Sommerfeld Theory of Metals

Pauli exclusion principle, part of quantum theory changed the understanding of electrons in metals and solved several important problems from Drude theory.

it all has to do with the velocity distribution

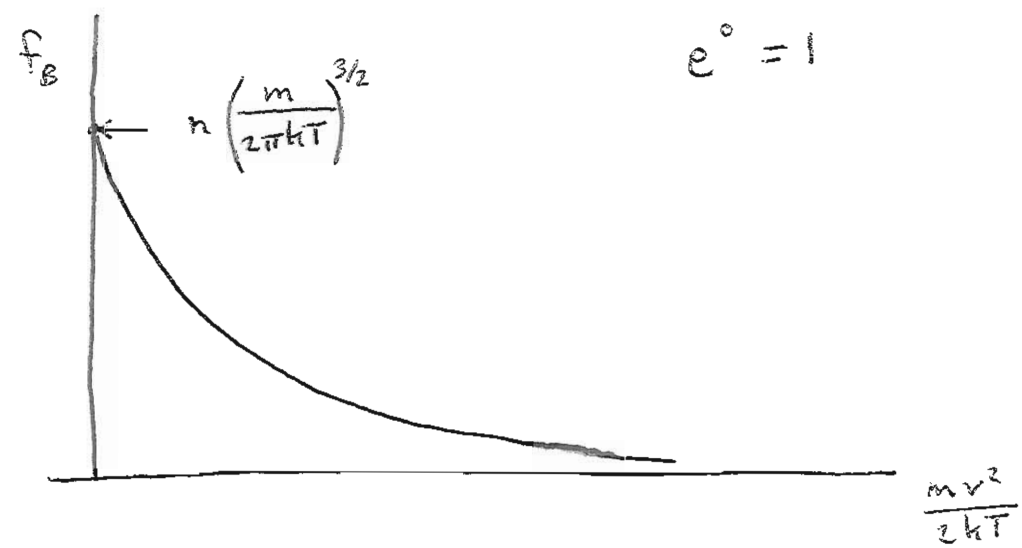
For a classical gas, v is distributed according to Maxwell-Boltzmann distribution

The probability for speed v is:

$$f_B(v) = n\left(\frac{m}{2\pi kT}\right)^{3/2} e^{-mv^2/2kT}$$

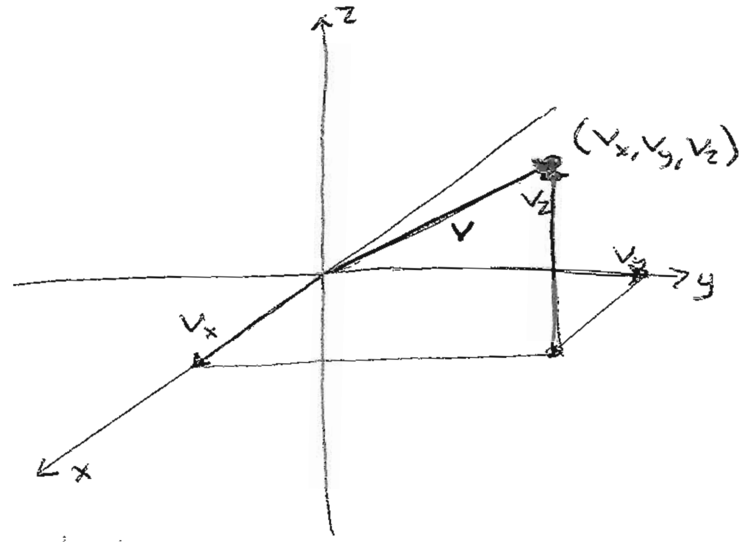
M-B speed probability

This looks like:



$e^0 = 1$

$\vec{v}$ is 3-D with components v_x v_y v_z

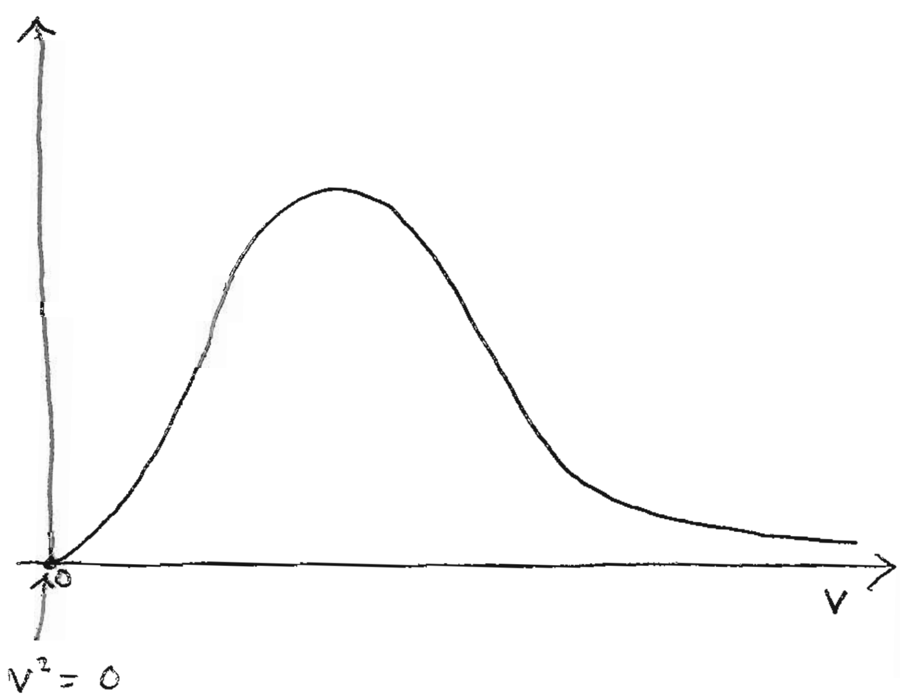


The actual number of particles per unit volume with speeds between v and v + dv is

$$n(v)\,dv = f_B(v)\, d\vec{v}$$

in spherical coords., $d\vec{v} = 4\pi v^2 dv$

The factor of $4\pi v^2 dv$ results in:

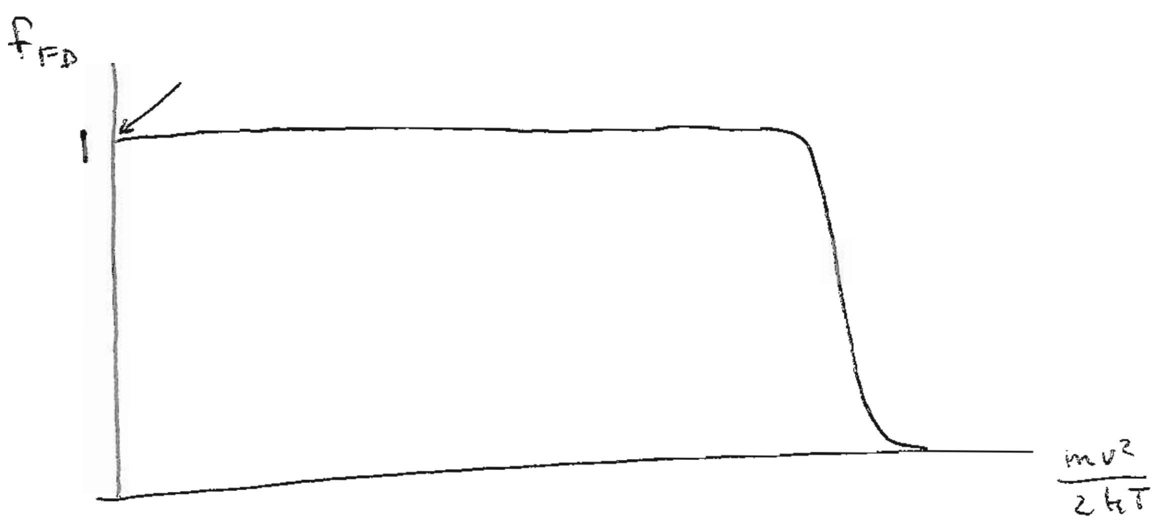


With advent of quantum theory and Pauli exclussion, it was found that electrons should follow Fermi-Dirac distribution:

$$f_{F\text{-}D}(v) = \frac{(m/\hbar)^3}{4\pi^3} \frac{1}{\exp[(\frac{1}{2}mv^2 - kT_0)/kT + 1}$$

The total number of electrons per unit volume is

$$n = \int f_{F\text{-}D}(v)\, dv$$



Ground State Properties of Electron Gas

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r}) = \mathcal{E}\,\psi(\vec{r})$$

how are electrons confined?

Born-von Karman boundary conditions

$$\psi(x, y, z+L) = \psi(x, y, z)$$
$$\psi(x, y+L, z) = \psi(x, y, z)$$
$$\psi(x+L, y, z) = \psi(x, y, z)$$

solution is
$$\psi_k(\vec{r}) = \frac{1}{\sqrt{V}}\,e^{i\vec{k}\cdot\vec{r}}$$

$\vec{k}$ is the wave vector

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

ψ is normalized to 1 in volume V

ψ is an eigenstate of the momentum operator

$$\vec{p} = \frac{\hbar}{i}\frac{\partial}{\partial\vec{r}} = \frac{\hbar}{i}\nabla \quad \Big\}\ \text{momentum operator}$$

i.e. $\vec{p}|\psi = \vec{p}\,\psi$

$$\left(\frac{\hbar}{i}\frac{\partial}{\partial\vec{r}}\right)\left(e^{i\vec{k}\cdot\vec{r}}\right) = \left(\frac{\hbar}{i}\,i\vec{k}\right)\left(e^{i\vec{k}\cdot\vec{r}}\right)$$

$$\Rightarrow \quad \vec{p} = \hbar\vec{k} \quad \Big\}\text{ eigenstate of } \vec{p}|$$

$$\vec{v} = \frac{\hbar\vec{k}}{m}$$

$$\varepsilon = \frac{p^2}{2m} = \frac{1}{2}mv^2$$

$e^{i\vec{k}\cdot\vec{r}}$ is a plane wave with wavelength

$$\lambda = \frac{2\pi}{k} \quad \Big\}\text{ spatial period of the wavefunction}$$

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boundary conditions

$$\Rightarrow \quad e^{i\vec{k}\cdot(\vec{r}+L_x\hat{x})} = e^{i\vec{k}\cdot\vec{r}}$$

$$\Rightarrow \quad e^{ik_xL_x} = 1$$

similarly $e^{ik_yL_y} = 1$

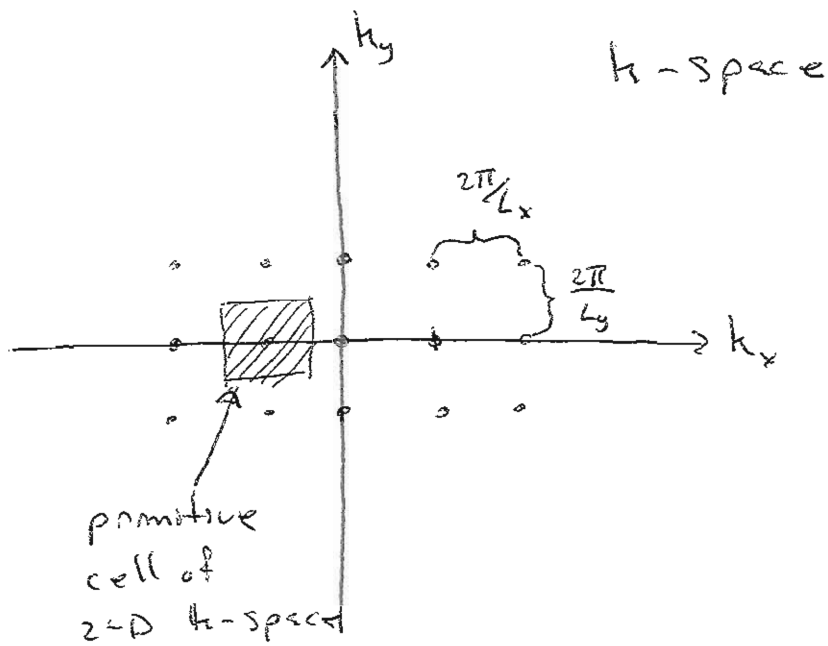
$+ \quad e^{ik_zL_z} = 1$

$$e^{ik_x L_x} = 1 \Rightarrow k_x = \frac{2\pi n_x}{L_x}$$

similarly $\Rightarrow$ & $k_y = \dfrac{2\pi n_y}{L_y}$

& $k_z = \dfrac{2\pi n_z}{L_z}$ $\quad$ n_x n_y n_z integers

$\Rightarrow$ allowed wave vectors are integral multiples of $\dfrac{2\pi}{L_x}$ etc



If we have a k-space region of size Ω,

the # of k-space pts. is

$$N_k = \frac{\Omega}{(2\pi)^3/L_x L_y L_z} = \frac{\Omega V}{(2\pi)^3}$$

$$\Rightarrow \text{density of levels} = \frac{V}{(2\pi)^3}$$