Physics of Electronics:

4. Conduction in Metals

July – December 2008

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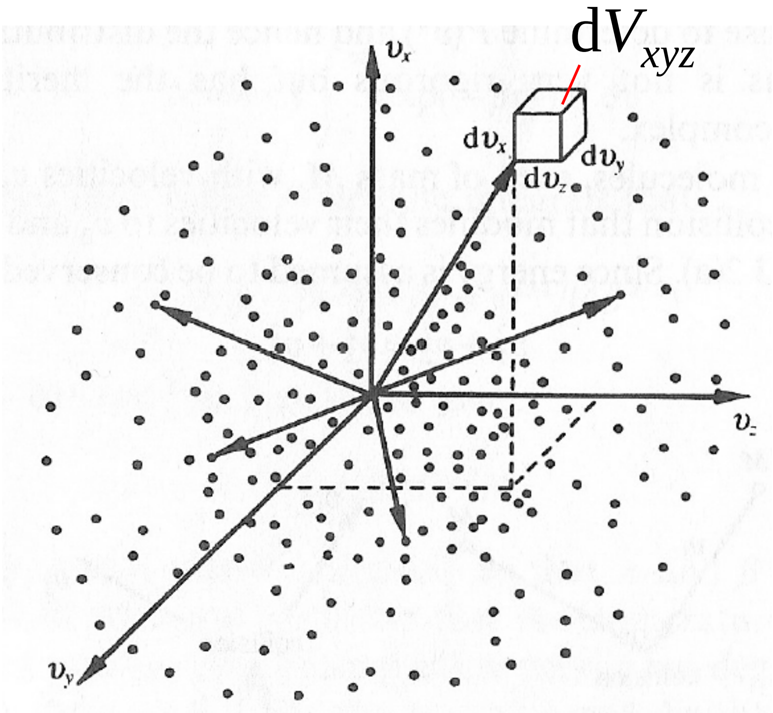
- Assemblies of classical particles.
- Collection of particles obeying the exclusion principle.
- A simple model of a conductor.
- Electrons in a 3D box.
- Maximum number of possible energy states.
- Energy distribution of electrons in a metal.
- Fermi level in a metal.
- Conduction processes in metals.

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 d*v* is

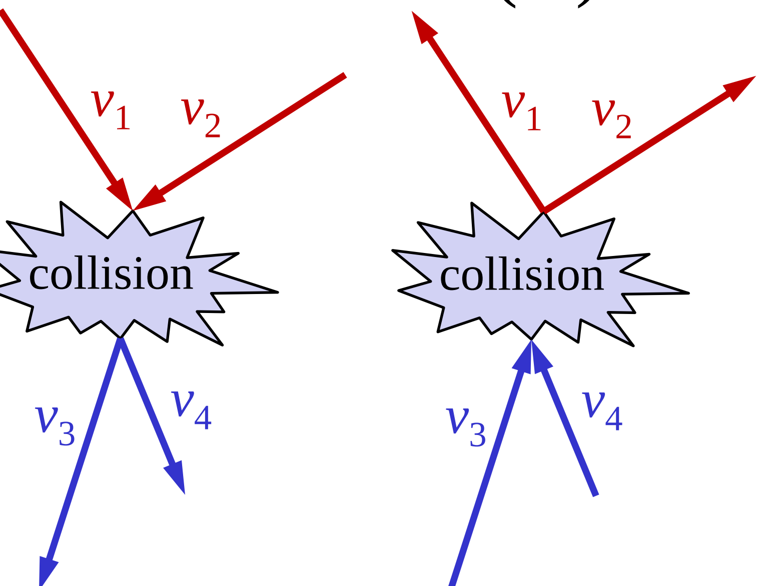
$$dN_v = P(v^2) 4\pi v^2\, dv$$

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



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: $N = 4\pi A \int_0^\infty \exp(-\beta v^2) v^2 \, dv$

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

$$\Rightarrow \quad \beta = M/(2kT), \qquad A = N\left(\frac{M}{2\pi k T}\right)^{3/2}$$

Maxwell-Boltzmann Distribution Function

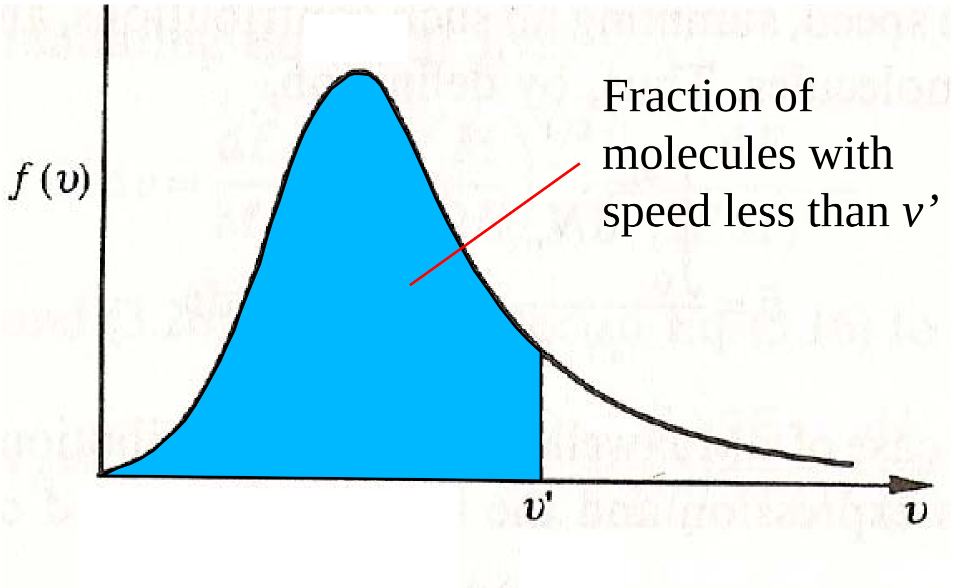
- Relation between $P(v^2)$ and $f(v)$:
  - Number of particles in a shell of thickness dv:

$$\mathrm{d}N_v = P(v^2) 4\pi v^2 \,\mathrm{d}v$$

$$\mathrm{d}N_v = N f(v)\,\mathrm{d}v$$

$$\Rightarrow \quad f(v) = 4\pi \left(\frac{M}{2\pi kT}\right)^{3/2} \exp\left(-\frac{Mv^2}{2kT}\right) v^2$$

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



Energy Distribution Function

- From speed to energy distribution:
  - Considering only kinetic energy:

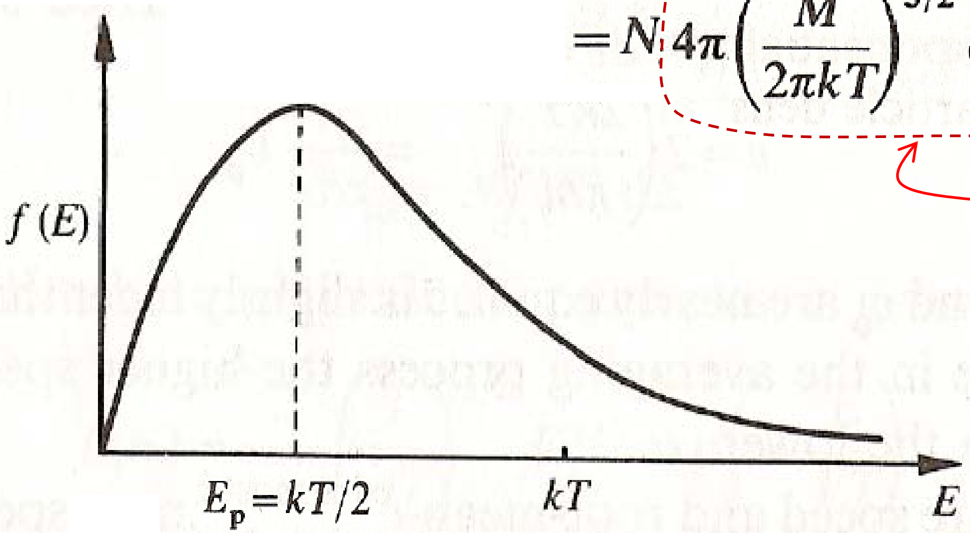
$$E = \frac{Mv^2}{2} \quad \Longrightarrow \quad \mathrm{d}v = \frac{\mathrm{d}E}{Mv} = \frac{\mathrm{d}E}{M}\left(\frac{M}{2E}\right)^{1/2} = \frac{\mathrm{d}E}{(2EM)^{1/2}}$$

  - Replacing on dN_v:

$$\mathrm{d}N_v = Nf(v)\,\mathrm{d}v = N\,4\pi\left(\frac{M}{2\pi kT}\right)^{3/2}\exp\left(-\frac{Mv^2}{\mathrm{d}v}\right)v^2$$

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

$f(E)$



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

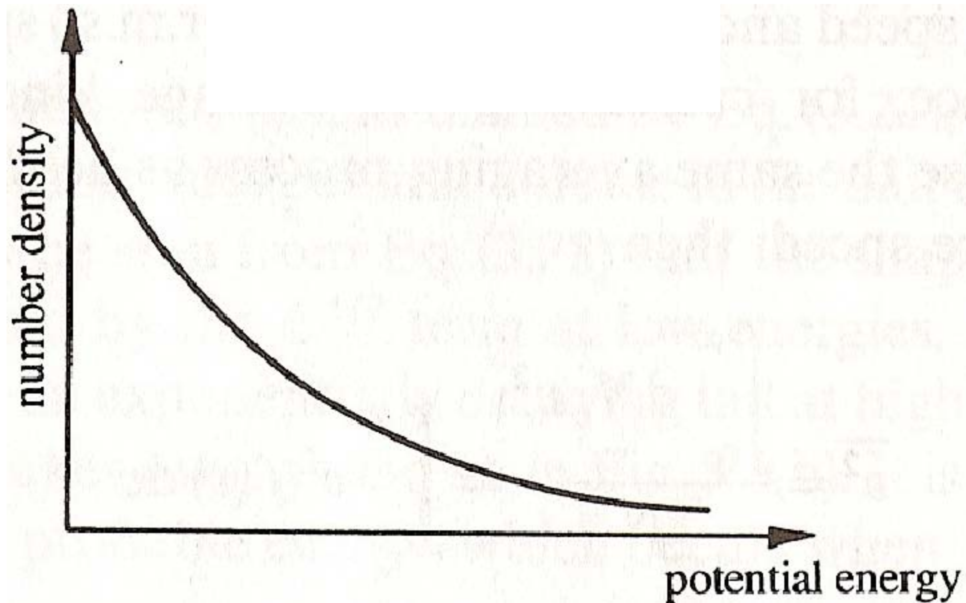
Boltzmann Distribution Function

- 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).

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

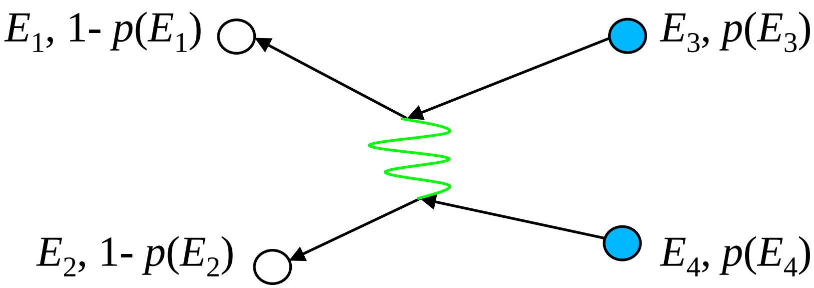
  - If the PE depends on the position so does the density of the ensemble:

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



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:



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

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

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

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

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

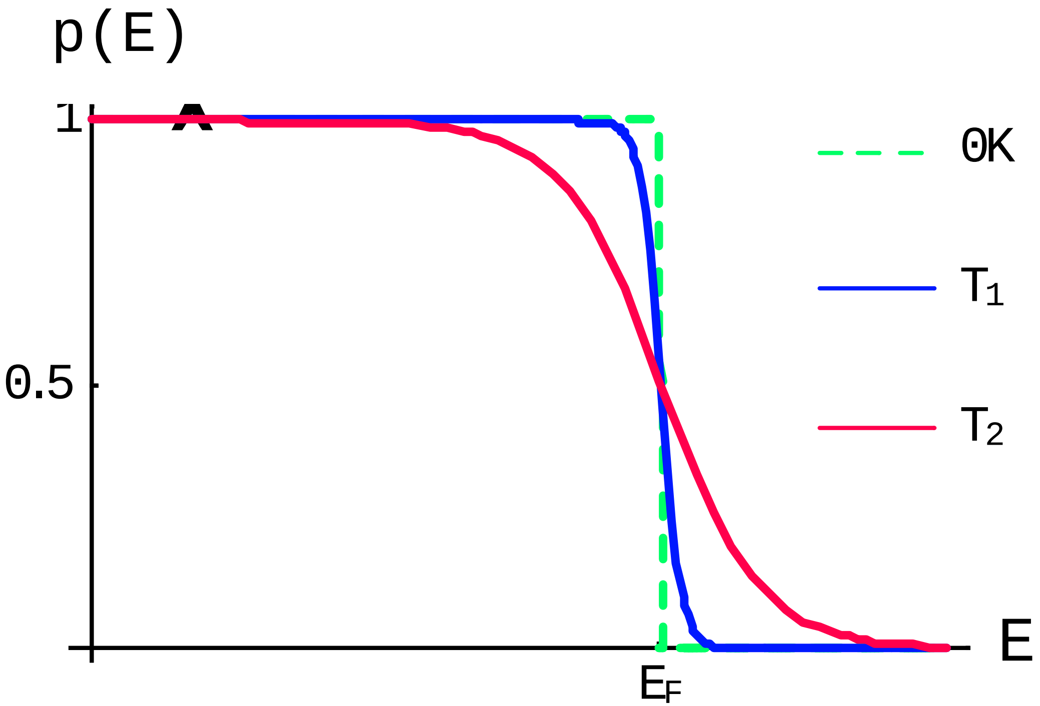
$$p(E)\simeq A\ \exp(-\beta E) \qquad \beta=1/kT$$

Fermi-Dirac Distribution

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

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

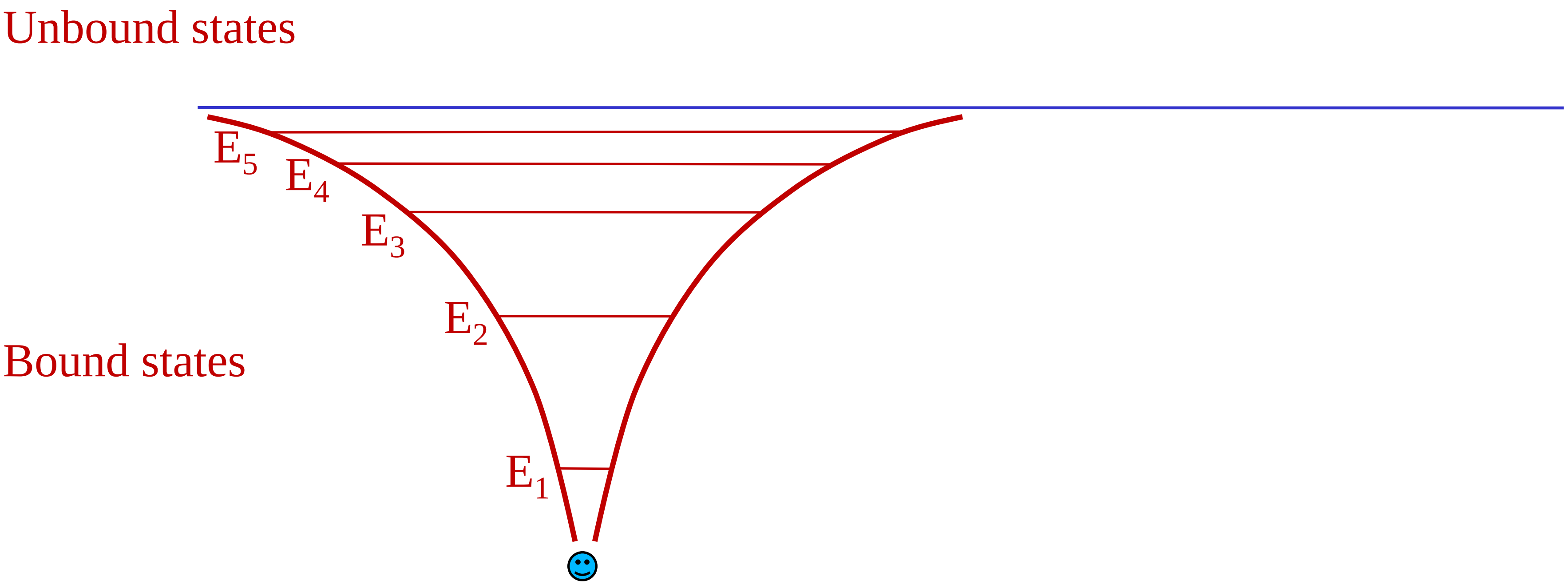
$$p(E) = \frac{1}{1 + \exp\left[(E - E_F)/kT\right]}$$



Note that for T = 0, $p(E)$ reduces to a step function. It means that all the states with energies $E \le E_F$ 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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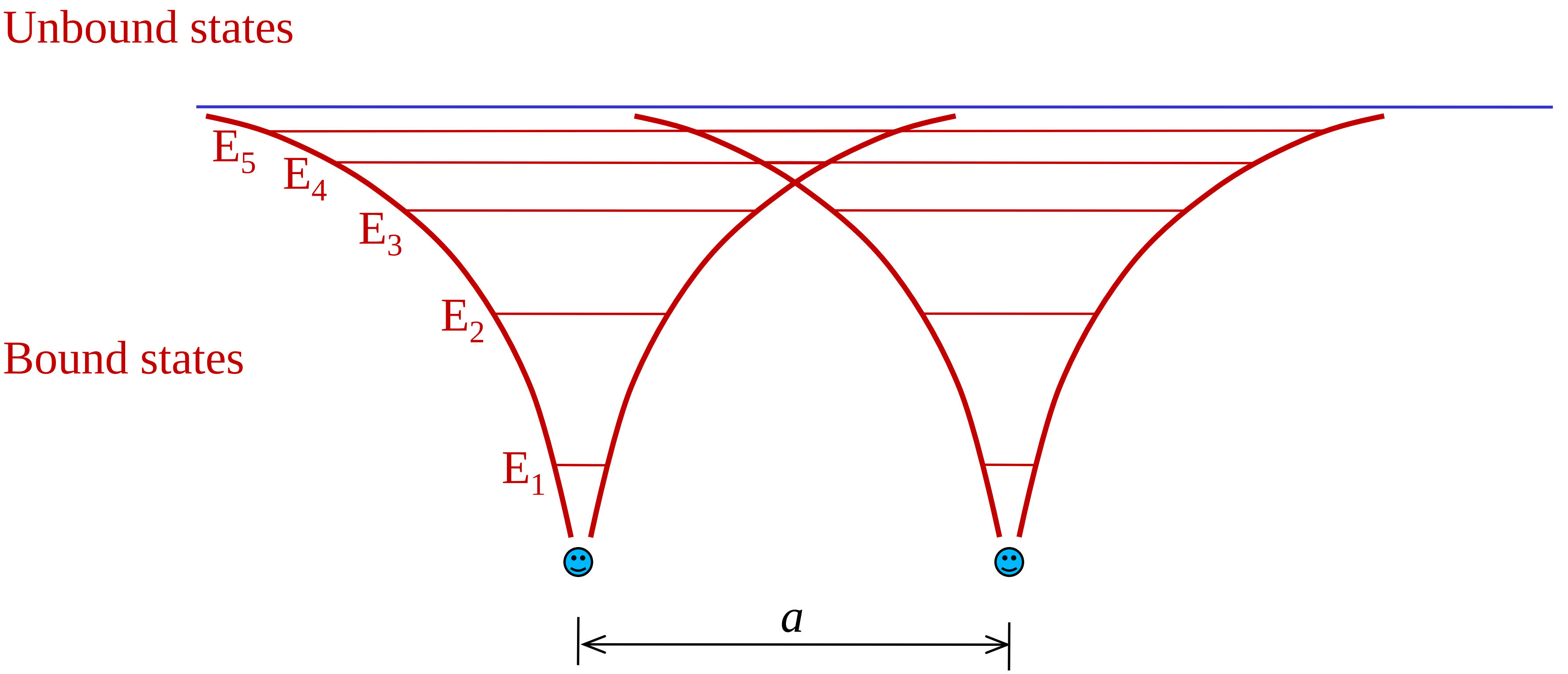

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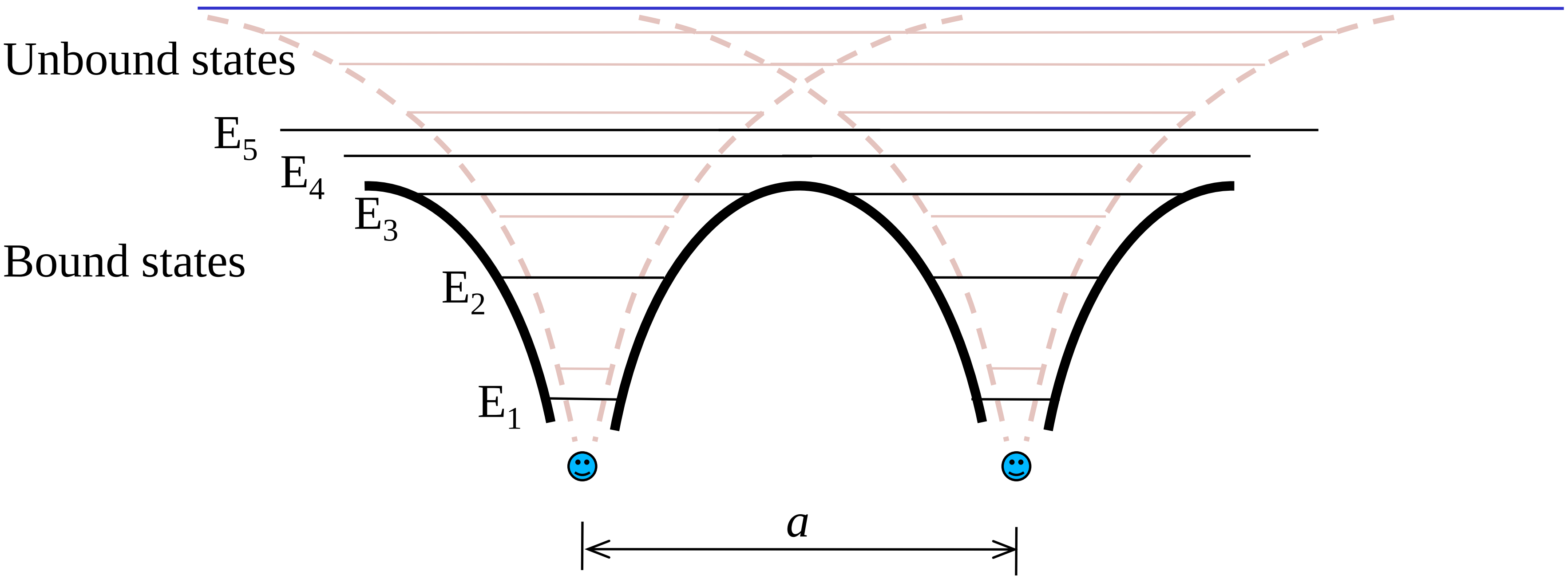

A Simple Model of a Conductor

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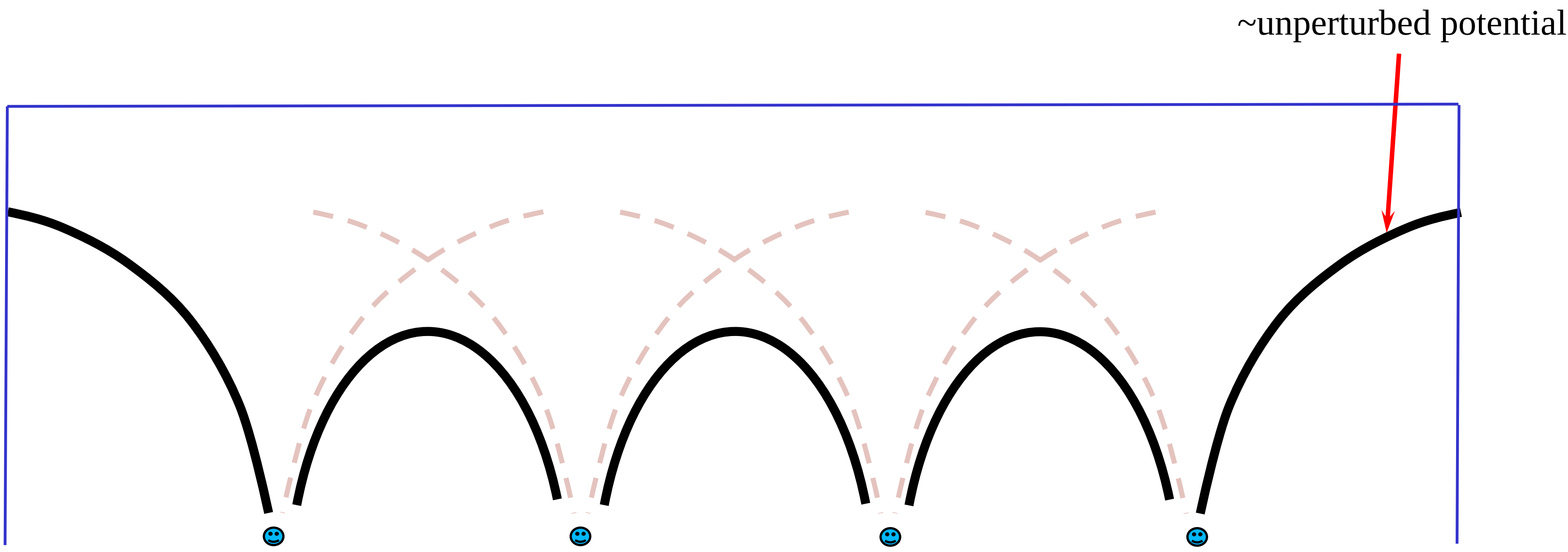
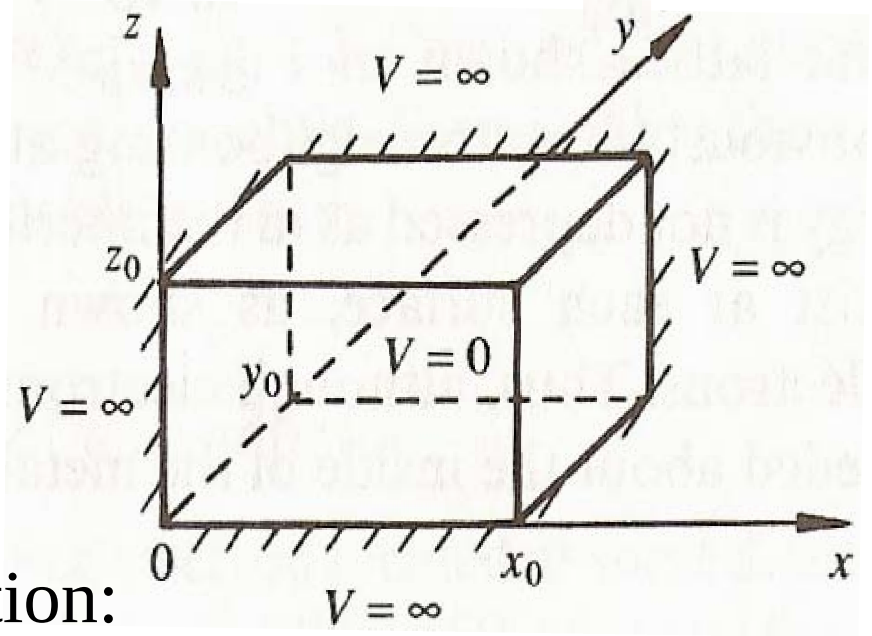


The potential barrier confines the electrons inside the faces of the conductor. Therefore we can model a conductor as unbound or free electrons confined to a potential box.

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*

Electrons in a 3D box

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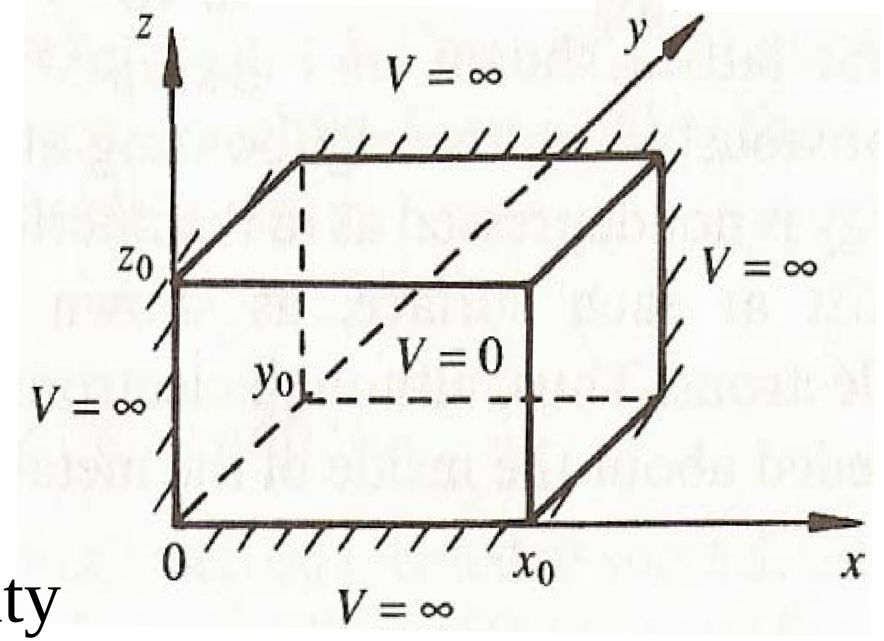
$$\nabla^2\Psi + \frac{2m}{\hbar^2}(E - V)\Psi = 0$$

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



  - Solving and using continuity ($\Psi = 0$ at the walls)

$$f_x = A\ \sin(n_x\pi x/x_0) \qquad f_y = B\ \sin(n_y\pi y/y_0)$$

$$f_z = C\ \sin(n_z\pi z/z_0)$$

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 we obtain the energy of every state

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

where

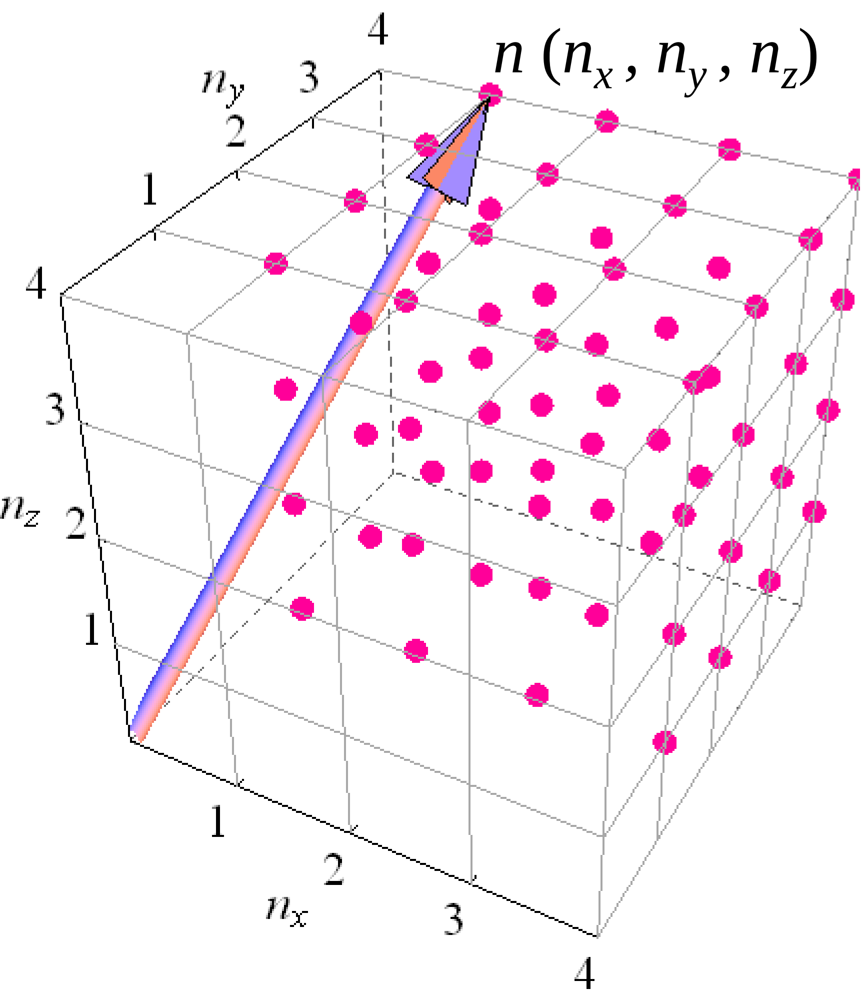
$$d = x_o = y_o = z_o$$

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

  – Note that results are similar to 1D well

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.

Space of States

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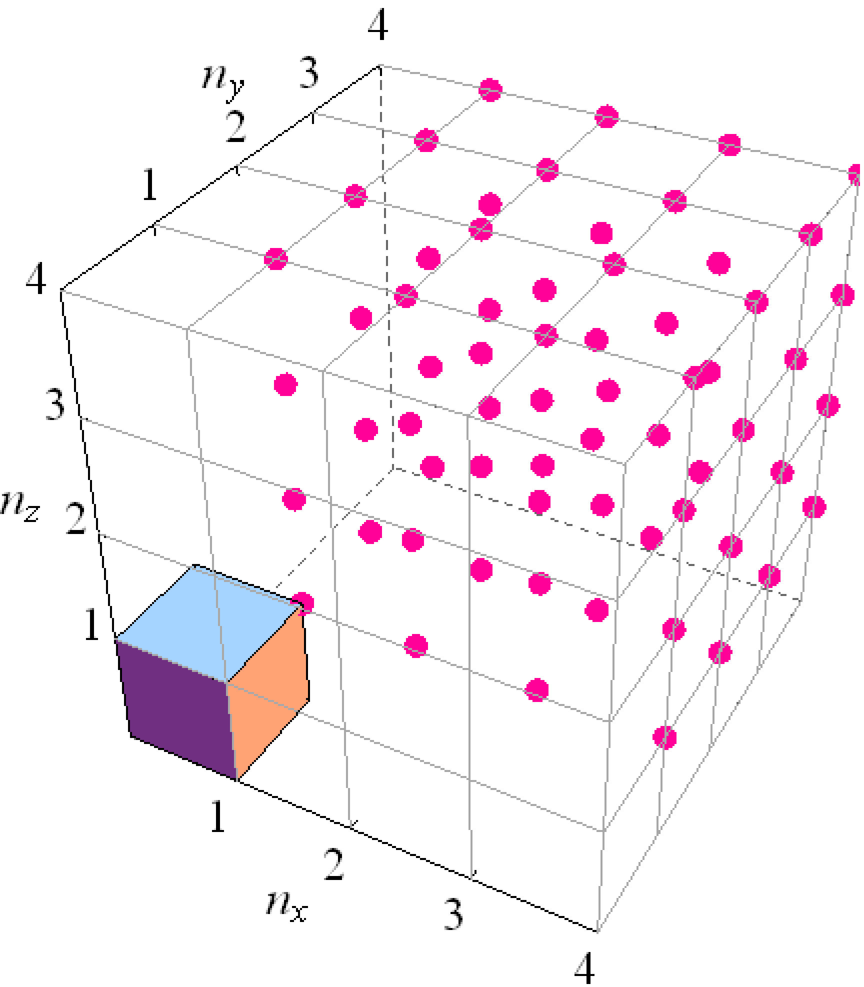
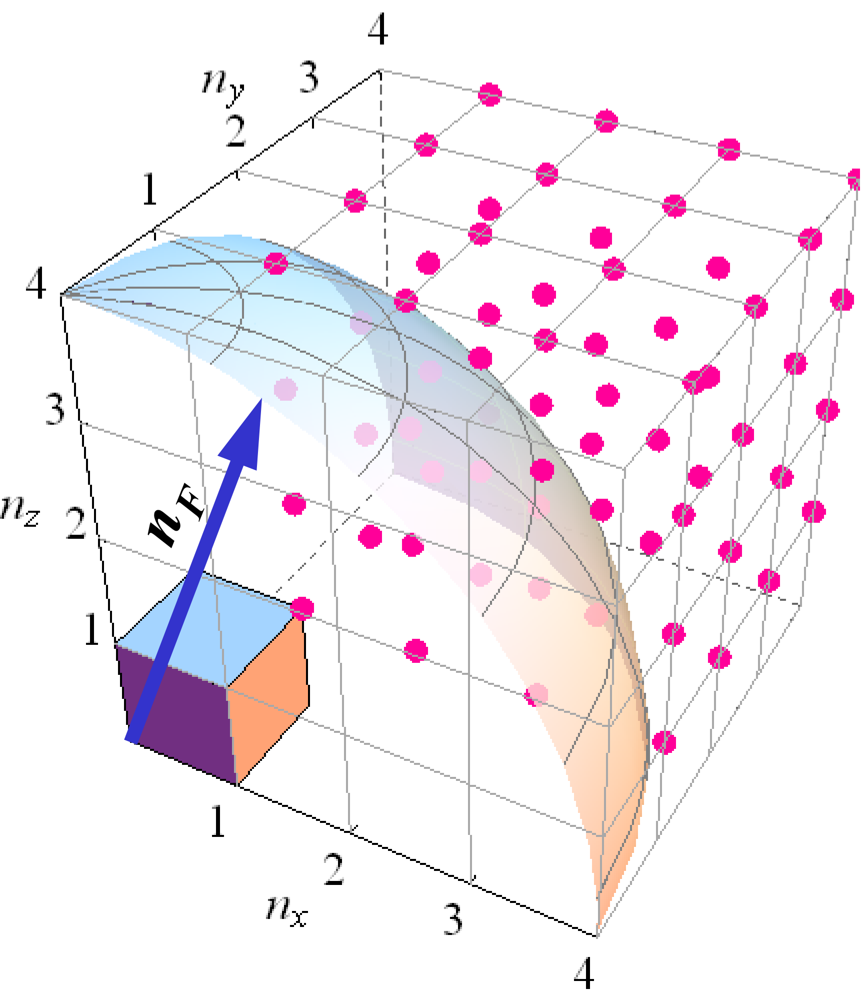


- In this representation, each point corresponds to one available state.
- To each unit of volume corresponds one available state.
- We will consider large number of points (continuum limit).

Maximum Number of States

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



- How many triplets (n_x, n_y, n_z) are there such that:

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

- The loccus of n_F is a sphere.

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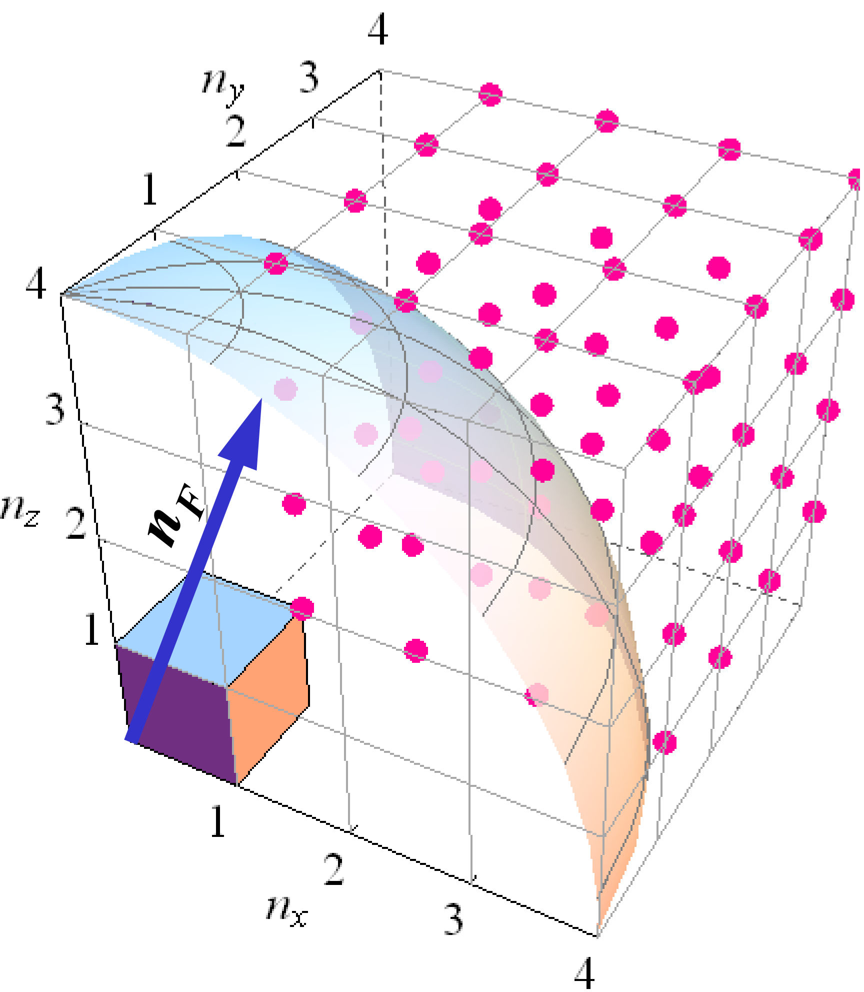

- How many triplets (n_x, n_y, n_z) are there such that:

  $n_F \geq n = (n_x^2 + n_y^2 + n_z^2)^{1/2}$?

- The loccus of n_F is a sphere.

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

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

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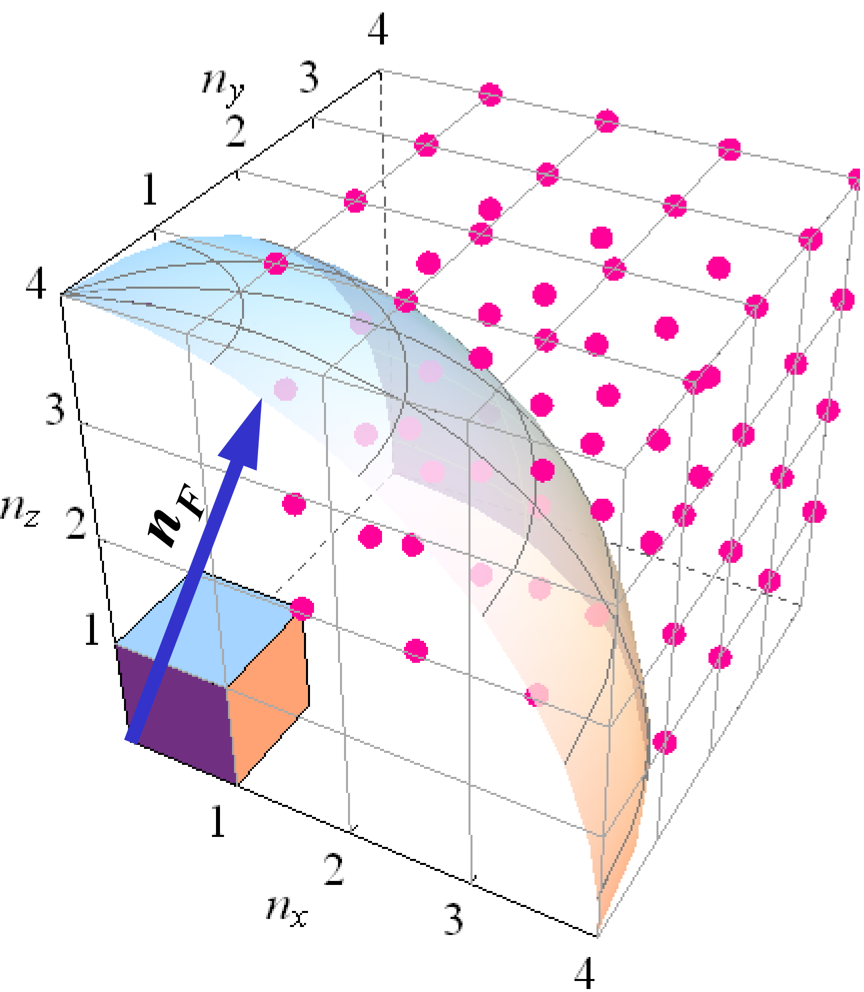
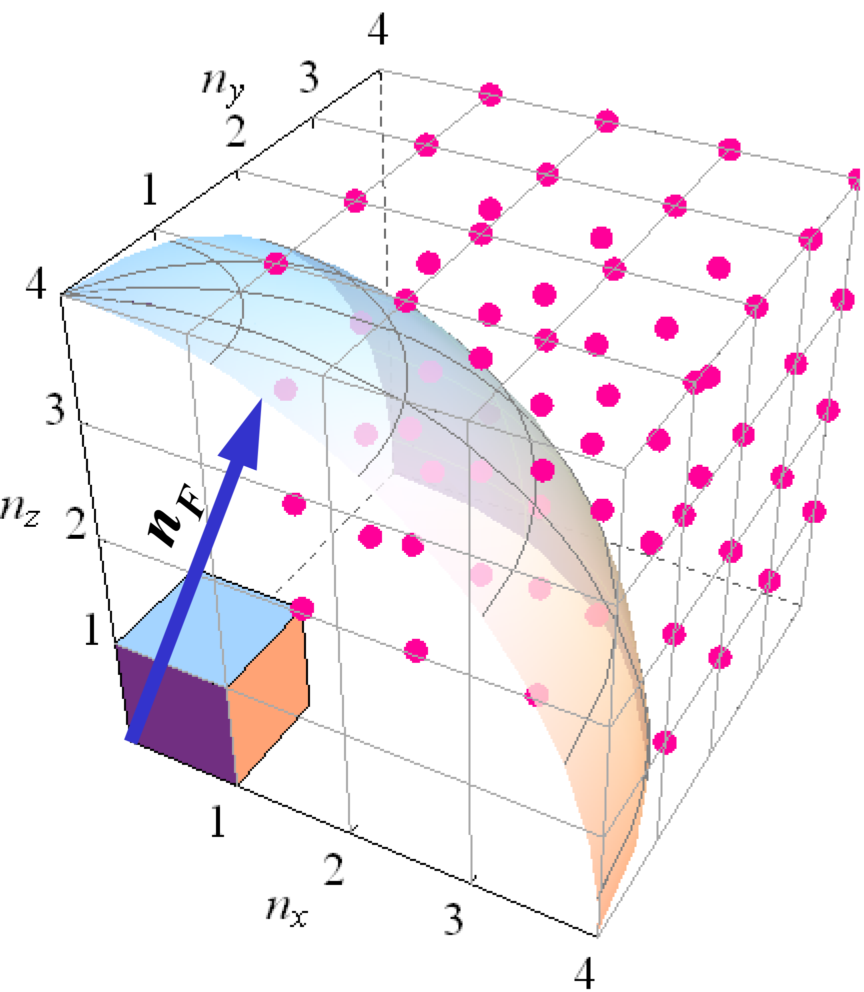


- How many triplets (n_x, n_y, n_z) are there such that:
  $n_F \geq n = (n_x^2 + n_y^2 + n_z^2)^{½}$?
- The loccus of n_F is a sphere.
- The number of states such that $n \leq n_F$ corresponds to the volume generated by n_F (spin) :

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

Maximum Number of States

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



- At 0 K we have:

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

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

- Therefore:

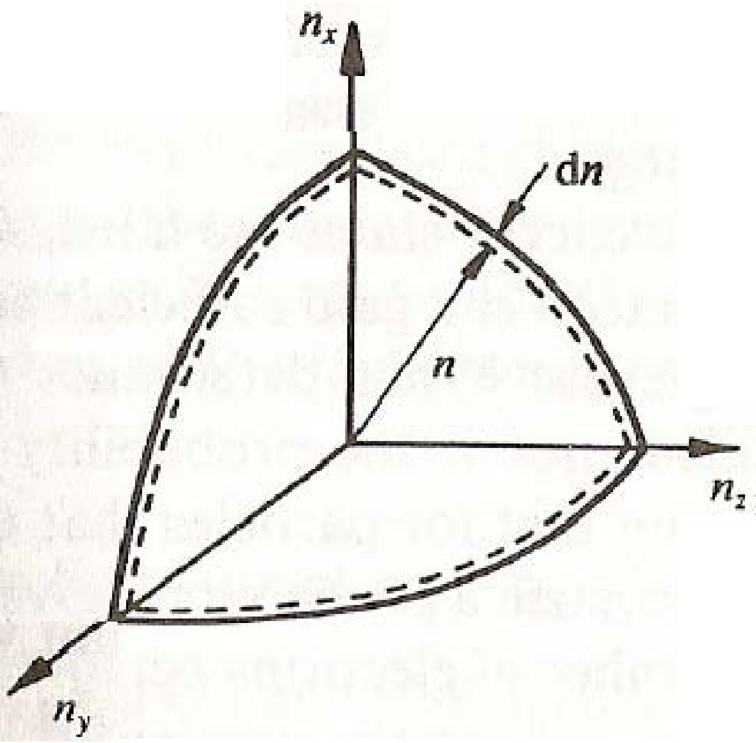
$$n_F = (3N/\pi)^{1/3} d$$

- The energy corresponding to 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 ?



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

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

Energy Distribution of e- in a Metal

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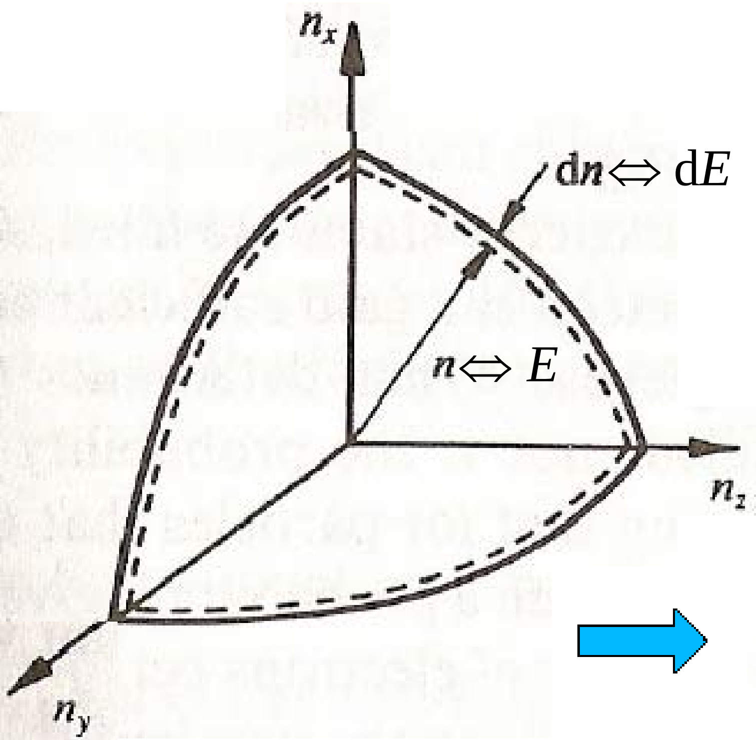


- Number of states in shell dn is equal to twice its volume:

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

- Density of (available) states, S(E): S(E)dE gives the number of states with energies in the range E and E+dE

$$S(E)\, dE\, d^3 = \pi n^2\, dn \;\Rightarrow\; S(E) = \frac{\pi n^2}{d^3}\frac{dn}{dE}$$

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

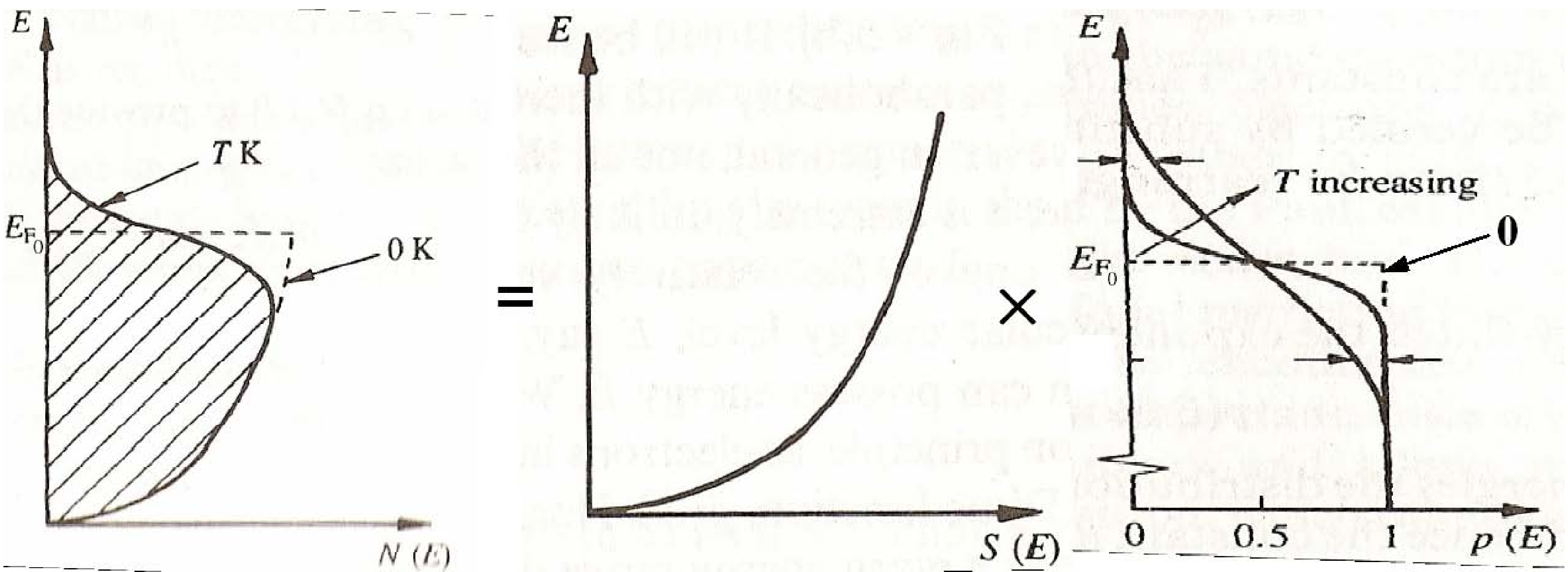
Energy Distribution of e- in a Metal

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

$N(E)dE$	=	$S(E)dE$	×	$p(E)$
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:

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

- At T = 0:

$$n=\frac{(8\sqrt{2})\pi m^{3/2}}{h^3}\int_0^{E_{\mathrm{F}0}} E^{1/2}\,\mathrm{d}E \quad\Rightarrow\quad E_{\mathrm{F}0}=\frac{h^2}{8m}\left(\frac{3n}{\pi}\right)^{2/3}=3.65\times10^{-19}\,n^{2/3}\ \mathrm{eV}$$

  - 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:

$$E_\mathrm{F}\approx E_{\mathrm{F}0}\left[1-\frac{\pi^2}{12}\left(\frac{kT}{E_{\mathrm{F}0}}\right)^2\right]$$

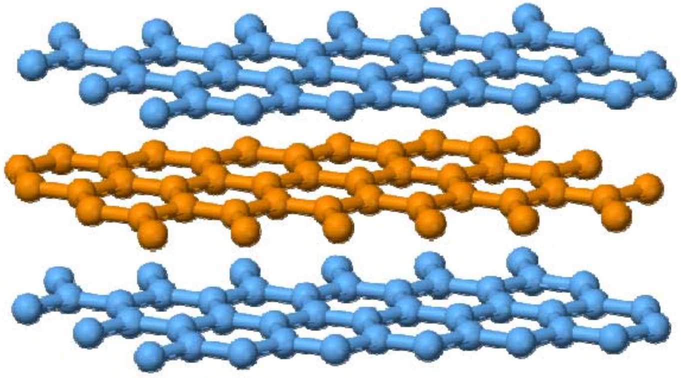
  - At usual temperatures kT ~ meV E_F depends slowly on T.

Conclusions

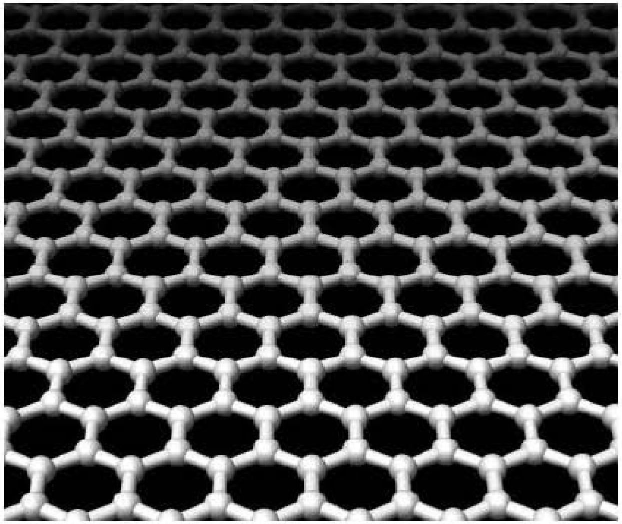
- We have introduced a simple model for electrons in a solid: free electron model.
- We simulated it using a 3D box potential.
- We have introduced the concept of Fermi energy: energy of the last occupied state.
- We have deduced the energy distribution of this electrons.

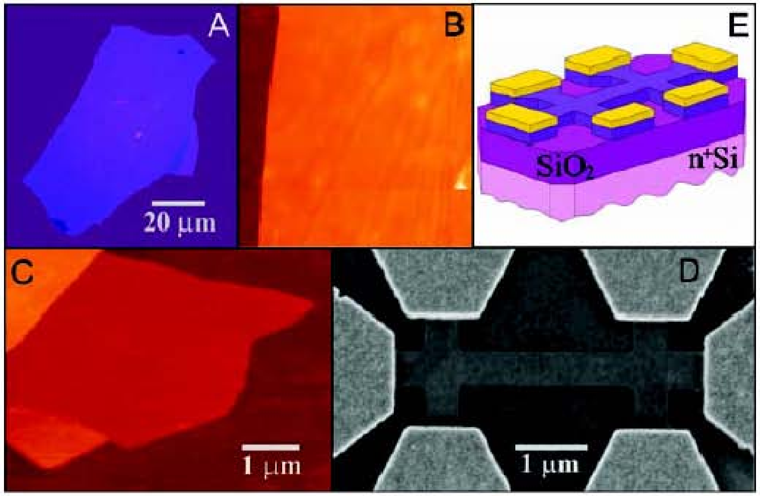
A 2D metal?

- Consider graphite:



- Single layers obtained from exfoliation:





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