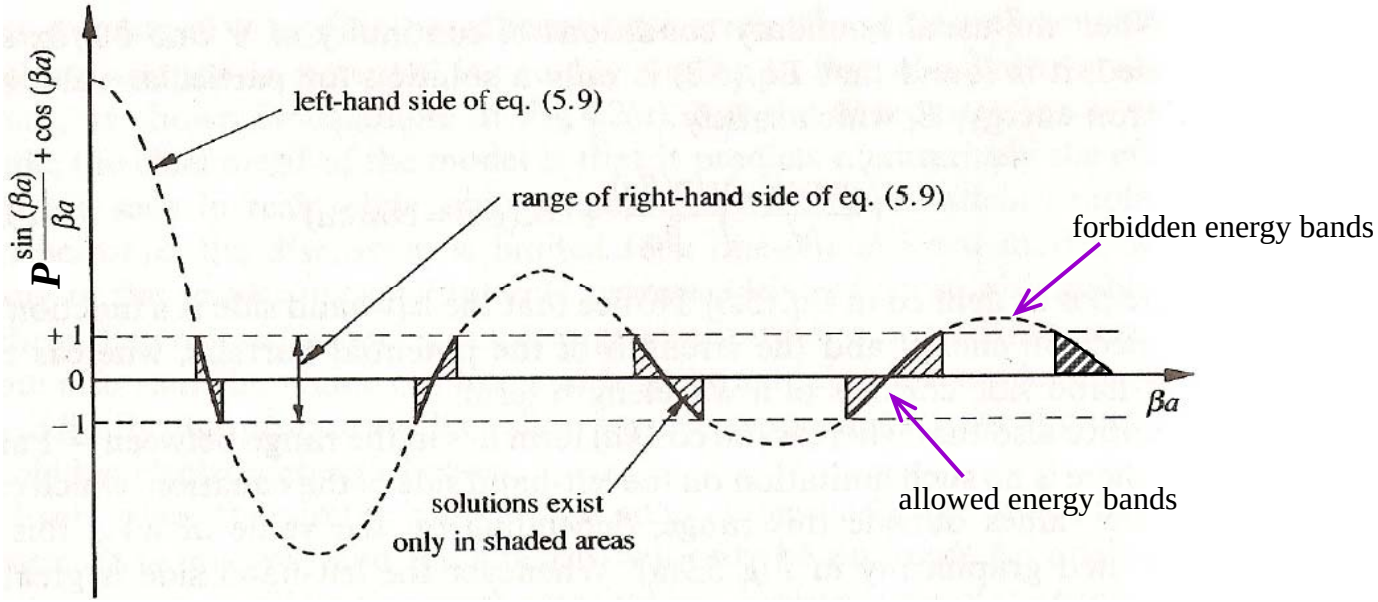
  - For simplicity, let's consider the case $\boldsymbol{b \to 0}$ & $\boldsymbol{V_0 \to \infty}$ but such that $\boldsymbol{\alpha^2 ba/2 = P}$ remains constant.

  - In this limit $\boldsymbol{\alpha \gg \beta}$ & $\boldsymbol{\alpha b \ll 1}$. Then:

$$(P/\beta a)\sin \beta a + \cos \beta a = \cos ka$$

Allowed Energy Bands

- Kronig-Penney model.
  - What are the allowed electron energies $E = \hbar\beta^2/2m$?
  - We have to solve $(P/\beta a)\sin \beta a + \cos \beta a = \cos ka$



  - As P becomes larger (i.e. the product bV_0), the allowed bands become narrower.
  - As $P \to 0$, $\beta \to k$ (i.e. towards the free electron model)

Conclusions

- We have introduced a simple model for conduction. Not all electrons conduce but those close to the Fermi energy.
- When going from isolated atoms to an assembly of them, energy bands start to form.
- Electrons can only exist in those bands. Not all energies are permitted.