Physics of Electronics:

4. Conduction in Metals

July – December 2008

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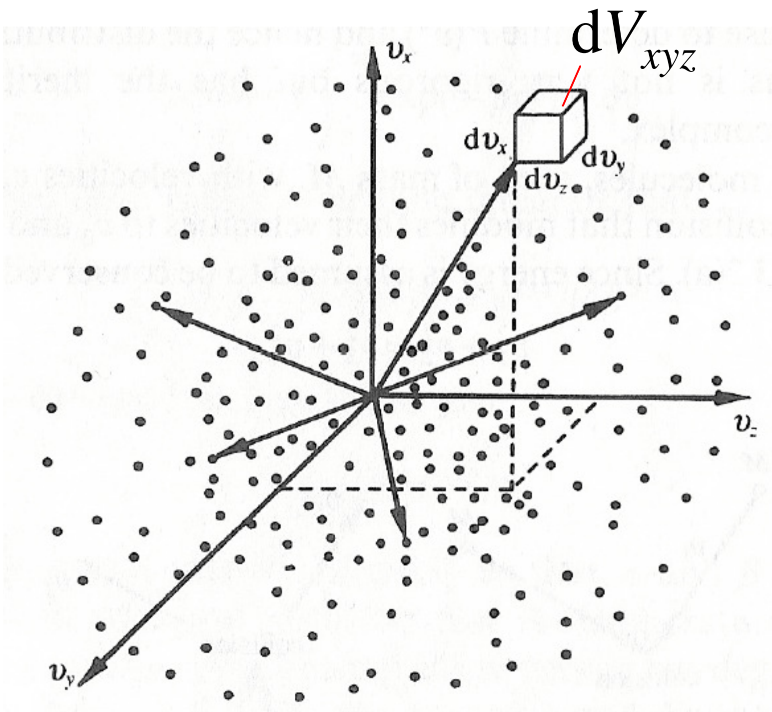
- Assemblies of classical particles.
- Collection of particles obeying the exclusion principle.
- A simple model of a conductor.
- Electrons in a 3D box.
- Maximum number of possible energy states.
- Energy distribution of electrons in a metal.
- Fermi level in a metal.
- Conduction processes in metals.

Assemblies of Classical Particles

- Consider a gas of N neutral molecules



The number of particles in dV_{xyz} is

$$dN_{xyz} = P(v^2)\, dv_x\, dv_y\, dv_z$$

and in a shell of thickness dv is

$$dN_v = P(v^2) 4\pi v^2\, dv$$

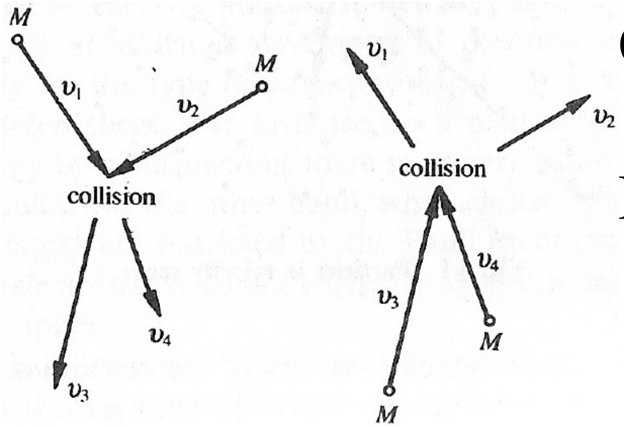
where $P(v^2)$ is the density of particles having a speed v (i.e. density of points in v-space).

Total number of particles is: $\int_0^\infty dN_v = \int_0^\infty P(v^2) 4\pi v^2\, dv = N$

Assemblies of Classical Particles

- The distribution function (distribution of speeds):
  - To find $P(v^2)$ let's consider collisions inside this gas

collison probability $\propto P(v_1^2)P(v_2^2)$



Collision and reversed collision:

$$P(v_1^2)P(v_2^2)=P(v_3^2)P(v_4^2)$$

Energy conservation:

$$v_1^2+v_2^2=v_3^2+v_4^2$$

$$\Rightarrow\quad P(v^2)=A\ \exp(-\beta v^2)$$

  - Constants A and β are found from:

Total number of particles: $N=4\pi A\int_0^\infty \exp(-\beta v^2)v^2\,\mathrm{d}v$

Definition of T: $\underbrace{\int_0^\infty \tfrac{1}{2}(M\,v^2)\,[A\exp(-\beta\,v^2)]\,4\pi v^2\,\mathrm{d}v}_{\text{Mean kinetic energy}}=\tfrac{3}{2}NkT$

$$\Rightarrow\quad \beta=M/(2kT)$$

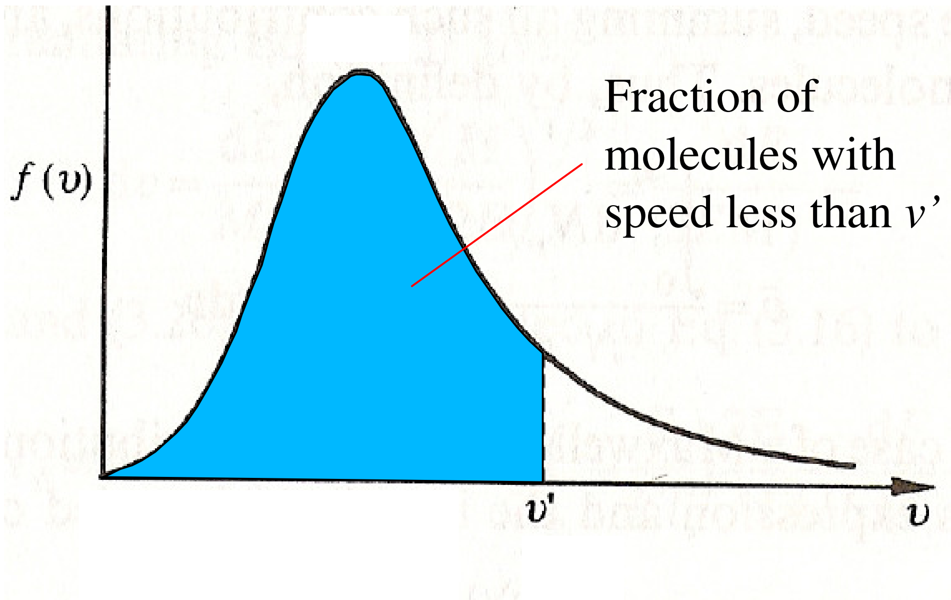
$$A=N\left(\frac{M}{2\pi kT}\right)^{3/2}$$

Maxwell-Boltzmann Distribution Function

- Relation between $P(v^2)$ and $f(v)$:
  - Number of particles in a shell of thickness dv:

$$\left.\begin{aligned} dN_v &= P(v^2)4\pi v^2\,dv \\ dN_v &= Nf(v)\,dv \end{aligned}\right\} \Rightarrow \boxed{f(v) = 4\pi\left(\frac{M}{2\pi kT}\right)^{3/2}\exp\left(-\frac{Mv^2}{2kT}\right)v^2}$$

  - $f(v)$ gives the fraction of molecules (per unit volume) in a given speed range (per unit range of speed).



Energy Distribution Function

- How the energy is distributed in the ensemble
  - The particles in the ensemble we have considered so far only have kinetic energy:

$$E = Mv^2/2 \quad \Rightarrow \quad dv = \frac{dE}{Mv} = \frac{dE}{M}\left(\frac{M}{2E}\right)^{1/2} = \frac{dE}{(2EM)^{1/2}}$$

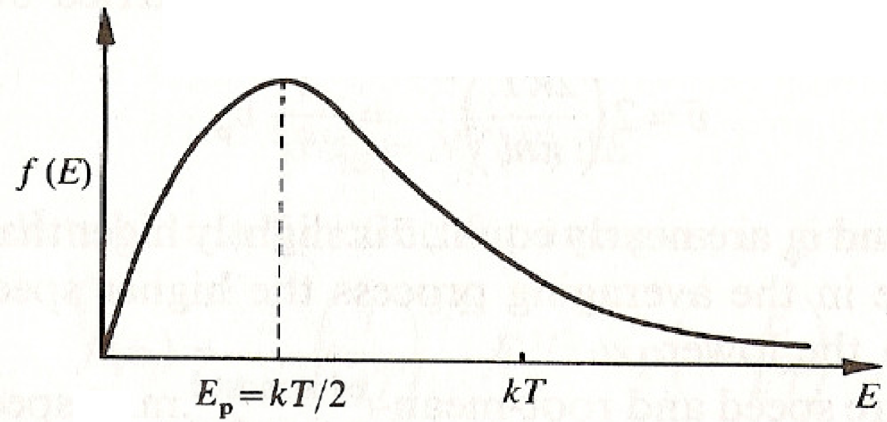
  - Replacing in the expression for dN_v:

$$dN_E = 4\pi N\left(\frac{M}{2\pi kT}\right)^{3/2} \exp\left(-\frac{E}{kT}\right)\frac{2E}{M}\frac{dE}{(2EM)^{1/2}}$$

  - But $dN_E = Nf(E)\,dE$ then:

$$\boxed{f(E) = \frac{2}{\pi^{1/2}}\left(\frac{1}{kT}\right)^{3/2} E^{1/2} \exp\left(-\frac{E}{kT}\right)}$$

Note that the density of the particles is independent of the position



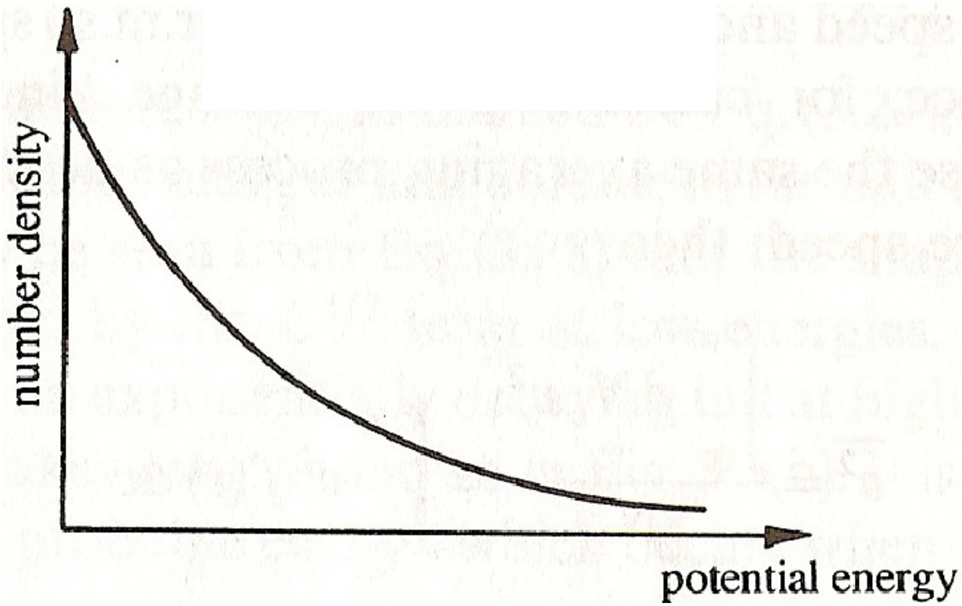
Boltzmann Distribution Function

- How the energy is distributed in the ensemble
  - We now consider that the particles in the ensemble not only have KE but also PE (gravitational or electrical field).

$$f(E) \propto \exp(-E/kT) \propto \exp[-(\mathrm{KE}+\mathrm{PE})/kT]$$

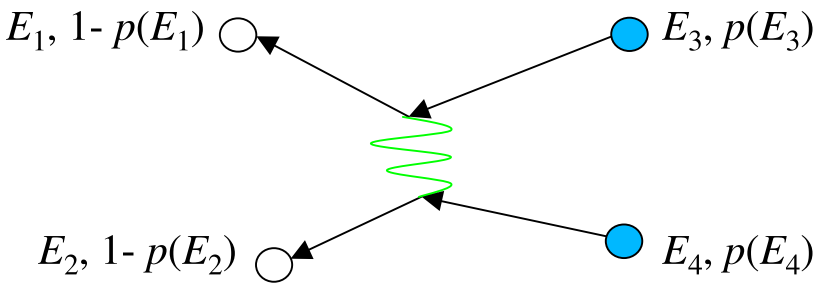
  - If the PE depends on the position so does the density of the ensemble:

$$n_2/n_1 = \exp[-e(V_2 - V_1)/kT]$$



Fermi-Dirac Distribution

- Ensembles obeying exclusion principle
  - Two quantum particles (E_3, E_4) interact and end up in two states (E_1, E_2) previously empty:



$$p(E_1)p(E_2)[1-p(E_3)][1-p(E_4)] = p(E_3)p(E_4)[1-p(E_1)][1-p(E_2)]$$

$$\Rightarrow \left(\frac{1}{p(E_1)}-1\right)\left(\frac{1}{p(E_2)}-1\right)=\left(\frac{1}{p(E_3)}-1\right)\left(\frac{1}{p(E_4)}-1\right)$$

$$\boldsymbol{E_1 + E_2 = E_1 + E_2}$$

$$\Rightarrow [1/p(E)]-1 = A\ \exp(\beta E)$$

$$p(E) = 1/[1 + A\exp(\beta E)]$$

  - When $E \to \infty$ it reduces to the Boltzmann distribution:

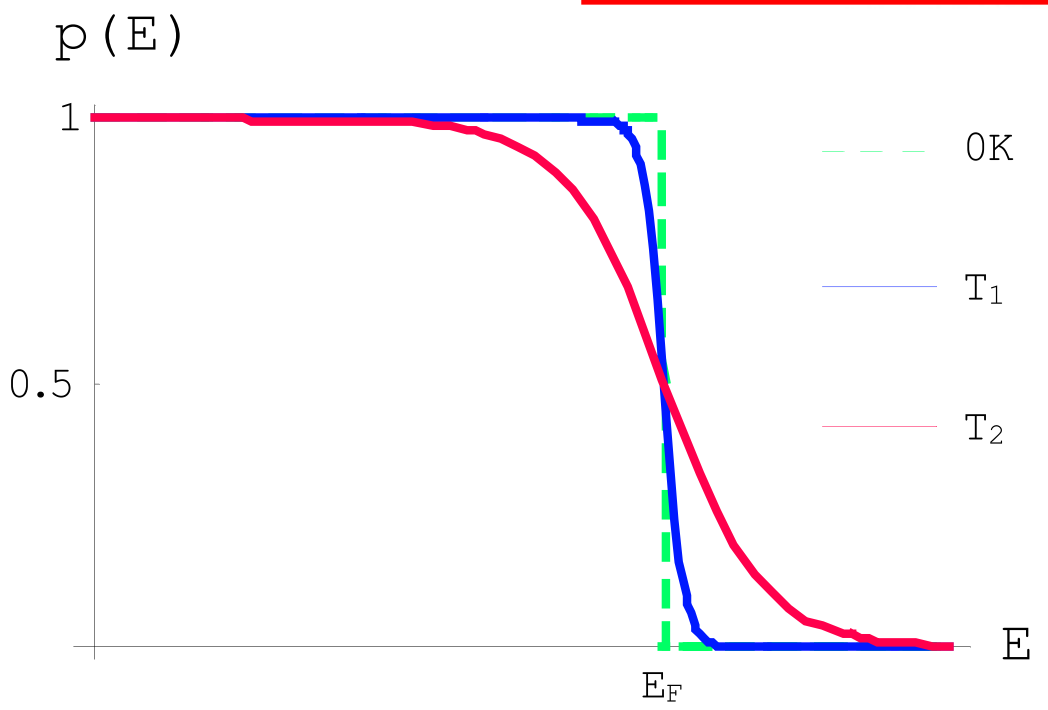
$$p(E) \simeq A\ \exp(-\beta E) \Rightarrow \beta = 1/kT$$

Fermi-Dirac Distribution

- Ensembles obeying exclusion principle
  - The constant A is redefined through E_F and can be found via normalization

$$A = \exp(-E_F/kT)$$

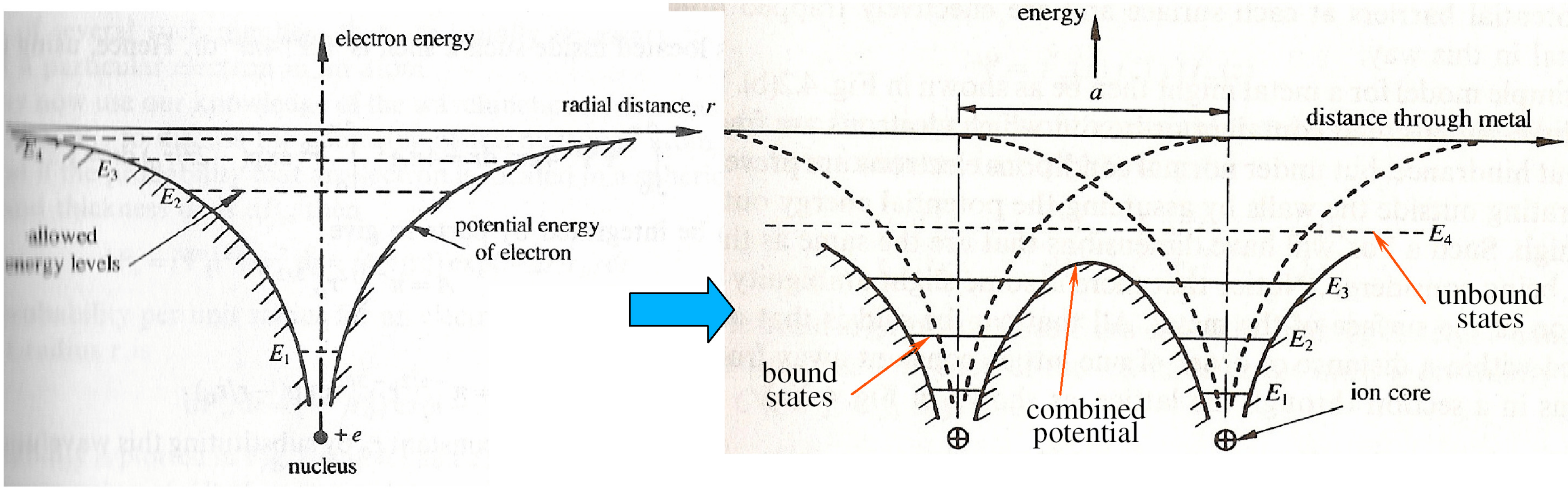
  - Therefore: $$\boxed{p(E) = \frac{1}{1+\exp[(E-E_F)/kT]}}$$



Note that for T = 0, $p(E)$ reduces to a step function. It means that all the states with energies $E \leq E_F$ are occupied and those above, are empty. When T > 0, some states below E_F are emptied and some are occupied due to thermal energy.

A Simple Model of a Conductor

- From one atom to a collection of atoms:



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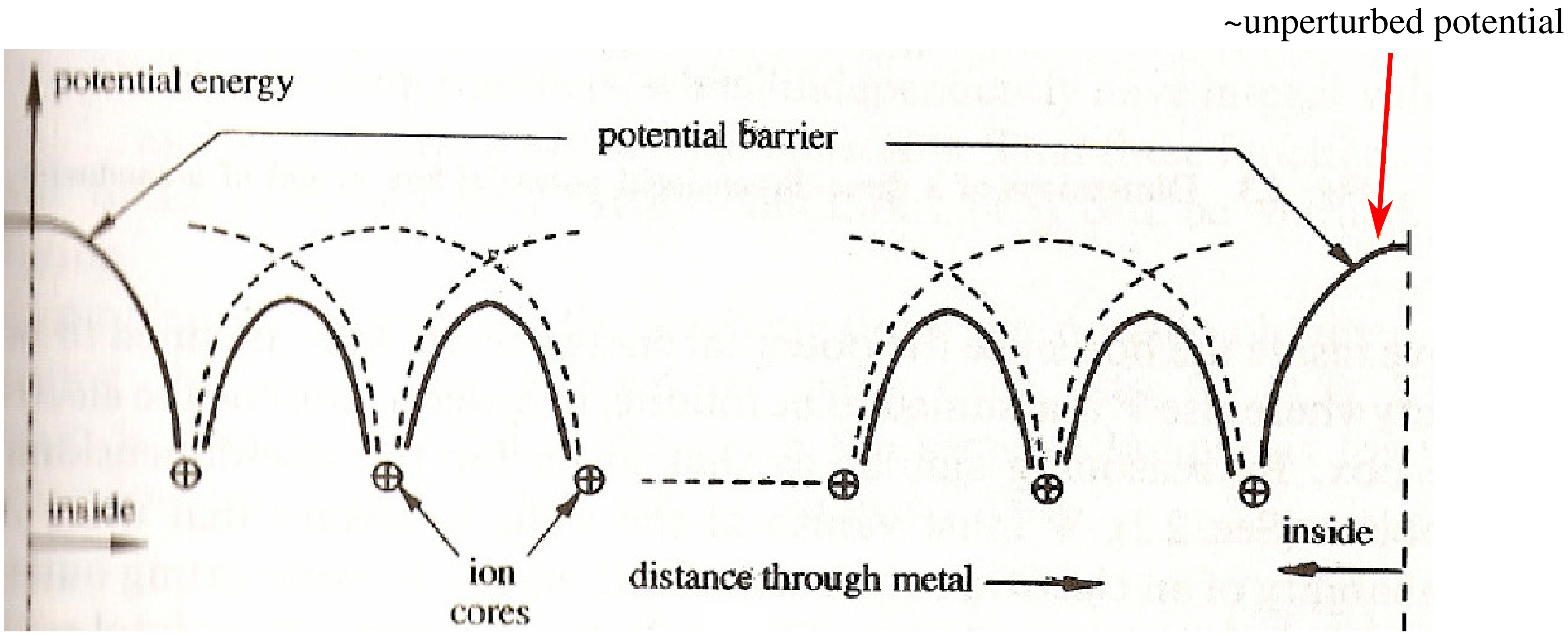
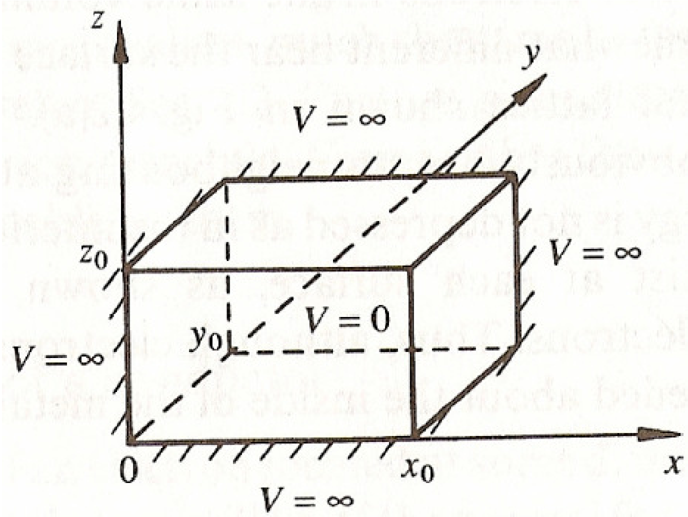


The potential barrier confines the electrons inside the faces of the conductor. Therefore we can model a conductor as unbound or free electrons confined to a potential box.

Electrons in a 3D box

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



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

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

  - Solving by variable separation

$$\Psi = f_x(x) f_y(y) f_z(z) \Rightarrow \frac{1}{f_x}\frac{d^2 f_x}{dx^2} + \frac{1}{f_y}\frac{d^2 f_y}{dy^2} + \frac{1}{f_z}\frac{d^2 f_z}{dz^2} = -\frac{2mE}{\hbar^2} \Rightarrow \frac{d^2 f_x}{dx^2} = C_1^2 f_x$$

(idem for y & z)

  - Solving and using continuity (Ψ=0 at the walls)

$$f_x = A\sin(n_x \pi x/x_0) \qquad f_y = B\sin(n_y \pi y/y_0) \qquad f_z = C\sin(n_z \pi z/z_0)$$

where n_x, n_y, n_z = 1, 2, 3, ...

Electrons in a 3D box

- Free electron model: V = 0 inside box & V = ∞ outside box
  - After normalization

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

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

  - Back into SE to obtain the energies of every state

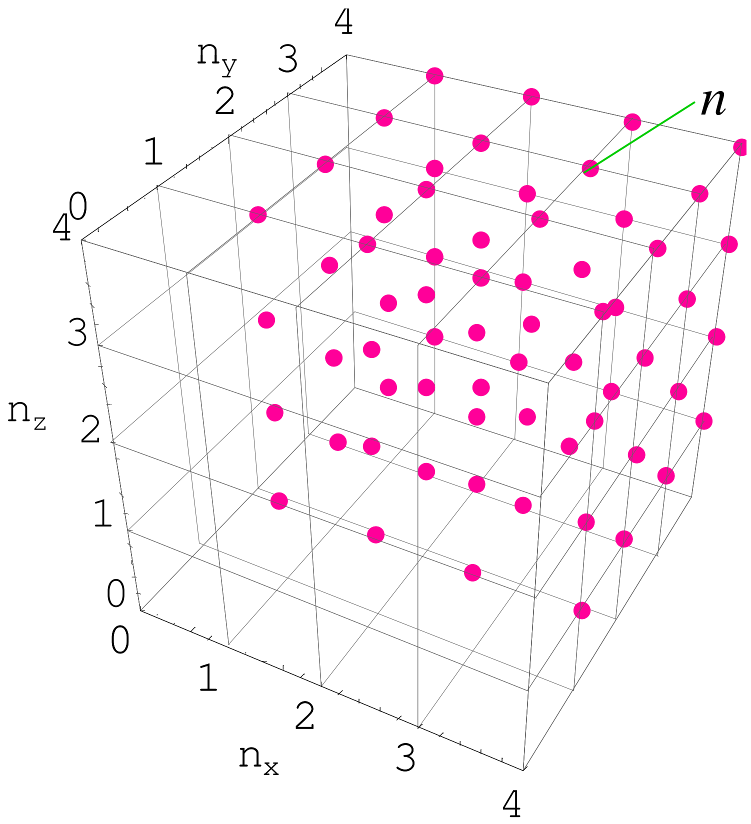
$$E = \frac{h^2}{8md^2} n^2$$

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

  - Note that results are similar to 1D well

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 $n_F \geq n = (n_x^2 + n_y^2 + n_z^2)^{½}$?



- In this representation, each point corresponds to one available state.

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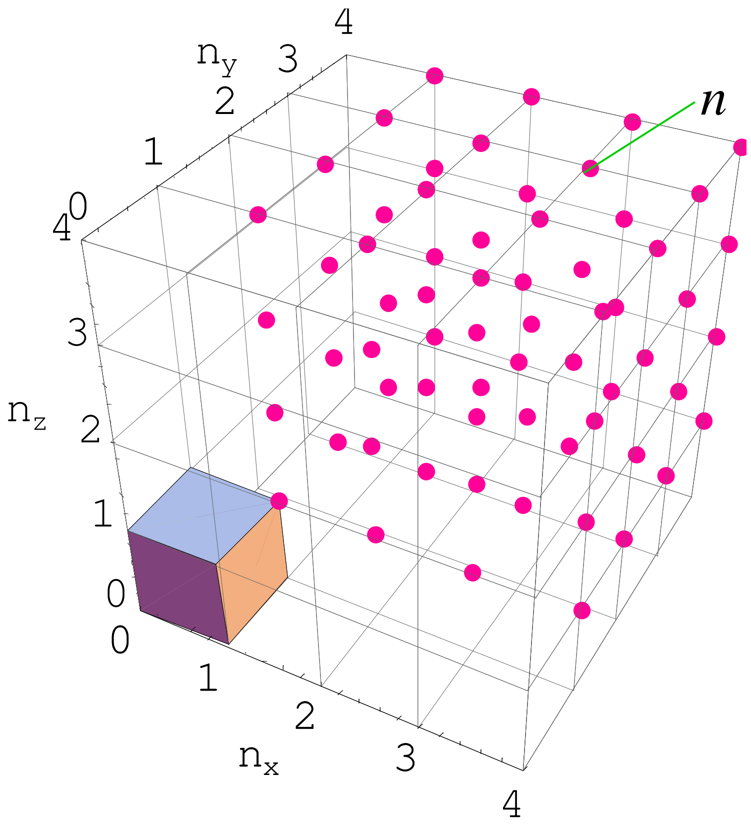

- In this representation, each point corresponds to one available state.
- To each unit of volume corresponds one available state.

Maximum Number of States

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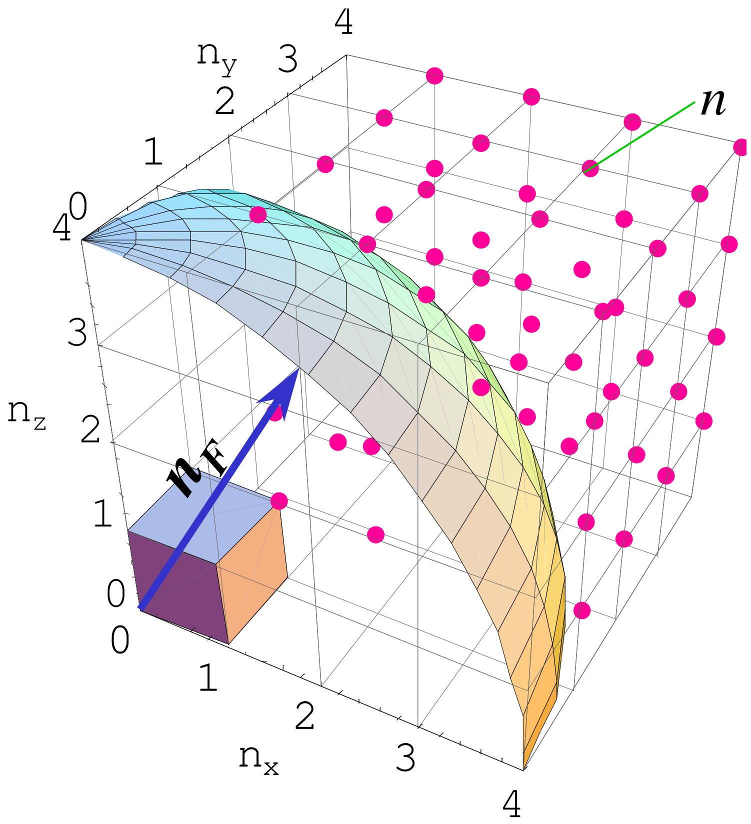

- In this representation, each point corresponds to one available state.
- To each unit of volume corresponds one available state.
- Then, the number of states such that $n \leq n_F$ corresponds to the volume generated by n_F:

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

- If we take into account the spin:

$$2(\pi n_F^3/6) = \pi n_F^3/3$$

Maximum Number of States

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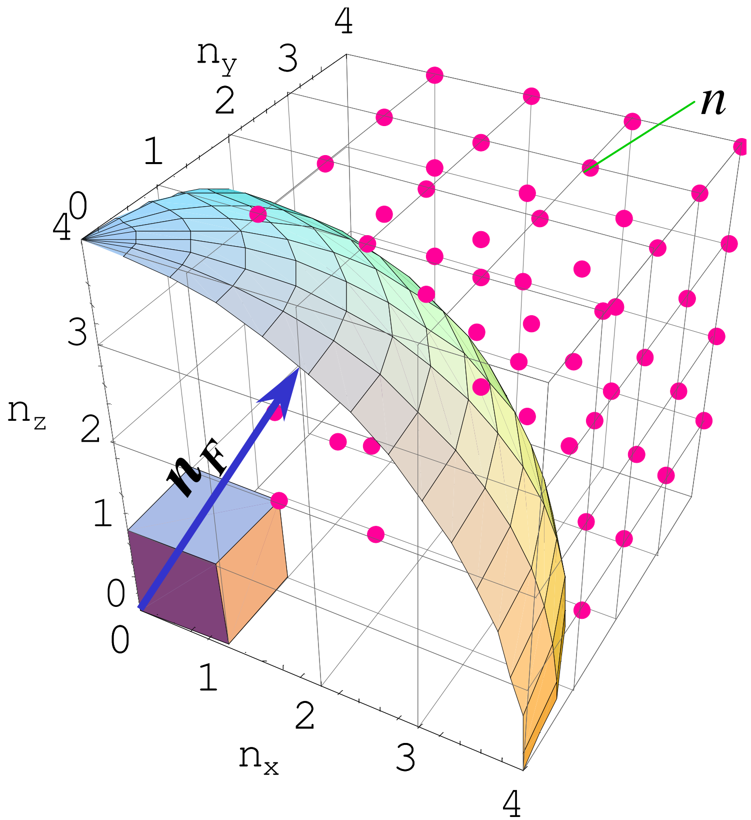


- At 0 K we have:

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

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

- Therefore:

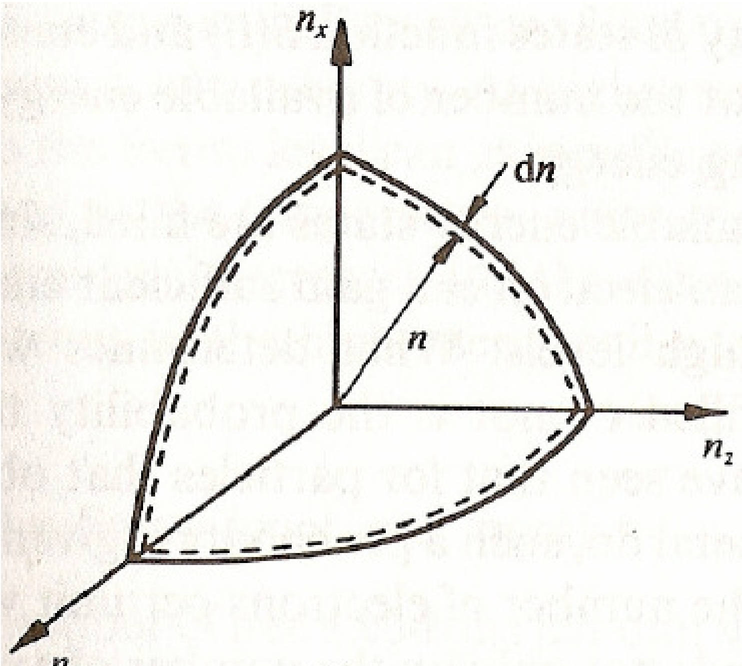
$$n_F = (3N/\pi)^{1/3} d$$

- The energy corresponding to nF:

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

Energy Distribution of e- in a Metal

- What is the number of (available) states with energies in the range E and $E+\mathrm{d}E$?
  - Since N is large, we can consider that n varies continuously.



(a)

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

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

- We define the density of (available) states, S(E), such that S(E)dE gives the number of states with energies in the range E and $E+\mathrm{d}E$ (or equivalently in the range n and $n + \mathrm{d}n$).

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

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

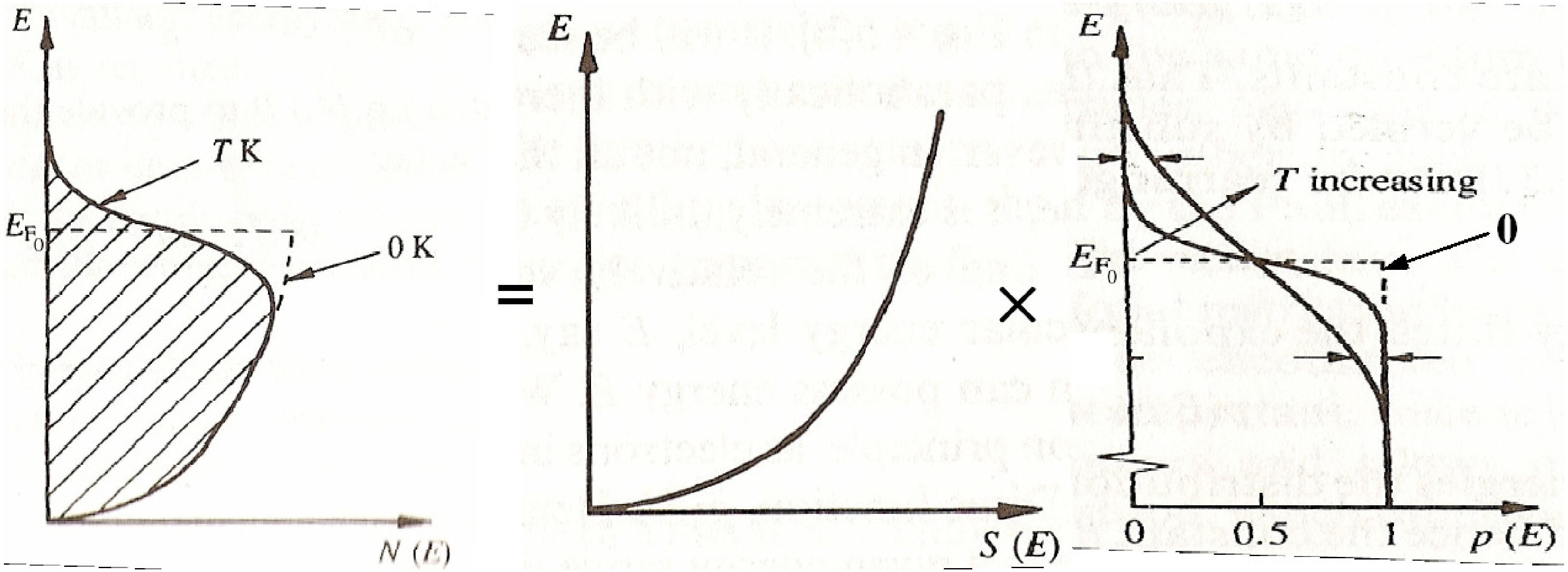
Energy Distribution of e- in a Metal

- What is the number of (available) states with energies in the range E and E+dE ?

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

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

$\Rightarrow$ $\boxed{\boldsymbol{N(E) = S(E)\,p(E)}}$ 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:

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

- At T = 0:

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

  - 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).

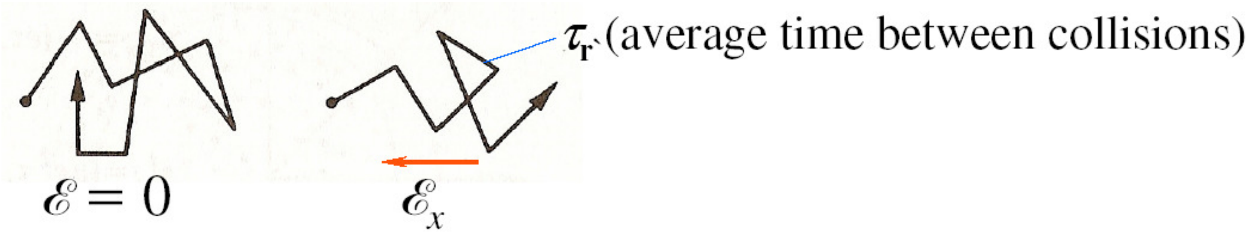
- At T > 0:

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

  - 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:

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

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

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

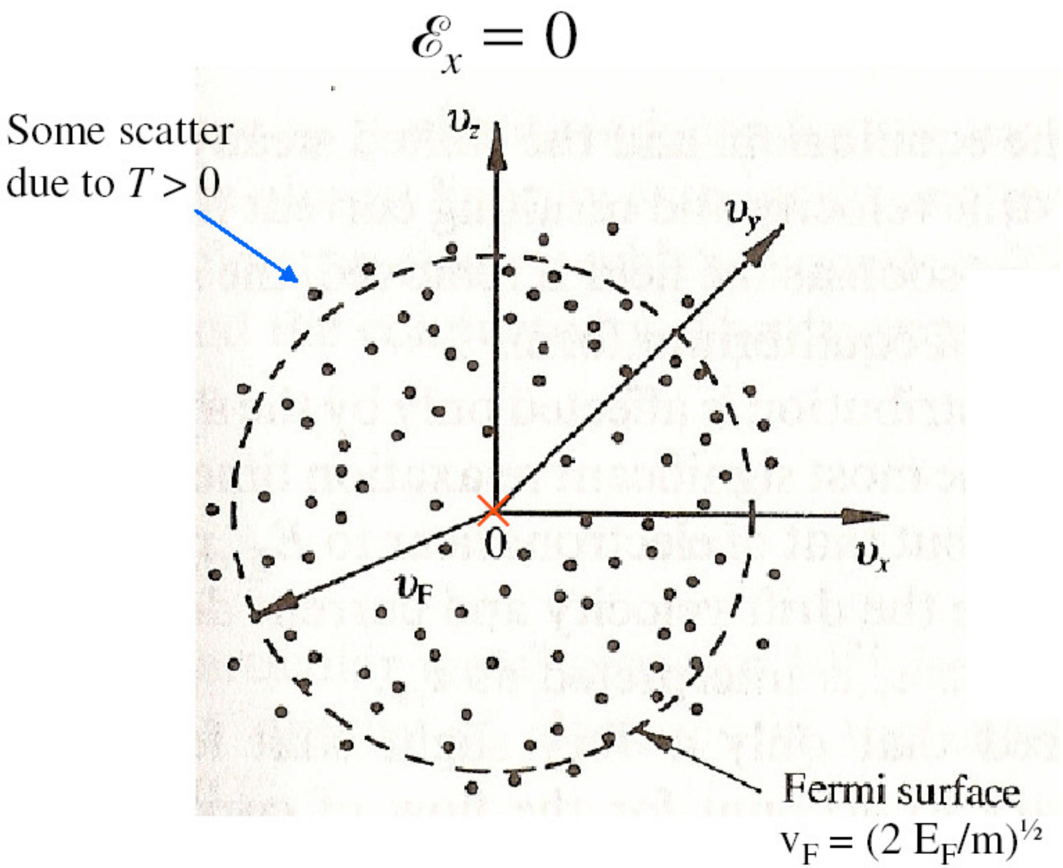
$$J_x = (ne^2\,\tau_r/m)\mathscr{E}_x = ne\mu\,\mathscr{E}_x$$

  - 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 ($E = ½\, mv^2$) :



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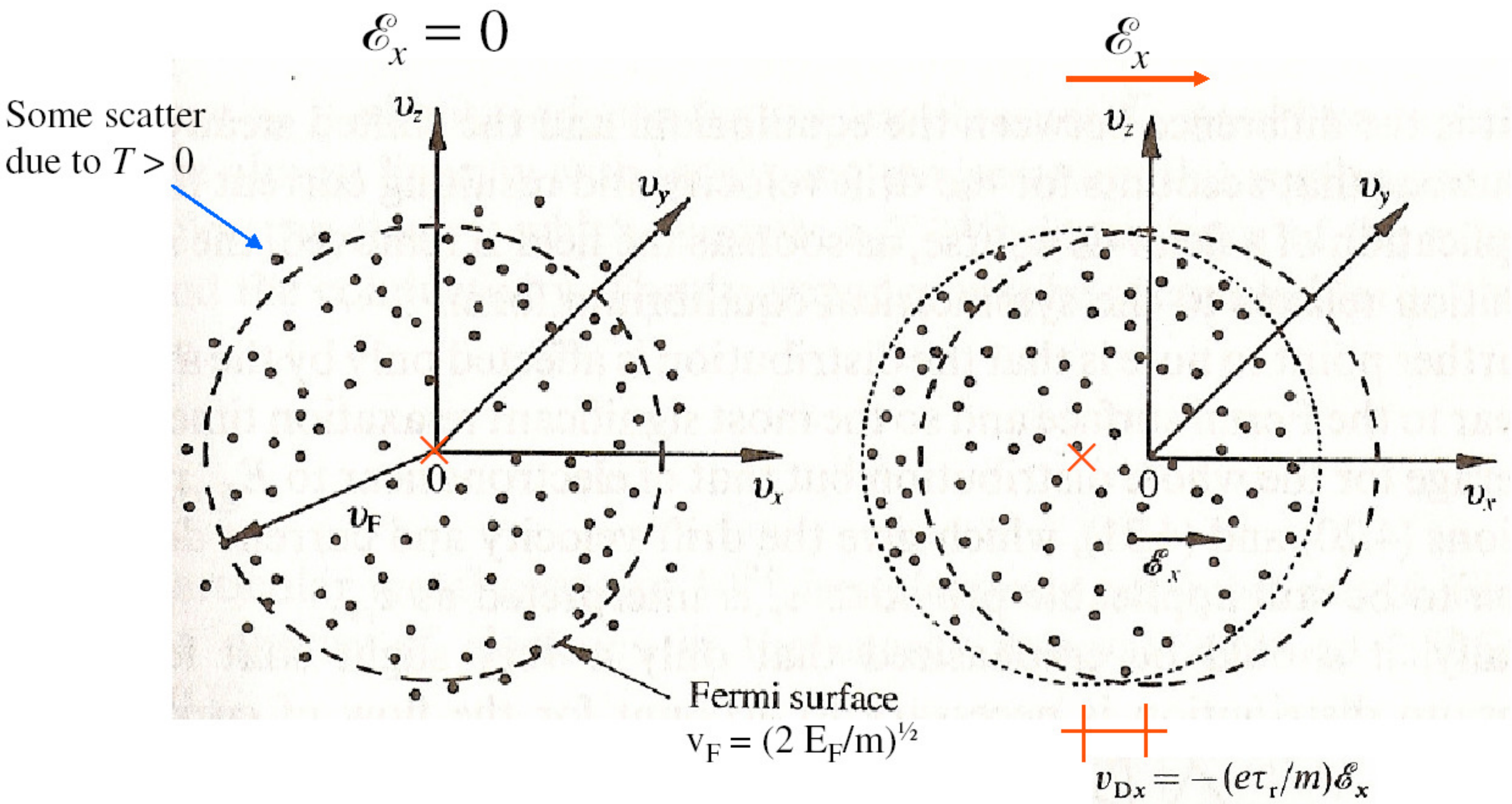
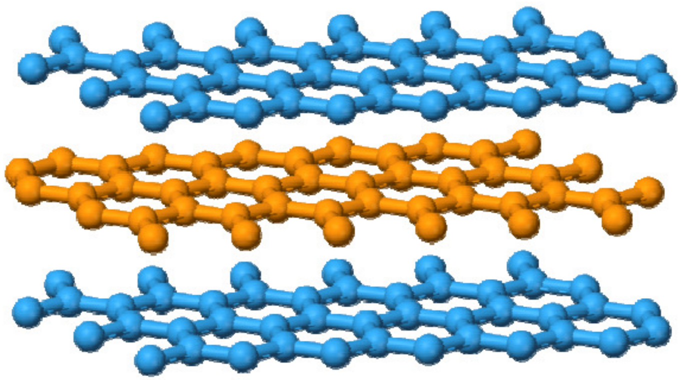
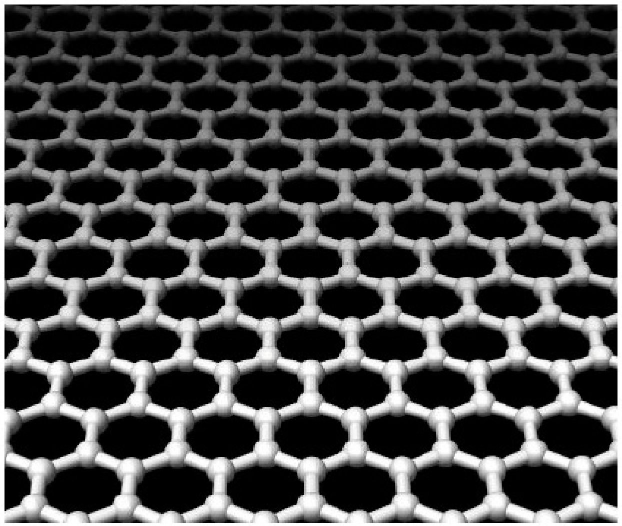


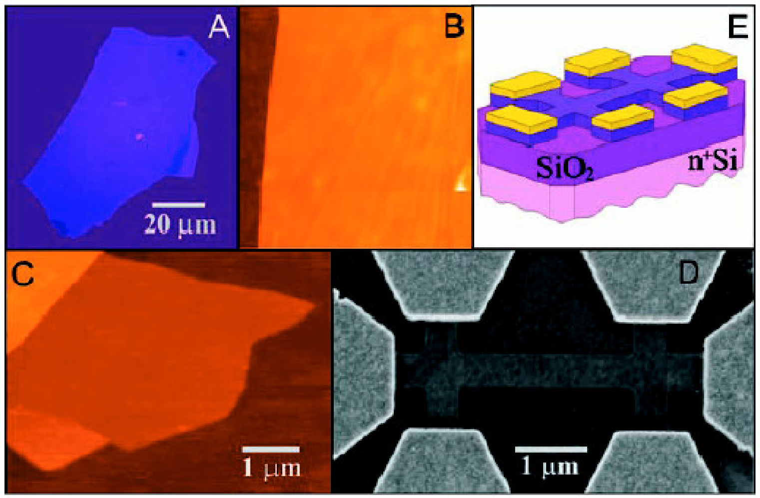
A 2D metal?

- Consider graphite:



- Single layers obtained from exfoliation:





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