

Physics 410/510 - Solid State Physics

Spring 2015

Wednesday, Week 6

Review:

$$\langle E \rangle = 3 \int_0^{\infty} D(\omega) \hbar \omega (n_B + 1/2) d\omega$$

$$\frac{4\pi V}{(2\pi)^3} k^2 \frac{1}{d\omega/dk} \quad (\text{spherically symmetric } \omega(\vec{k}) = \omega(k))$$

With Debye, $\omega(\vec{k}) = v_s k$, we calculate C :

$$C = \frac{2\langle E \rangle}{T} = 9Nk_B \left(\frac{T}{T_D}\right)^3 \int_0^{\hbar\omega_D/k_B T} \frac{x^4 e^x}{(e^x - 1)^2} dx$$

$$T_D \equiv \frac{\hbar\omega_D}{k_B}$$

$$\omega_D \equiv (6\pi^2 n v_s^3)^{1/3}$$

$$\hookrightarrow 3N = 3 \int_0^{\omega_D} D(\omega) d\omega$$

At low T ,

$$C(T) \propto T^3$$

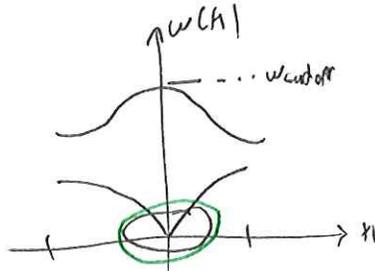
At $T \gg T_D$,

$$C(T) \rightarrow 3Nk_B$$

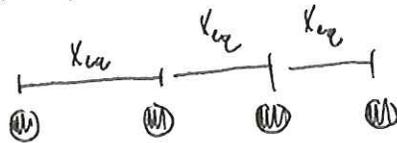
Remarks:

• T^3 behavior occurs when $T \ll T_D$:

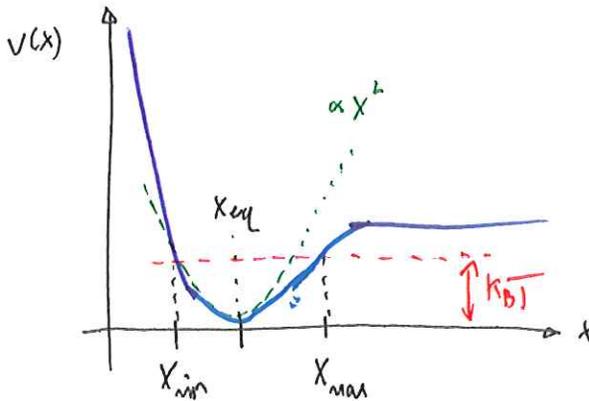
• Here $\omega \ll \omega_D = \omega_{cutoff}$, ω implies where acoustic phonon live
 $\hat{\epsilon}$ the Debye approximation holds, $\omega = v_s \cdot k$:



• For Metals, $C = \gamma T + \beta T^3$



Thermal Expansion:



$V(X_{min}) = V(X_{max}) = k_B T$

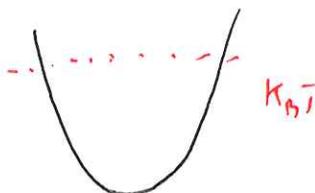
$|X_{max} - X_{eq}| > |X_{min} - X_{eq}|$

so $\langle X \rangle > X_{eq}$ because of asymmetric potential.

$\hat{\epsilon}$ $\langle X \rangle$ will increase for higher T 's

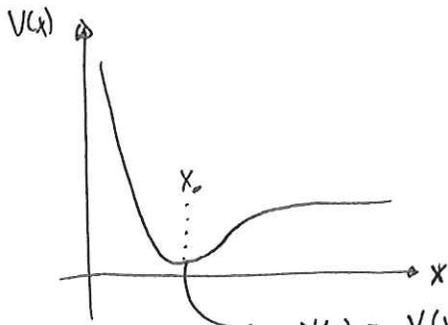


If only $\frac{1}{2} kx^2$



$\langle X \rangle = 0$

Can we approximate \downarrow behavior of thermal expansion?



$$V(x) = V(x_0) + V'(x_0)x + \frac{1}{2}V''(x_0)x^2 + \frac{1}{6}V'''(x_0)x^3 + \dots$$

$$= a + 0 + cx^2 - dx^3 - ex^4 + \dots$$

\downarrow at minimum $V'(x_0) = 0$

\downarrow softening effect

Using Boltzmann's Distribution function:

$$\langle x \rangle = \frac{\int_{-\infty}^{\infty} x \exp(-\beta V(x)) dx}{\int_{-\infty}^{\infty} \exp(-\beta V(x)) dx}$$

$$\int x \exp(-\beta(a + cx^2 - dx^3 - ex^4)) dx$$

$$= \exp(-\beta a) \int x \exp(-\beta cx^2) \exp(\beta(dx^3 + ex^4)) dx$$

$$\approx C_0 \int \exp(-\beta cx^2) x (1 + \beta dx^3 + \beta ex^4) dx$$

$$= C_0 \int \exp(-\beta cx^2) (x + \beta dx^4 + \beta ex^5) dx$$

$$= C_0 \frac{3\pi^{1/2}}{4} \cdot \frac{d}{c^{3/2}} \cdot \frac{1}{\beta^{3/2}}$$

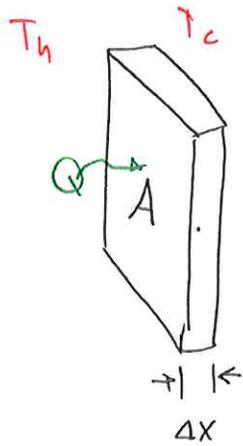
$$\int_{-\infty}^{\infty} \exp(-\beta V(x)) dx$$

$$= C_0 \int \exp(-\beta cx^2) (1 + \beta dx^3 + \beta ex^4 + \dots) dx$$

$$= C_0 \left(\frac{\pi}{\beta c} \right)^{1/2}$$

$$\langle x \rangle = \frac{3d}{4c^2} k_B T$$

Thermal Conductivity:



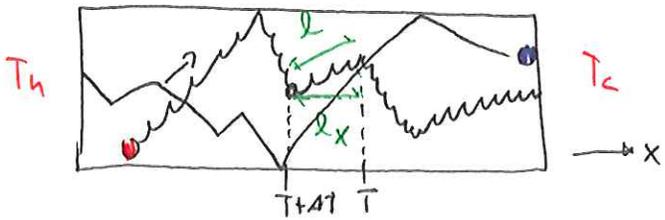
$$Q \propto \frac{(T_h - T_c) \cdot A}{\Delta x} \Delta t$$

$$\frac{Q}{A \Delta t} = -k \frac{\Delta T}{\Delta x}$$

$T_c - T_h$
thermal conductivity

$$\vec{J}_x = -k \frac{\partial T}{\partial x} \quad \text{Fourier heat Law}$$

$$\vec{J} = -K \vec{\nabla} T$$



$n \equiv$ number density of phonons

$$\text{Flux } \leftarrow = +\frac{1}{2} n v_x$$

$$\text{Flux } \rightarrow = \frac{1}{2} n v_x$$

Energy given up going from $T + \Delta T \rightarrow T$:

$$E = c \Delta T$$

$$= c \frac{\partial T}{\partial x} \cdot l_x$$

mean free path in x-direction

$$= c \frac{\partial T}{\partial x} v_x \cdot \tau$$

heat capacity
average collision time

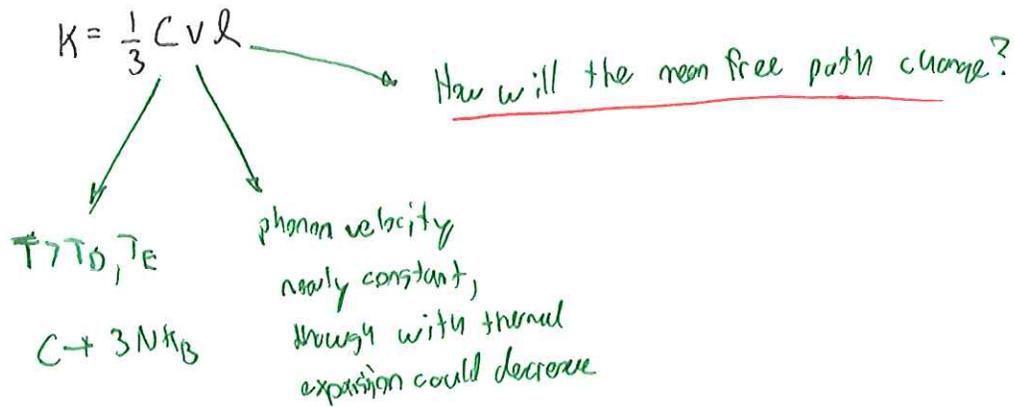
Then net flux of thermal energy is

$$\begin{aligned} J_x &= -n v_x \cdot c \frac{\partial T}{\partial x} v_x \tau \\ &= -n v_x^2 c \tau \frac{\partial T}{\partial x} \\ &= -\frac{1}{3} n v^2 c \tau \frac{\partial T}{\partial x} \\ &= -\frac{1}{3} \frac{Nc}{V} \cdot v l \frac{\partial T}{\partial x} = -\frac{1}{3} C_V \cdot v l \frac{\partial T}{\partial x} \end{aligned}$$

$$K = \frac{1}{3} C_V \cdot v l$$

ave. phonon velocity
mean free path
heat capacity per unit volume

How will the thermal conductivity depend on the temperature?



$l \propto \frac{1}{n} \rightarrow \# \text{ phonons}$
 $\propto \frac{1}{T}$

$n = n_B(\beta \hbar \omega)$
 $= \frac{1}{e^{\beta \hbar \omega} - 1}$
 $\approx \frac{1}{1 + \beta \hbar \omega} \propto T$

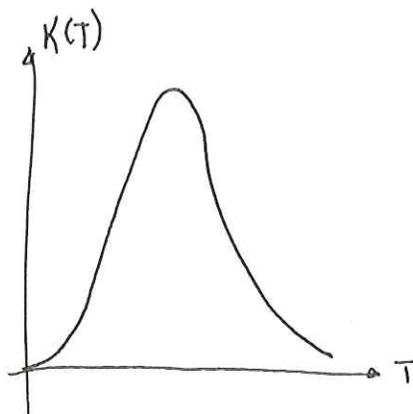
$\propto \frac{k_B}{\hbar \omega} \cdot T$

$T \gg \hbar \omega / k_B$

$\Rightarrow K \propto \frac{1}{T}$ at high T.

At low T, $C \propto T^3$

$K \propto T^3$

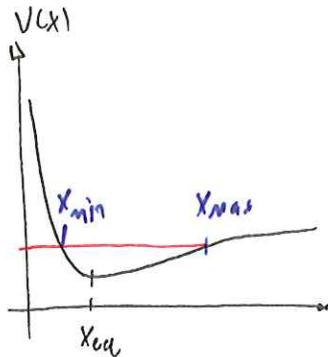


Physics 410/510 - Solid State Physics

Spring 2015

Friday, Week 6:

Review:



Anharmonic potential leads to

$$\langle x \rangle = \frac{3d}{4C^2} k_B T$$

Thermal energy flux: $J_x = -\frac{1}{3} C_v v l \frac{\partial T}{\partial x}$

$$K \equiv \frac{1}{3} C_v v l$$

\nearrow ave. phonon velocity
 \searrow mean free path
 \downarrow heat capacity per unit volume

In Debye Model,

$$T \ll T_D \quad C_v \propto T^3 \quad \Rightarrow \quad K \propto T^3$$

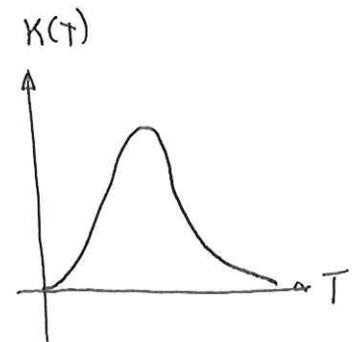
$$v = v_s$$

$$l \rightarrow \text{constant}$$

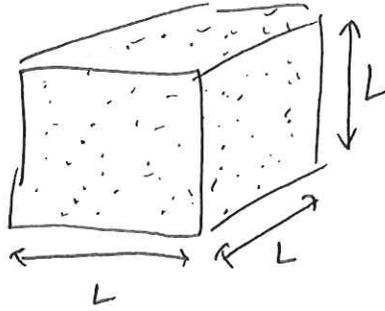
$$T \gg T_D \quad C_v \rightarrow 3Nk_B/V \quad \Rightarrow \quad K \propto \frac{1}{T}$$

$$v = v_s$$

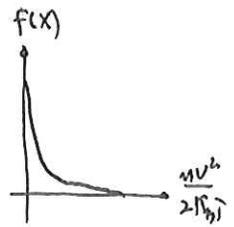
$$l \propto \frac{1}{n} = \frac{1}{T}$$



Now we turn to electrons in metals. First we consider a system of non-interacting electrons that obey the Pauli exclusion rule. We assume the electrons do not interact with other electrons, cores, etc. We call this a free electron Fermi gas:



If we treat the electron gas classically, the heat capacity will be derived from the Maxwell Boltzmann distribution:



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

Maxwell-Boltzmann Distribution:

of electrons per unit volume w/ velocity in range $d\vec{v}$ about \vec{v} is $f_B(\vec{v})d\vec{v}$

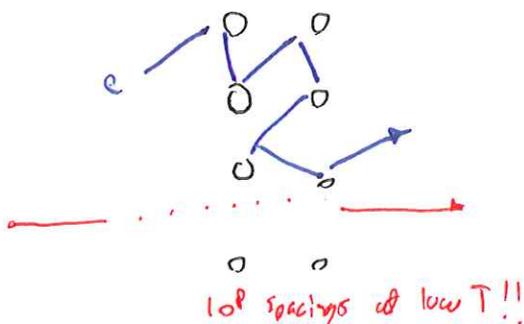
Don't confuse with prob. per unit speed of finding particles w/ speed near v : $f(v) \propto v^2 e^{-m v^2 / 2k_B T}$.

f_B will give

$$C_2 = \frac{3}{2} N k_B \quad \left[\text{Heat Capacity for electron gas} \right]$$

We don't see this experimentally!! We see $\frac{1}{100}$ this value at room T.

Also, the electron mean free path is expected to be short:



But observed \gg expected classically

This classical theory also fails w/ the correct distribution function:

- What determines whether material is metal or insulator?
- Hall coefficient $R_H = \frac{-1}{neL}$ is constant. Doesn't explain deviations
- How many conduction electrons?
- Magnetoresistance is \vec{B} field dependent.

But, the free electron model does get many things correct, including:

- Ohm's Law
- Wiedemann-Franz Law: $\frac{\kappa}{\sigma} \propto T$

Thermal cond.

$\kappa/\sigma \propto T$

electrical cond.

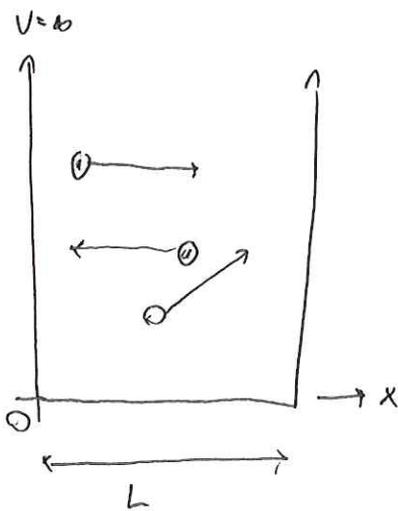
De Broglie λ

For e^- , $v_N \sim v_Q$

Q: When can we treat particles classically? $v_N \gg v_Q \equiv v_Q = \left(\frac{\hbar}{2\pi m \lambda} \right)^3$

Instead of modelling an electron gas classically, we will use Quantum & Quantum statistics

Electrons in a Box:



$$\begin{aligned}
 H\psi &= E\psi & \rightarrow & -i\hbar \vec{\nabla} = m\vec{v} \\
 &= \frac{p^2}{2m} \psi \\
 &= -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x)
 \end{aligned}$$

$$\Rightarrow \psi''(x) = -\left(\frac{2mE}{\hbar^2}\right) \psi(x) = -k^2 \psi(x)$$

$$\psi(x) = A \cos(kx) + B \sin(kx) = C e^{ikx} + D e^{-ikx}$$

$$\psi(0) = 0 = A \cdot 1 + B \cdot 0 \Rightarrow A = 0$$

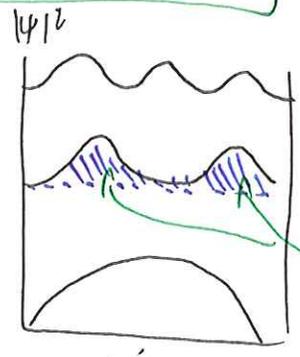
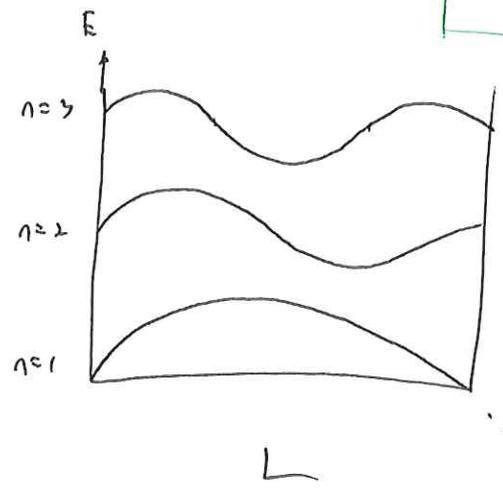
$$\psi(L) = 0 = B \sin(k \cdot L) = 0 \Rightarrow k \cdot L = \pi \cdot n$$

$$\Rightarrow \boxed{k_n = \frac{\pi}{L} \cdot n \quad n \in \mathbb{N}}$$

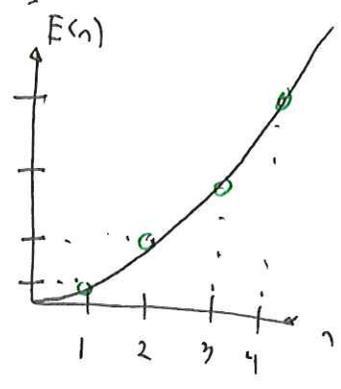
So,

$$\psi(x) = B \sin\left(\frac{\pi \cdot n \cdot x}{L}\right)$$

$$k_n \cdot \lambda = 2\pi \rightarrow \lambda_n = \frac{2\pi}{k_n} = \frac{2\pi L}{\pi n} = \frac{2L}{n}$$



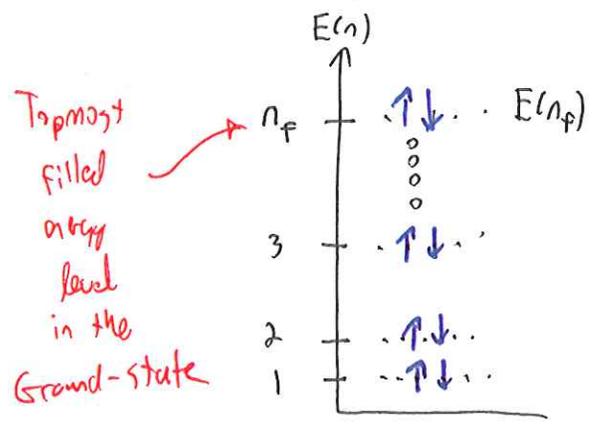
$$E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2 \pi^2}{2mL^2} \cdot n^2$$



The eigenstates are

$$|\psi\rangle = |n, m_s\rangle \quad m_s = \pm \frac{1}{2}$$

The Pauli Exclusion principle forbids two electrons occupying same state (contrast with photons) so each n has two spin states:



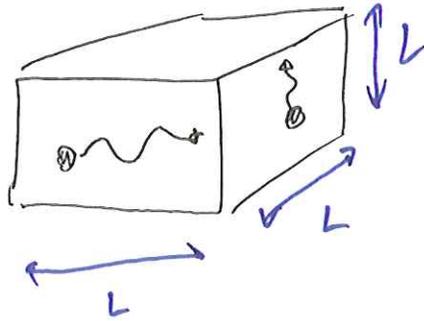
If we have N electrons, then

$$2n_f = N \rightarrow n_f = \frac{N}{2}$$

$$E_f = E(n_f) = \frac{\hbar^2 \pi^2}{2mL^2} \cdot \frac{N^2}{4} = \frac{\hbar^2}{2m} \left(\frac{N\pi}{2L}\right)^2$$

Fermi Energy ↑

Electrons in a 3D box:



$$\begin{aligned}
 H\psi &= E\psi \quad \Rightarrow \quad -\frac{\hbar^2}{2m} \nabla^2 \psi = E\psi \\
 &= -\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \psi \\
 &= (E_x + E_y + E_z) \psi
 \end{aligned}$$

Separation of variables:

$$\psi(x, y, z) = \psi_x \psi_y \psi_z$$

$$\text{Then} \quad -\frac{\hbar^2}{2m} \left(\psi_y \psi_z \frac{\partial^2}{\partial x^2} \psi_x + \psi_x \psi_z \frac{\partial^2}{\partial y^2} \psi_y + \psi_x \psi_y \frac{\partial^2}{\partial z^2} \psi_z \right) = (E_x + E_y + E_z) \psi_x \psi_y \psi_z$$

$$\Rightarrow \quad -\frac{\hbar^2}{2m} \left(\frac{1}{\psi_x} \frac{\partial^2}{\partial x^2} \psi_x + \frac{1}{\psi_y} \frac{\partial^2}{\partial y^2} \psi_y + \frac{1}{\psi_z} \frac{\partial^2}{\partial z^2} \psi_z \right) = E_x + E_y + E_z$$

$$\Rightarrow \quad -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi_x = E_x \psi_x \quad \Rightarrow \quad \boxed{\psi_x(x) = B_x \sin\left(\frac{\pi}{L} n_x \cdot x\right)}$$

$$\Rightarrow \quad \boxed{\psi(\vec{x}) = B_x \sin\left(\frac{\pi}{L} n_x \cdot x\right) \cdot B_y \sin\left(\frac{\pi}{L} n_y \cdot y\right) \cdot B_z \sin\left(\frac{\pi}{L} n_z \cdot z\right)}$$

$$\boxed{E = \frac{\hbar^2 \pi^2}{2mL^2} (n_x^2 + n_y^2 + n_z^2)}$$

$$n_i \in \mathbb{N}$$

Recall that $\psi(\vec{r}) = e^{i\vec{k}\cdot\vec{r}}$ is also a solution to the particle in a box Schrödinger equation. Here though, as with vibration waves, we use the Born-von Karman B.C.'s:

$$\begin{aligned}\psi(\vec{r} + L\hat{x}) &= e^{-ik_x(x+L)} e^{ik_y y} e^{ik_z z} \\ &= e^{ik_x x} e^{ik_y y} e^{ik_z z}\end{aligned}$$

$$\Rightarrow \underbrace{k_x \cdot L = 2\pi \cdot n}_{\substack{\downarrow \\ \text{contrast to } \sin(-) \text{ case where } k_x = \frac{\pi \cdot n}{L} \quad n \in \mathbb{N}}}} \quad n \in \mathbb{Z} \Rightarrow \boxed{k_x = \frac{2\pi \cdot n}{L}}$$

We'll use $\psi(\vec{r}) = e^{i\vec{k}\cdot\vec{r}}$ form instead to use all of \vec{k} -space.
 ↑
 travelling plane wave

∴ the energy is:

$$\boxed{E(\vec{k}) = \frac{\hbar^2}{2m} \vec{k}^2 = \frac{\hbar^2}{2m} (k_x^2 + k_y^2 + k_z^2)}$$

These electrons do also have momentum:

$$\vec{p}\psi = -i\hbar\nabla\psi(\vec{r}) = \hbar\vec{k}\psi(\vec{r}) \Rightarrow \boxed{\langle \vec{p} \rangle = \hbar\vec{k}}$$

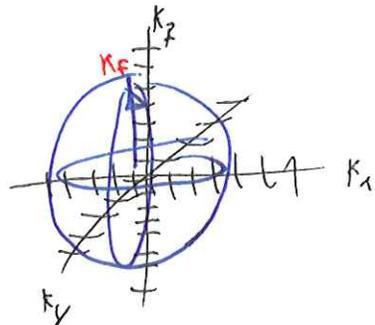
∴ velocity

$$\boxed{\vec{v} \equiv \vec{p}/m = \frac{\hbar\vec{k}}{m}}$$

In the ground state, the system will take on lowest values of \vec{k} up to a maximum \vec{k}_f .

The energy at this wavevector will be

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



The DOS $= 2 \cdot \left(\frac{2\pi}{L}\right)^3 = 2 \cdot \left(\frac{L}{2\pi}\right)^3$, so the # states up to k_f is # electrons

$$N = \text{DOS}_k \cdot \text{Volume}_k$$

$$= 2 \left(\frac{L}{2\pi}\right)^3 \cdot \frac{4\pi}{3} k_f^3$$

$$= \frac{V}{3\pi^2} k_f^3 \Rightarrow k_f = \left(3\pi^2 N/V\right)^{1/3}$$

Fermi wave vector.

So the Fermi Energy is:

$$E(k_f) = E_f = \frac{\hbar^2 k_f^2}{2m} = \frac{\hbar^2}{2m} \left(3\pi^2 N/V\right)^{2/3}$$

Fermi Energy for free electron gas
 $E_f \sim 1-10 \text{ eV}$

Fermi velocity:

$$v_f = \frac{\hbar k_f}{m} = \left(\frac{\hbar}{m}\right) \left(3\pi^2 N/V\right)^{1/3}$$

$T_f \equiv E_f/k_B$
 $T_f \sim 10^4 \text{ K}$

$v_f \sim 10^8 \text{ cm/s}$

We want to calculate Thermal properties of electron gas, so we'll need density of states (in Energy) [# states / Energy]:

$$N_{\leq k} = 2 \times \left(\frac{L}{2\pi}\right)^3 \cdot \frac{4\pi}{3} k^3$$

$$= \frac{V}{3\pi^2} k^3$$

$$N_{\leq E} = \frac{V}{3\pi^2} \left(\frac{2mE}{\hbar^2}\right)^{3/2}$$

$$D(E) = \frac{dN_{\leq k}}{dE} = \frac{V}{\pi^2} k^2 \frac{1}{dE/dk}$$

$$= \frac{V}{\pi^2} k^2 \frac{m}{\hbar k} = \frac{Vm}{\pi^2 \hbar^2} k = \frac{Vm}{\pi^2 \hbar^2} \sqrt{\frac{2mE}{\hbar^2}} = \frac{V}{2\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} E^{1/2} = D(E)$$

$\bar{v} = \frac{\hbar^2 k^2}{2m} \quad \frac{dE}{dk} = \frac{\hbar^2 k}{m} = \frac{2E}{k}$