Quantum mechanics of free electrons

- Important for quantized resistance calculation
- Important for single electron transistors
- Density of states
  - 3 dimensions
  - 2 dimensions
  - 1 dimensions
  - 0 dimensions
- Dimensionality (effective)
  - Set by size of nano-device compared to electron wavelength

Quantum mechanics of free particles

$$\left|\Psi(\vec{r},t)\right|^2$$

is probability of finding an electron at point r at time t.

Ψ is complex, and both real and imaginary parts are physical.

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For a free particle:

$$\Psi(\vec{r},t) \sim e^{i(\vec{k}\cdot\vec{r}-\omega t)}$$

Momentum:

$$\vec{p} = \hbar\vec{k}$$

Energy:

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

Schrodinger equation:

$$\boxed{i\hbar \frac{\partial}{\partial t}\Psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x,t)}$$

(1 dimension)

(Time dependent)

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A is a (complex) constant.

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$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\left(A\cdot e^{i(kx-\omega t)}\right) = \left(-\frac{\hbar^2}{2m}\right)(ik)^2\left(A\cdot e^{i(kx-\omega t)}\right)$$

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Schrodinger equation: (3 dimensions)

$$i\hbar\frac{\partial}{\partial t}\Psi(\vec{r},t) = -\frac{\hbar^2}{2m}\vec{\nabla}^2\Psi(\vec{r},t) = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\Psi(\vec{r},t)$$

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Let $\Psi(\vec{r},t) = A\cdot e^{i(\vec{k}\cdot\vec{r}-\omega t)} = A\cdot e^{i\left((k_x\cdot x+k_y\cdot y+k_z\cdot z)-\omega t\right)}$

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But:

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$$=\left(-\frac{\hbar^2}{2m}\right)\left((ik_x)^2+(ik_y)^2+(ik_z)^2\right)\left(A\cdot e^{i(\vec{k}\cdot\vec{r}-\omega t)}\right)=\left(\frac{\hbar^2(k_x{}^2+k_y{}^2+k_z{}^2)}{2m}\right)\Psi(\vec{r},t)$$

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$$= \frac{\hbar^2 k^2}{2m}\left(A\cdot e^{i(\vec{k}\cdot\vec{r}-\omega t)}\right) = \frac{p^2}{2m}\Psi(\vec{r},t)$$

Quantum mechanics of free particles:

$$\Psi(\vec{r},t) \sim e^{i(\vec{k}\cdot\vec{r}-\omega t)}$$

Generally,

$$\Psi(\vec{r},t) = \sum_n A_n e^{i(k_n x-\omega_n t)} \rightarrow \int dk A(k) e^{i(kx-\omega t)}$$

is also a possibility.

Time-independent Schrodinger equation

$$\Psi(\vec{r},t) = A \cdot e^{i(\vec{k}\cdot\vec{r}-\omega t)}$$

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Time-independent Schrodinger equation

$$\Psi(\vec{r},t) = A \cdot e^{i(\vec{k}\cdot\vec{r} - \omega t)}$$

$$= A \cdot e^{i\left((k_x \cdot x + k_y \cdot y + k_z \cdot z) - \omega t\right)} = \underbrace{A \cdot e^{i(k_x \cdot x + k_y \cdot y + k_z \cdot z)}}_{\text{Call this } \psi(\vec{r})} \cdot e^{-i\omega t}$$

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Call this $\psi(\vec{r})$

$$\Rightarrow \Psi(\vec{r},t) = \psi(\vec{r}) \cdot e^{-i\omega t}$$

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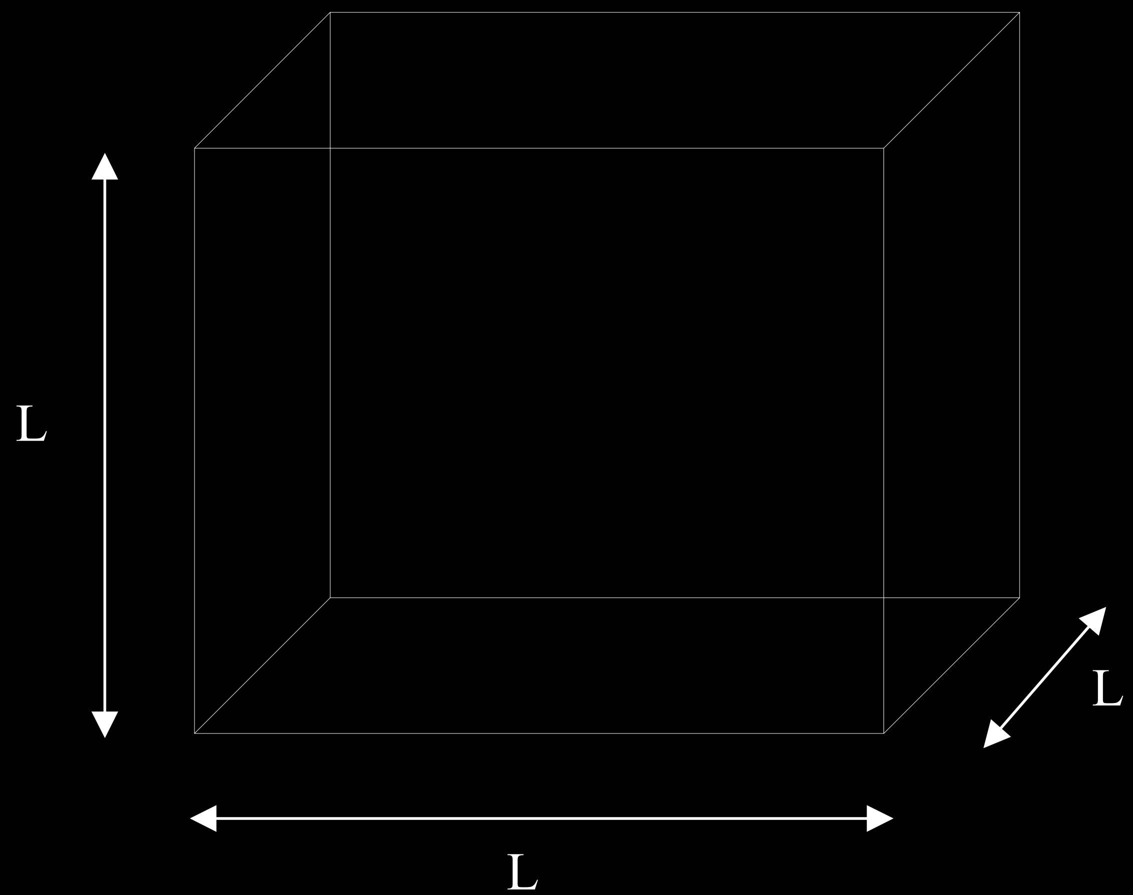
$$\boxed{\Rightarrow -\frac{\hbar^2}{2m}\vec{\nabla}^2\psi(\vec{r}) = E \cdot \psi(\vec{r})}$$

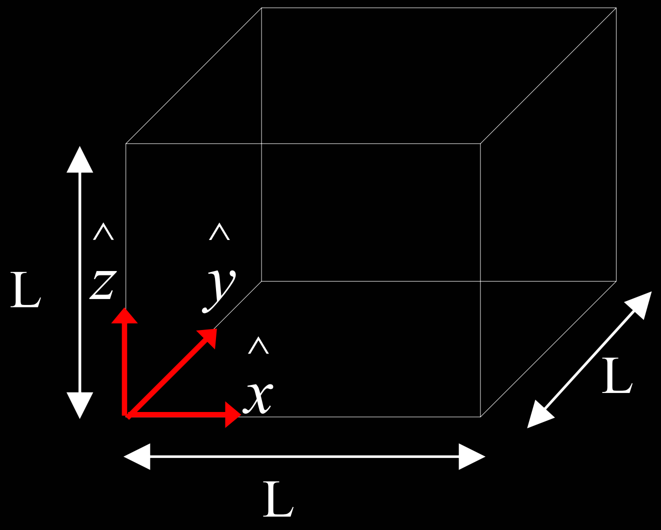
Confined particles: A box



Goal: find $\psi(\vec{r})$

Similar to electric field inside the box.

Goal: find $\psi(\vec{r})$



Everywhere outside the box

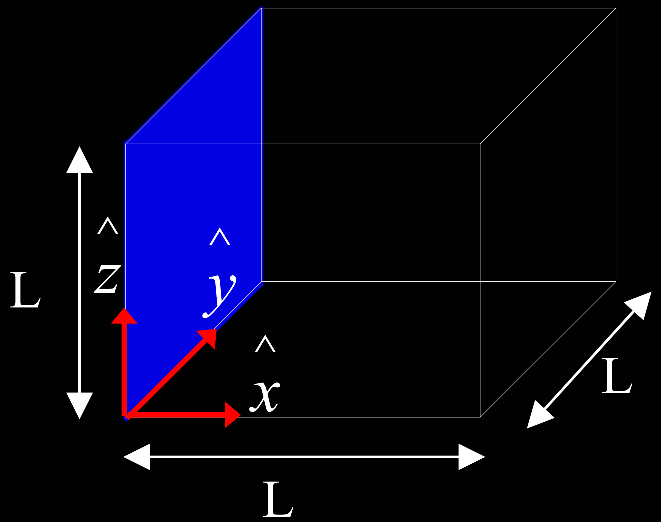
In particular,

$$\left|\psi(\vec{r})\right|^2 = 0$$

on the boundaries.

As before, we will consider all six surfaces:

Boundary conditions:



The plane x=0:

Try:

$$\psi(\vec{r}) = A \cdot e^{i(k_x \cdot x + k_y \cdot y + k_z \cdot z)}$$

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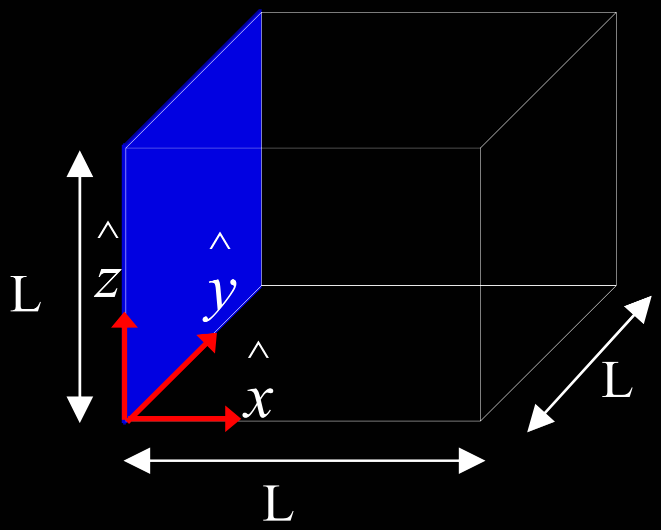

The plane x=0:

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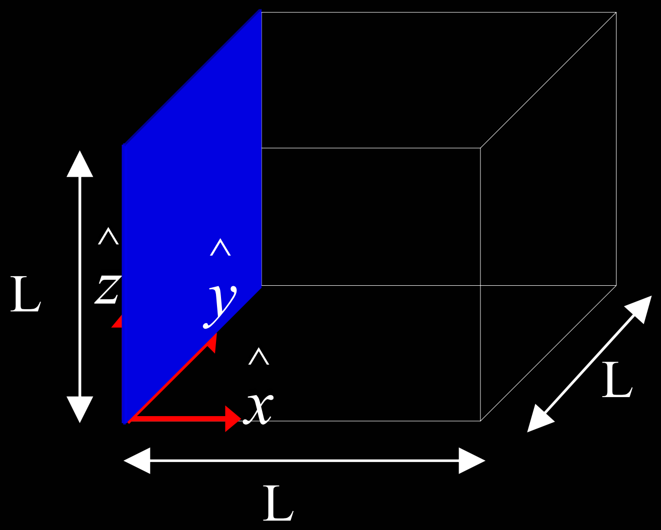
$$\psi(\vec{r}) = A \cdot e^{i(k_x \cdot x + k_y \cdot y + k_z \cdot z)}$$

$$\psi(x=0, y, z) = A \cdot e^{i(k_x \cdot \underbrace{x}_{0} + k_y \cdot y + k_z \cdot z)} = A \cdot e^{i(k_y \cdot y + k_z \cdot z)}$$

Does not solve boundary condition!!!

Boundary conditions:

The plane x=0:



Let's try something:

$$\psi(\vec{r}) = A \cdot e^{i(k_x \cdot x + k_y \cdot y + k_z \cdot z)}$$

$$-A \cdot e^{i(-k_x \cdot x + k_y \cdot y + k_z \cdot z)}$$

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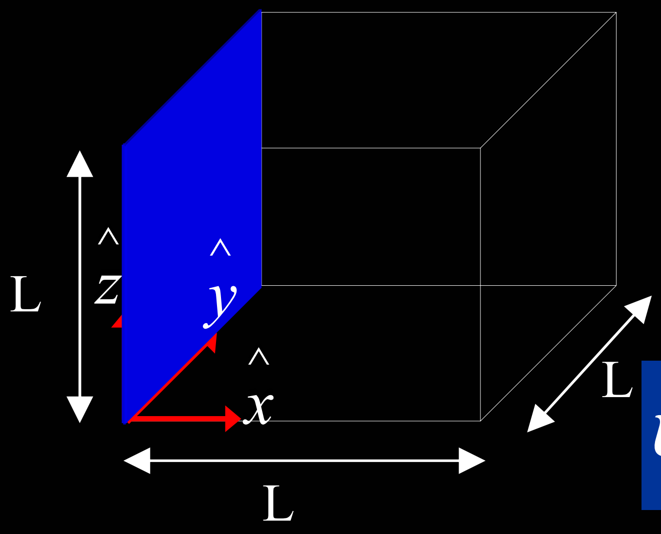

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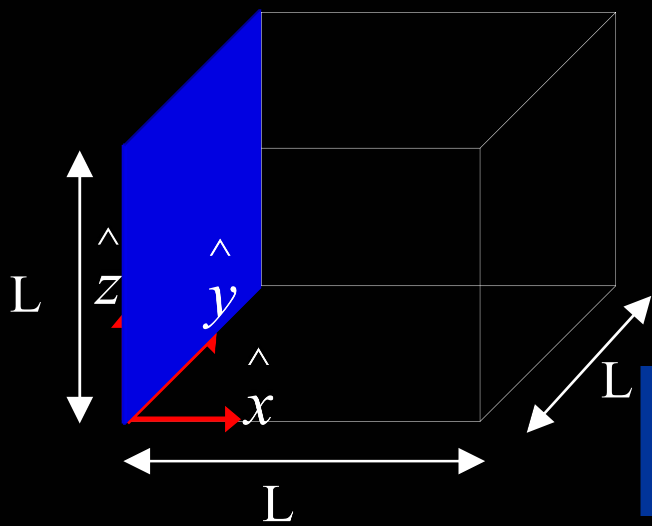
$$\psi(\vec{r}) = A \cdot \left(e^{ik_x \cdot x} - e^{-ik_x \cdot x} \right) \cdot e^{i(k_y \cdot y + k_z \cdot z)}$$

$$\boxed{e^{a \cdot b} = e^a \cdot e^b}$$

Boundary conditions:

The plane x=0:



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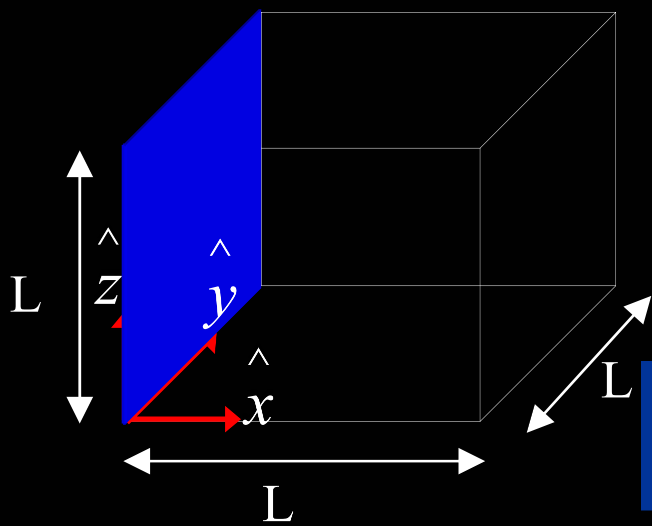

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$$= A\cdot\left(e^0 - e^0\right)\cdot e^{i(k_y\cdot y + k_z\cdot z)} = 0$$

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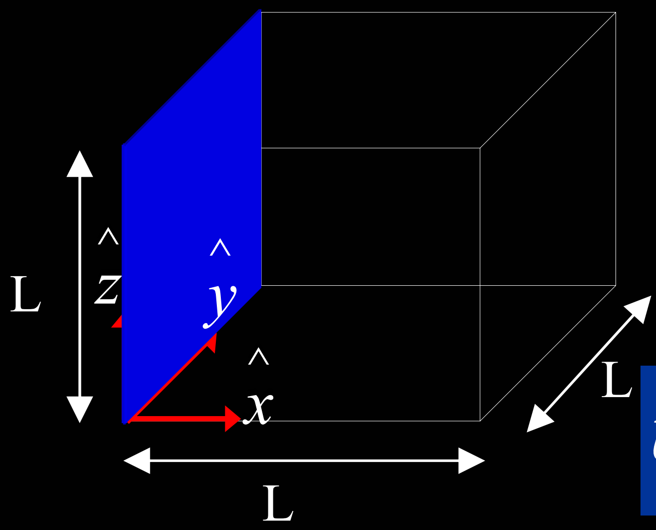
The plane x=0:



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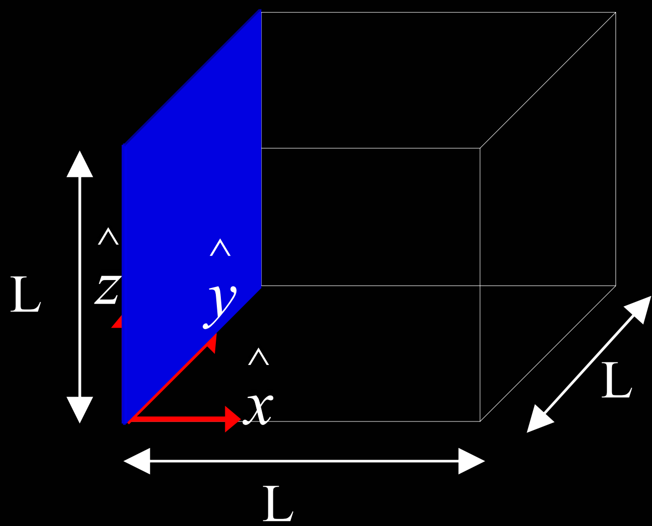
Does solve boundary condition!!!

Boundary conditions: The plane x=L:



$$\psi(\vec{r}) = A\cdot\left(e^{ik_x\cdot x} - e^{-ik_x\cdot x}\right)\cdot e^{i(k_y\cdot y + k_z\cdot z)}$$

$$= 2iA\cdot\sin(k_x x)\cdot e^{i(k_y\cdot y + k_z\cdot z)}$$

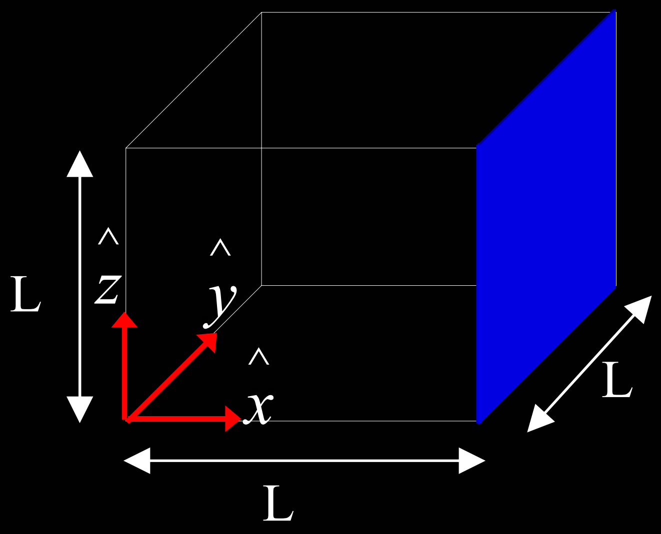
$$\boxed{\sin(\theta) = \frac{1}{2i}\left(e^{i\theta} - e^{-i\theta}\right)}$$

$$\psi(x = L, y, z) = 2iA\cdot\sin(k_x L)\cdot e^{i(k_y\cdot y + k_z\cdot z)} = 0\,?$$

If and only if:

$$\boxed{k_n = n\pi / L}$$

Boundary conditions: The plane x=L:



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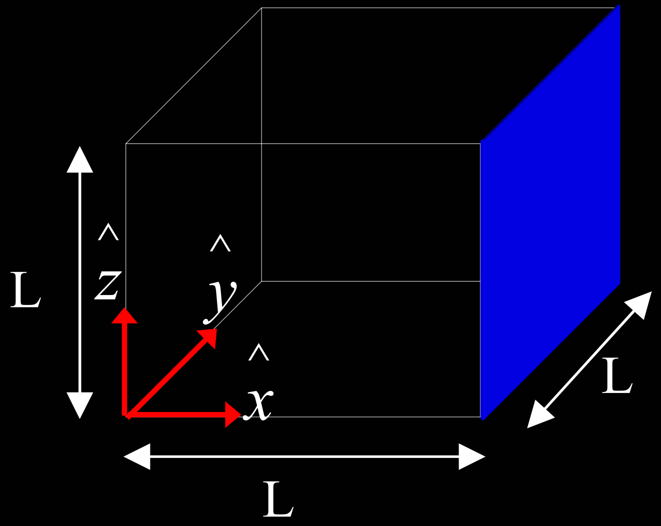

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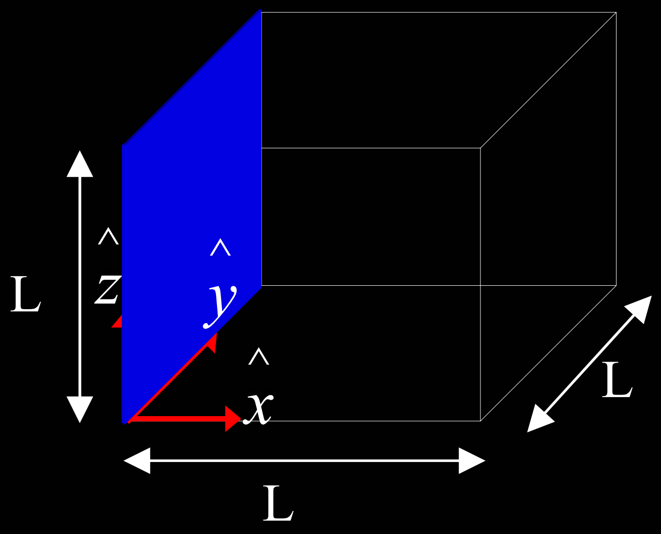
Boundary conditions:

The plane x=L:



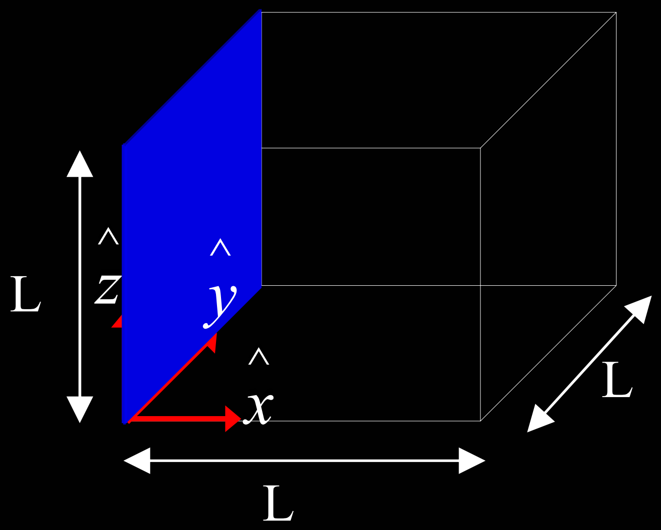
$$\psi(\vec{r}) = A\cdot\left(e^{ik_x\cdot x} - e^{-ik_x\cdot x}\right)\cdot e^{i(k_y\cdot y + k_z\cdot z)}$$

$$= 2iA\cdot\sin(k_x x)\cdot e^{i(k_y\cdot y + k_z\cdot z)}$$

$$\boxed{\sin(\theta) = \frac{1}{2i}\left(e^{i\theta} - e^{-i\theta}\right)}$$

$$\psi(x = L, y, z) = 2iA\cdot\sin(k_x L)\cdot e^{i(k_y\cdot y + k_z\cdot z)} = 0\,?$$

Boundary conditions: The plane x=L:



$$\psi(\vec{r}) = A\cdot\left(e^{ik_x\cdot x} - e^{-ik_x\cdot x}\right)\cdot e^{i(k_y\cdot y + k_z\cdot z)}$$

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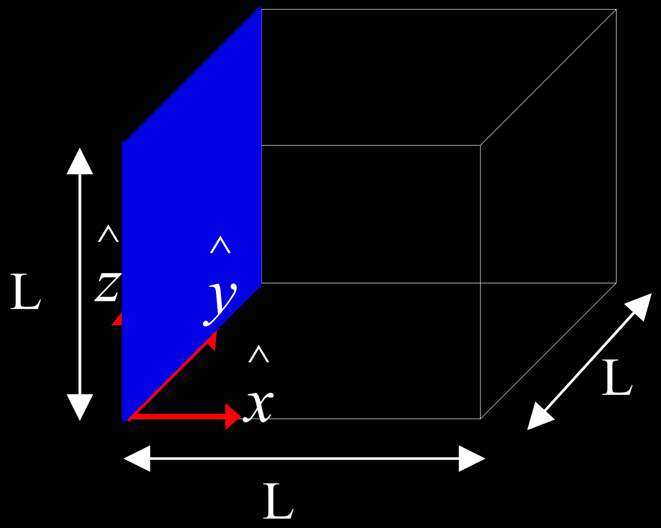
If and only if:

$$\boxed{k_n = n\pi / L}$$

Boundary conditions:



We can do the same for y, z:

$$\psi(\vec{r}) = (2i)^3 A \cdot \sin(k_{n_x} x) \cdot \sin(k_{n_y} y) \cdot \sin(k_{n_z} z)$$

$$k_{n_x} = n_x \pi / L$$

$$k_{n_y} = n_y \pi / L$$

$$k_{n_z} = n_z \pi / L$$

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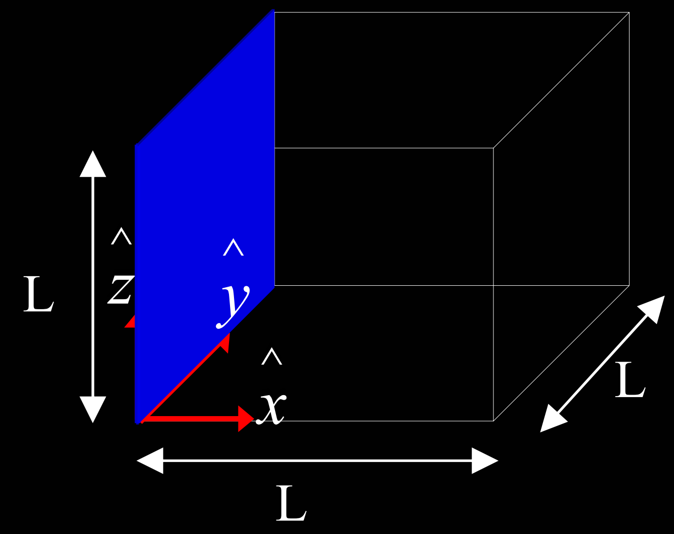

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$$k_{n_x} = n_x \pi / L$$

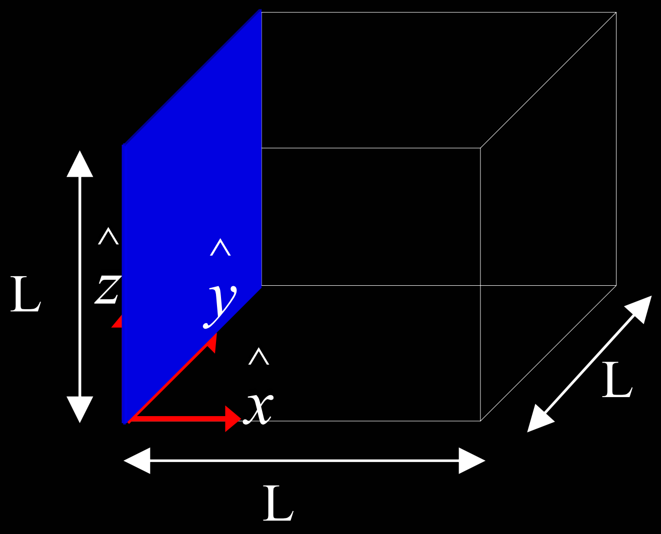
$$k_{n_y} = n_y \pi / L$$

$$k_{n_z} = n_z \pi / L$$

$$E = \frac{\hbar^2 (k_{n_x}{}^2 + k_{n_y}{}^2 + k_{n_z}{}^2)}{2m} = \frac{\hbar^2 (\pi / L)^2}{2m} (n_x{}^2 + n_y{}^2 + n_z{}^2)$$

These are the allowed energy levels, or "quantum states"

Many electrons:

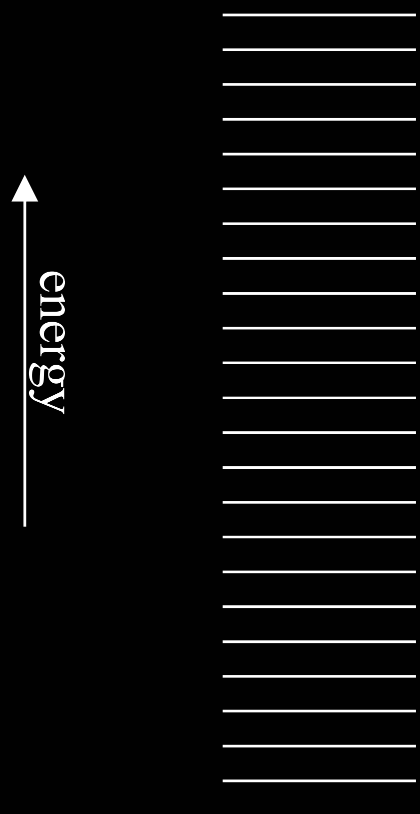


$$E = \frac{\hbar^2 (\pi / L)^2}{2m} (n_x{}^2 + n_y{}^2 + n_z{}^2)$$

These are the allowed energy levels, or "quantum states"

Pauli exclusion principle: Each unique combination of n_x, n_y, n_z can only have two electrons (spin up, spin down).

Energy spectrum of free particles:



Etc.

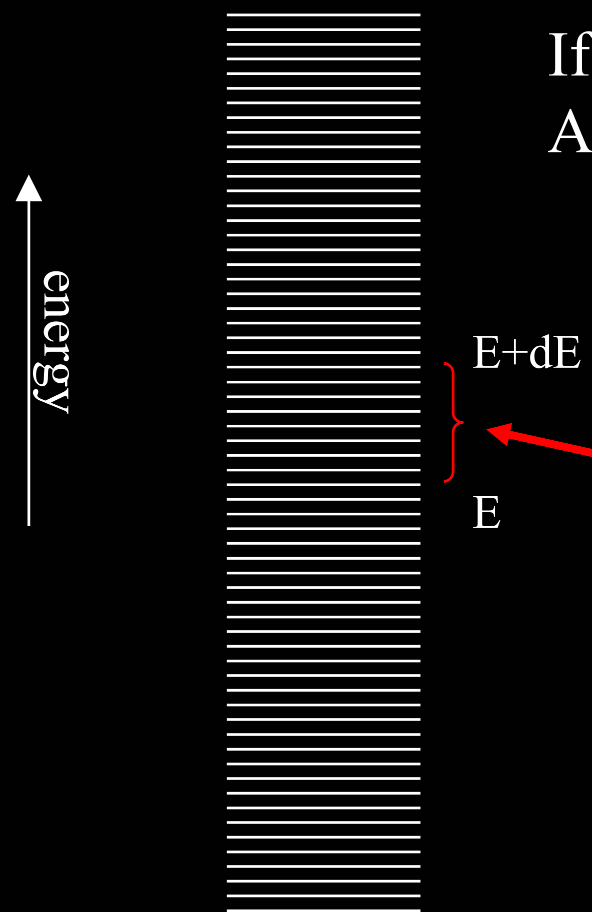
$n_x=2, n_y=1, n_z=1$

$n_x=1, n_y=2, n_z=1$

$n_x=1, n_y=1, n_z=2$

$n_x=1, n_y=1, n_z=1$

Density of states:



If L is large, states are very close together.
Approximate as a continuum.

How many states?

Number of states with energy between E and E + dE

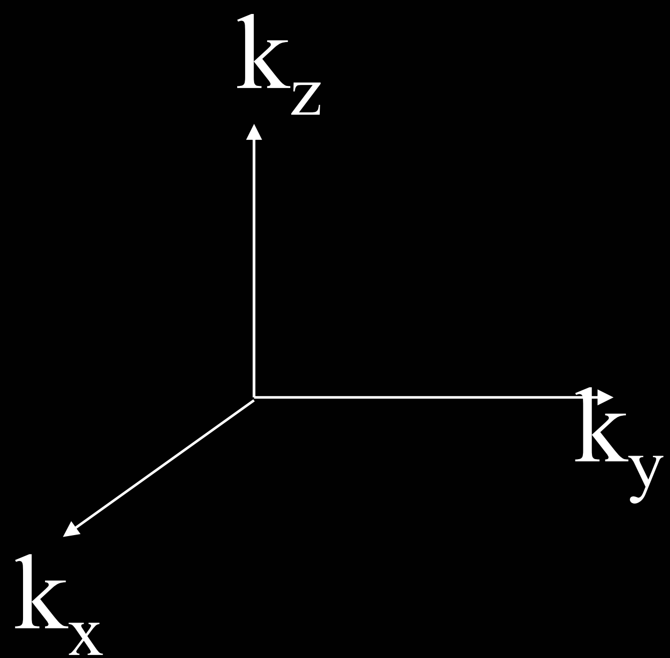
Number of states with energy between E and E + dE *per volume.*

Density of states:

Easier first to think of in k-space:

Density of states in k-space is uniform:

One state per $(\pi/L)^3$:



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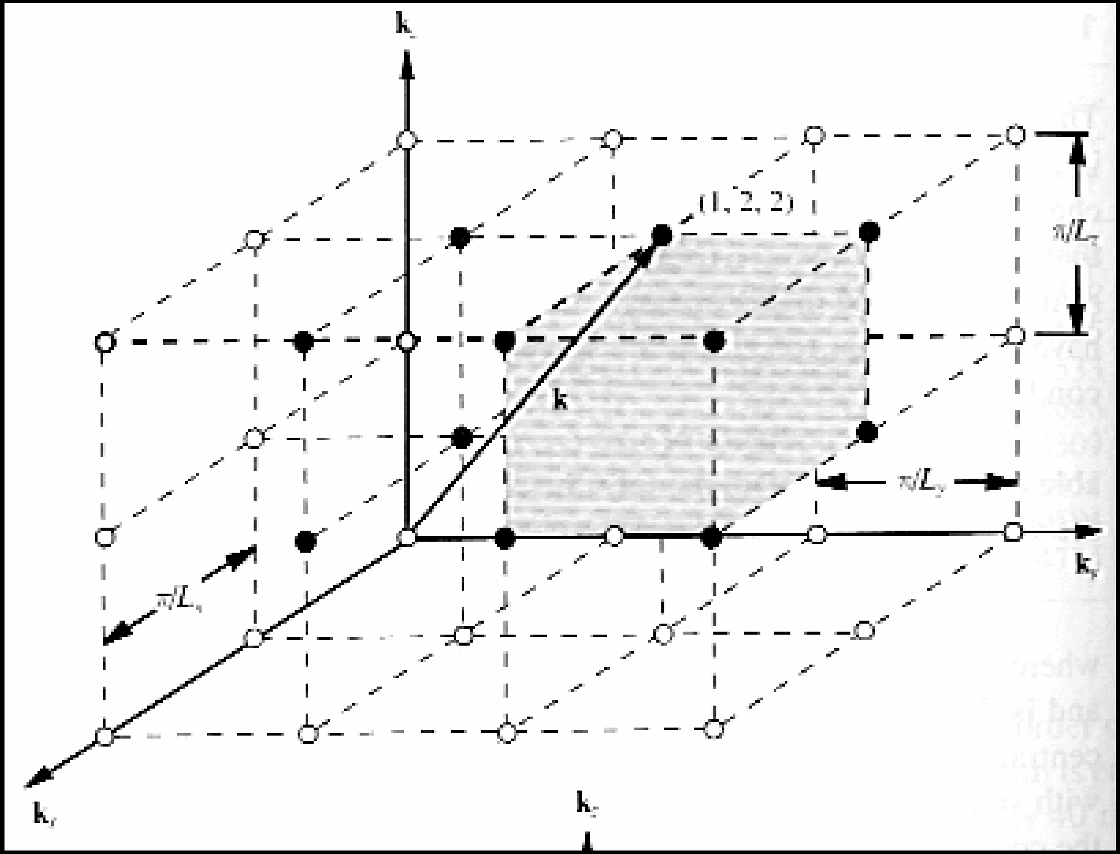
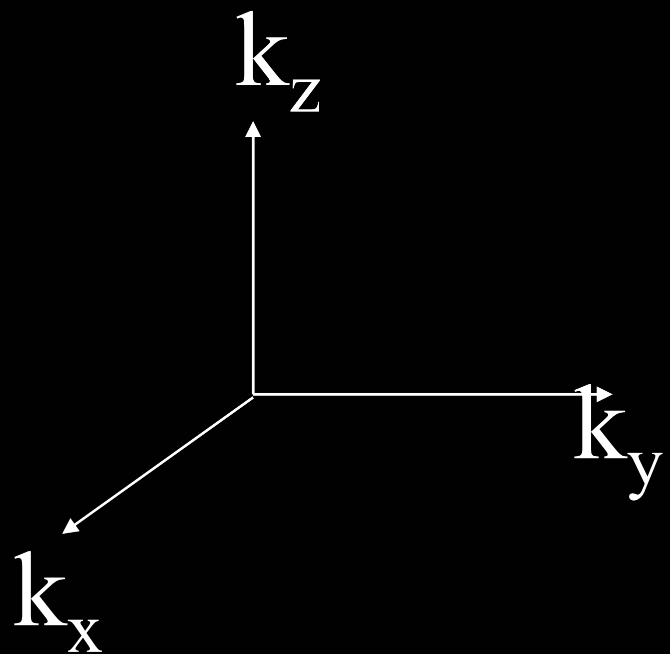
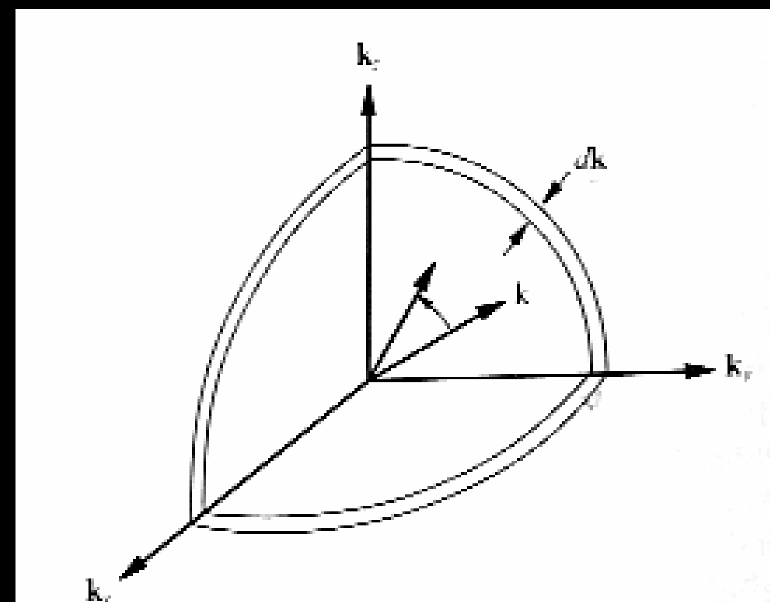


From Verdeyen

Density of states: Number of states between k, k+dk:





Verdeyen

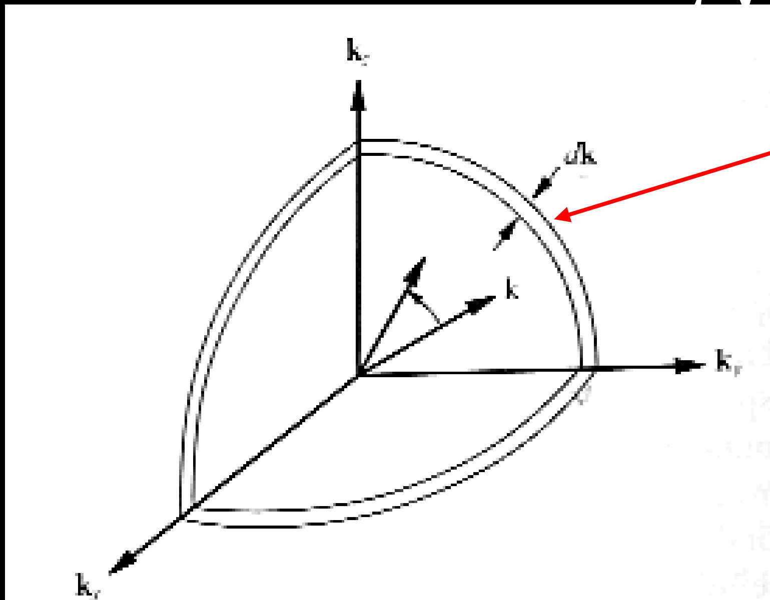
$$k_{n_x} = n_x \pi / L$$

$$k_{n_y} = n_y \pi / L$$

$$k_{n_z} = n_z \pi / L$$

$$k \equiv \sqrt{k_x^2 + k_y^2 + k_z^2}$$

$N_k dk = ?$



Volume of spherical shell
$=4\pi k^2 dk/8$
8 is for upper right quadrant

Number of states in volume=
Volume x States/volume

States/volume = 1 / $(\pi/L)^3$:

$$N_k dk = \left(4\pi k^2 dk/8\right)\cdot\left(\frac{1}{(\pi/L)^3}\right)\cdot 2 = L^3\frac{k^2 dk}{\pi^2}$$

$$\boxed{\rho_k dk \equiv \frac{N_k dk}{\text{volume}} = \frac{k^2 dk}{\pi^2}}$$

HW you will do calculation for 2 dimensional world.

$$\rho(E)dE = ?$$

$$\rho(E)dE = ?$$

We use:

$$\boxed{\rho_k dk = \rho(E)dE}$$

$$\rho(E)dE = ?$$

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$$\boxed{\rho_k dk = \frac{k^2 dk}{\pi^2}}$$

$$\rho(E)dE = ?$$

We use:

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$$\boxed{\rho_k dk = \frac{k^2 dk}{\pi^2}}$$

$$\boxed{E = \frac{\hbar^2 k^2}{2m} \Rightarrow k = \sqrt{\frac{2mE}{\hbar^2}} \Rightarrow dk = \sqrt{\frac{2m}{\hbar^2}}\frac{dE}{2\sqrt{E}}}$$

$$\rho(E)dE = ?$$

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$$E = \frac{\hbar^2 k^2}{2m} \Rightarrow k = \sqrt{\frac{2mE}{\hbar^2}} \Rightarrow dk = \sqrt{\frac{2m}{\hbar^2}} \frac{dE}{2\sqrt{E}}$$

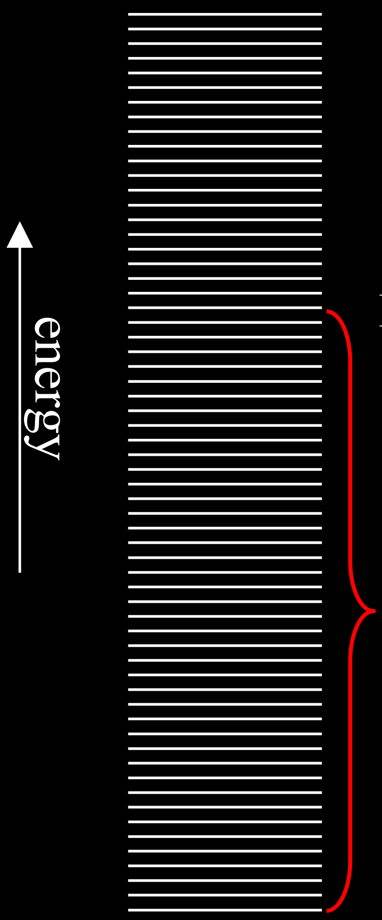
$$\boxed{\rho(E)dE = \frac{2^{3/2} m^{3/2}}{\pi^2 \hbar^{3/2}} \cdot E^{1/2} dE}$$

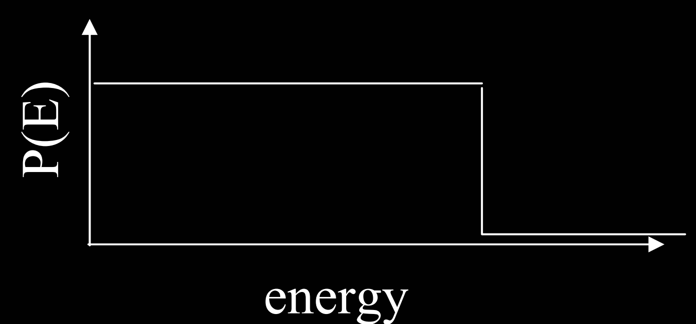
Fermi gas:

At zero temperature, as we add electrons to the box, we gradually fill up all the states. (DISCUSS PAULI EXCLUSION PRINCIPLE -IMPORTANT!)

When we are done filling the box, the energy of the last electron is called the "Fermi energy."

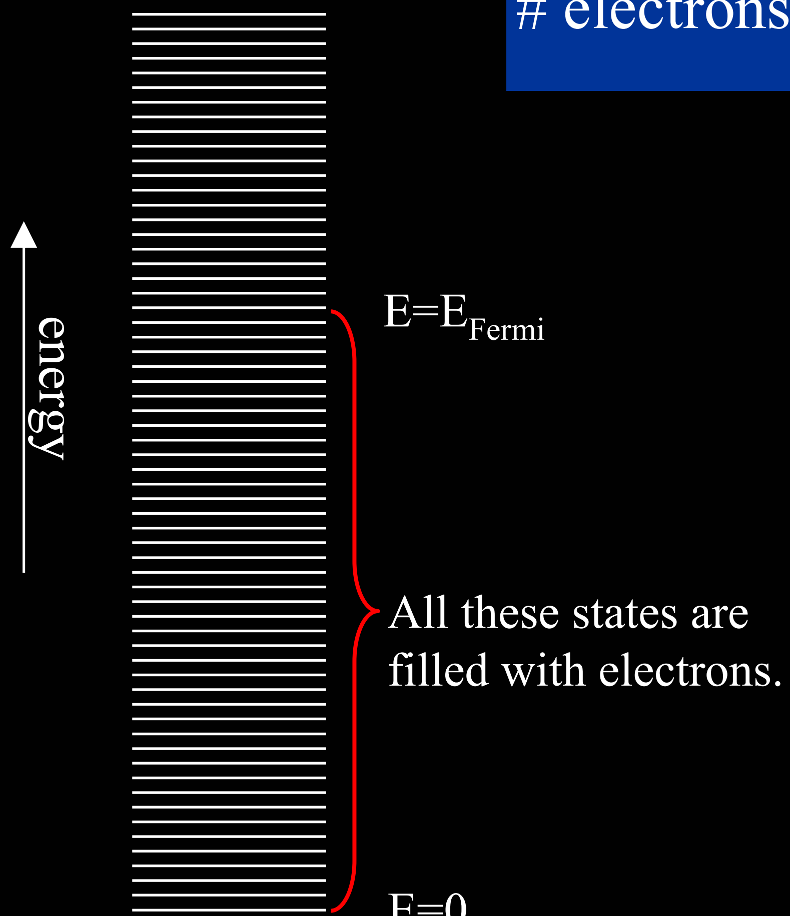
"Gas" means we neglect electron-electron interactions.





Fermi energy:

$$\#\ \text{electrons} = \int_0^{E_f} N_{\mathrm{E}}\, \mathrm{dE} = \int_0^{E_f} L^3 \frac{2^{1/2} m^{3/2}}{\pi^2 \hbar^{3/2}} \cdot E^{1/2} dE$$



Fermi energy:

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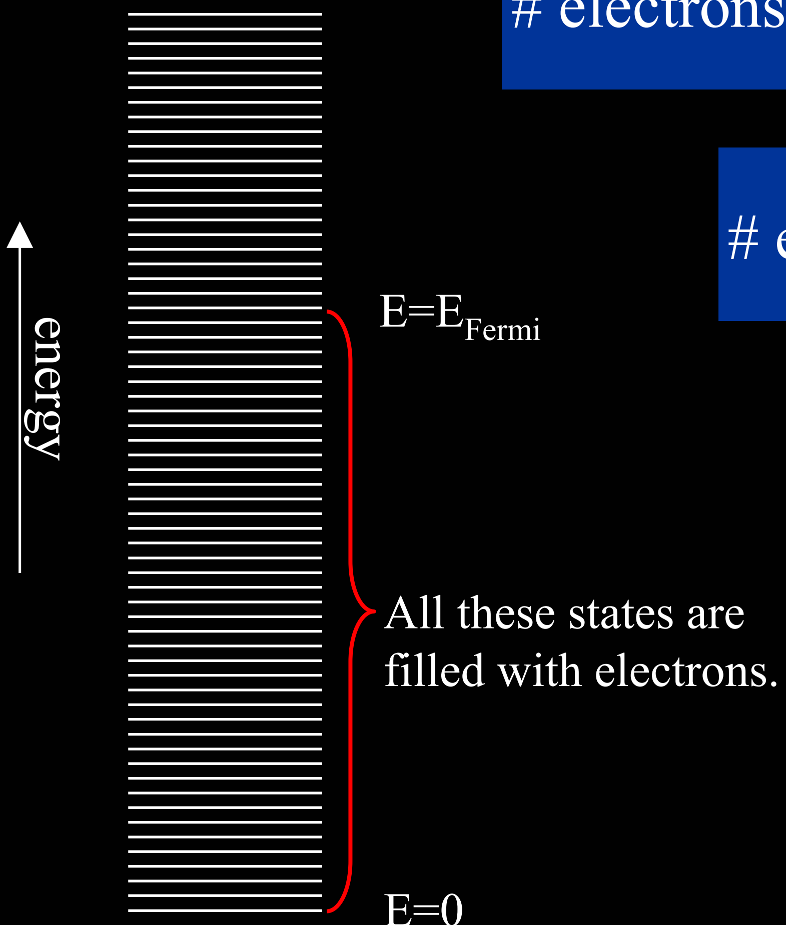
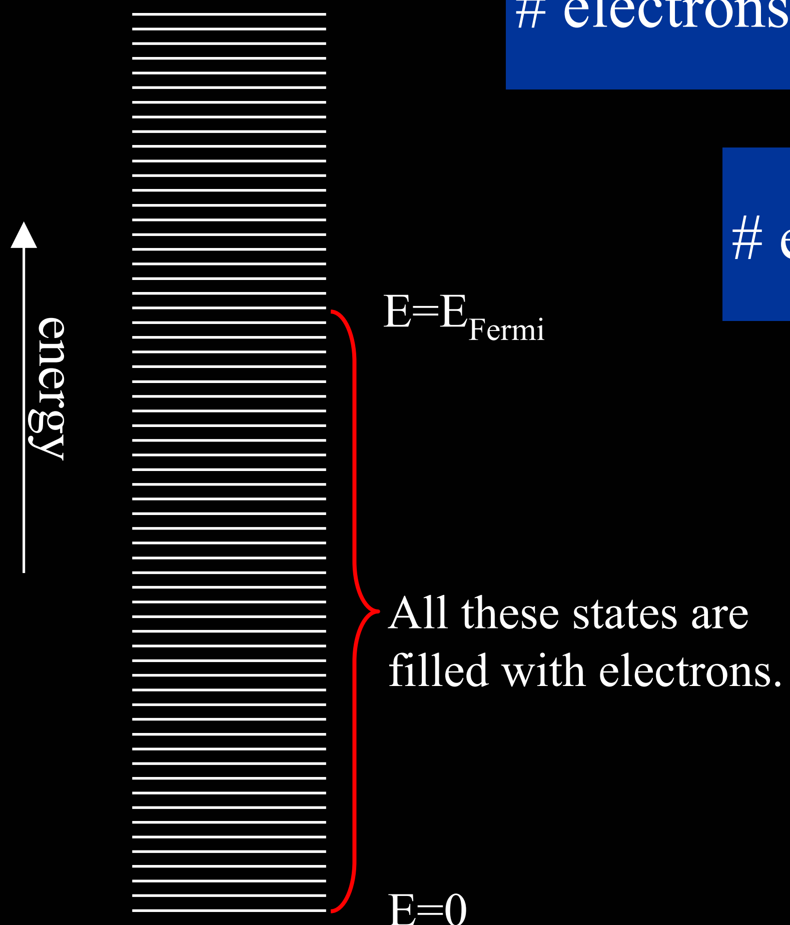
$$\#\ \text{electrons} = L^3 \frac{2^{1/2} m^{3/2}}{\pi^2 \hbar^{3/2}} \frac{2}{3} E_f^{3/2}$$



Fermi energy:



$$\#\text{ electrons} = \int_0^{E_f} N_{\mathrm{E}}\,\mathrm{dE} = \int_0^{E_f} L^3 \frac{2^{1/2} m^{3/2}}{\pi^2 \hbar^{3/2}} \cdot E^{1/2} dE$$

$$\#\text{ electrons} = L^3 \frac{2^{1/2} m^{3/2}}{\pi^2 \hbar^{3/2}} \frac{2}{3} E_f^{3/2}$$

$$\boxed{\Rightarrow E_f = \frac{\hbar^2 3^{2/3} \pi^{4/3}}{2m} \left(\frac{\#\text{ electrons}}{L^3} \right)^{2/3}}$$

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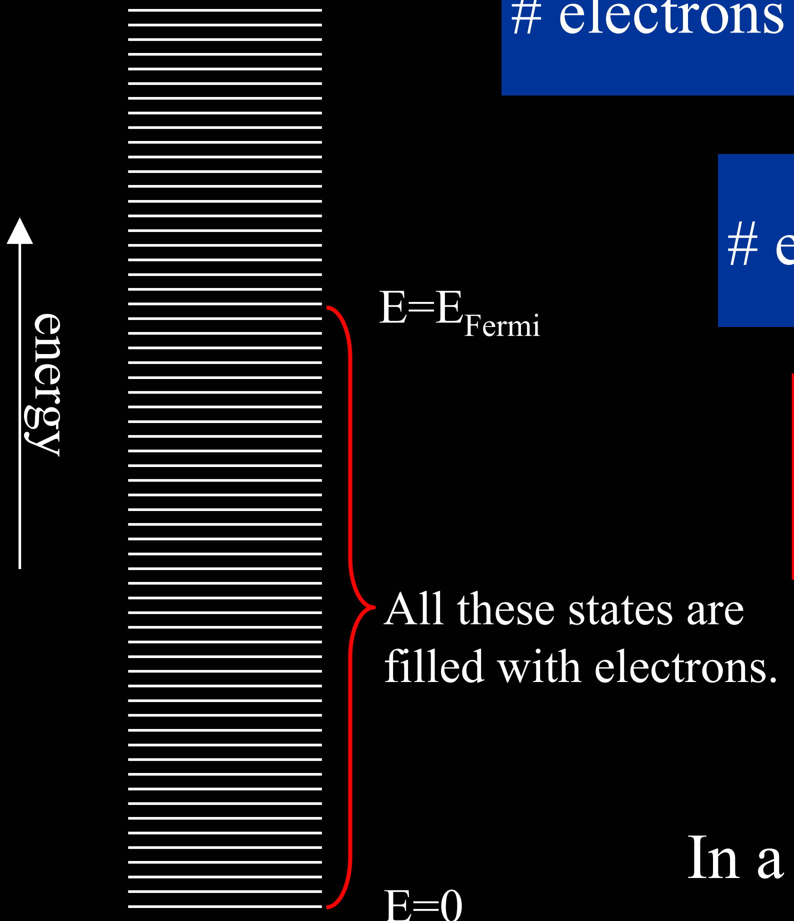
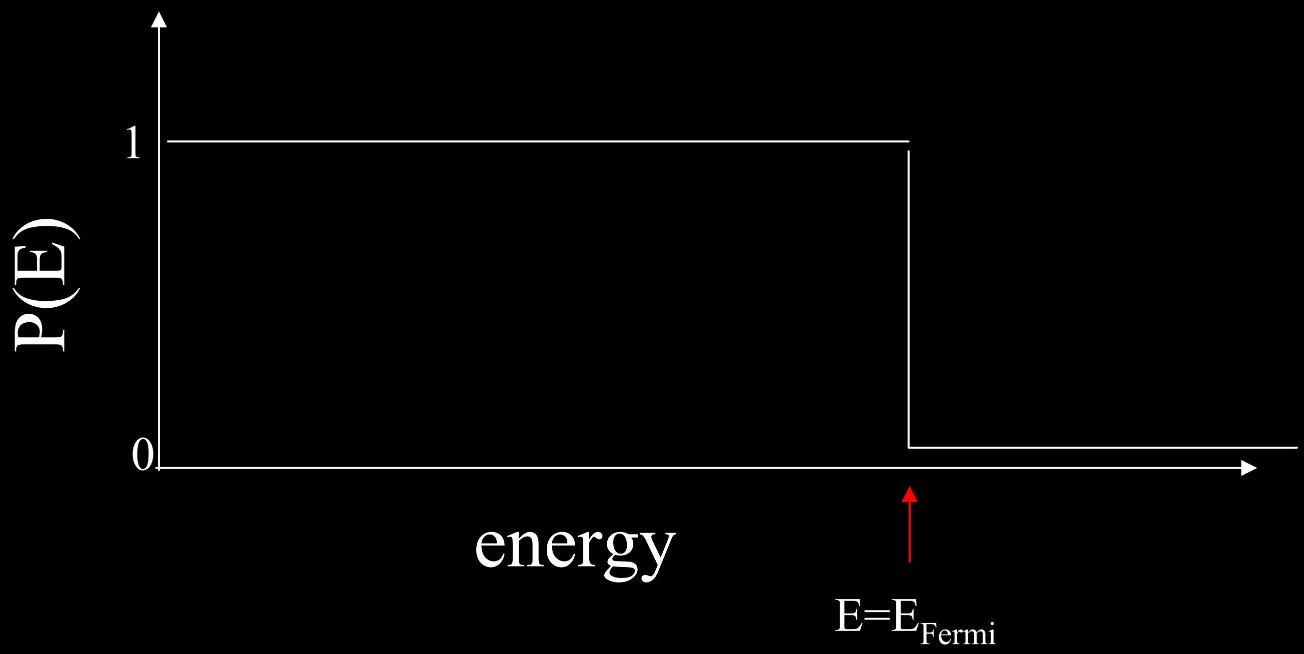
$$\Rightarrow \boxed{E_f = \frac{\hbar^2 3^{2/3} \pi^{4/3}}{2m} \left(\frac{\#\text{ electrons}}{L^3} \right)^{2/3}}$$



In a typical metal, 1 electron $/(0.1\ \mathrm{nm})^3$.

$E_f \sim 10$ eV

Occupation probability:



P(E) = probability of occupying a state with energy E

What about finite temperature?

Boltzmann:

Recall Boltzmann factor P(ε):

"The probability for a physical system to be in a state with energy ε is proportional to $e^{-\varepsilon / k_B T}$."

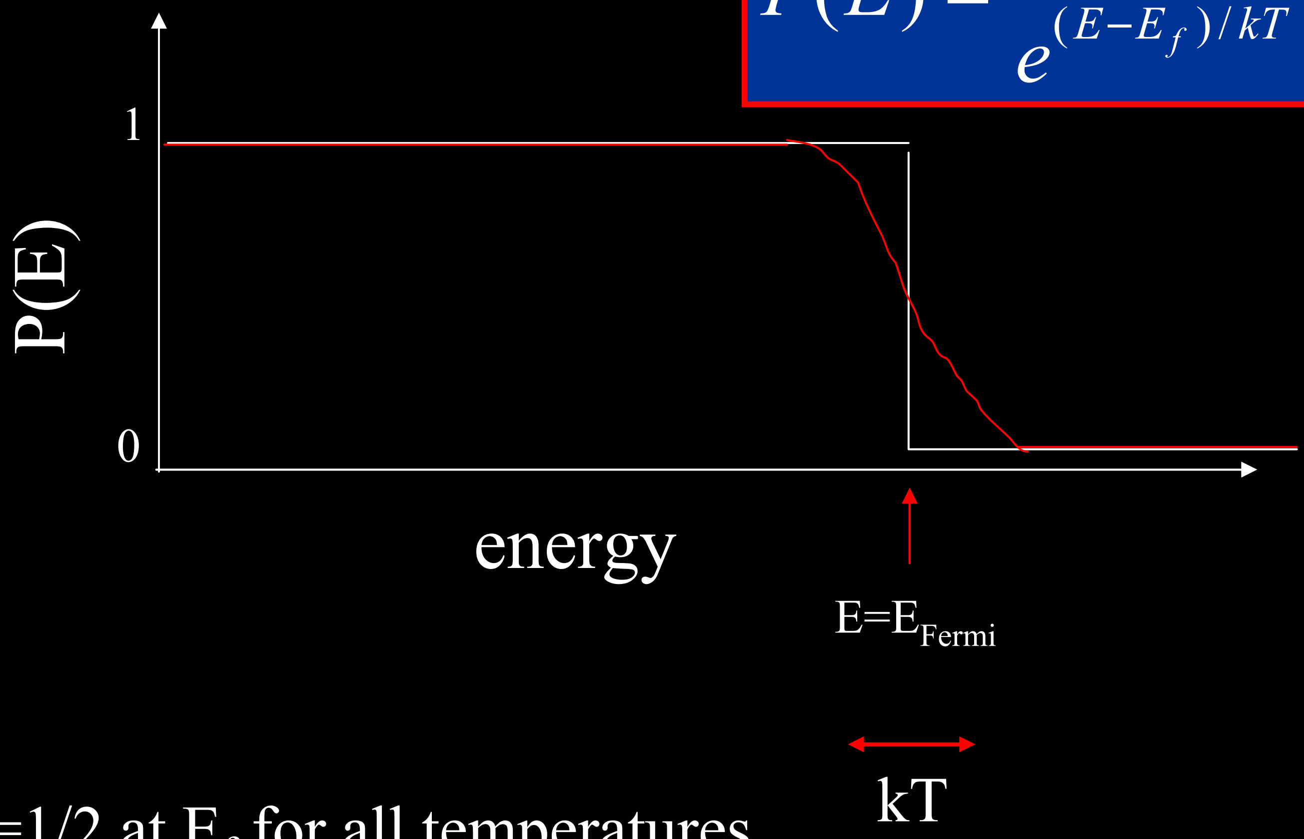
This is actually not quite true. It is classical. A quantum calculation shows for electrons:

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

Called Fermi-Dirac distribution function. Boltzman is high-energy limit (discuss!)

Fermi-Dirac:

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



P=1/2 at E_f for all temperatures.