HW - Friday!

Lecture 4 - More Solid State

Last time, started talking about solids (Sect. 5.3)

0^{th} order model: free electron gas

→ Non interacting electrons in ∞ square well (l_x, l_y, l_z)

Single particle states

$$\psi_{\vec{k}} = \sqrt{\frac{8}{V}} \sin k_x x \sin k_y y \sin k_z z$$

$$\vec{k} = \left(\frac{\pi n_x}{l_x}, \frac{\pi n_y}{l_y}, \frac{\pi n_z}{l_z} \right) \quad \text{integers } n_x, n_y, n_z$$

Energy $\quad E_k = \dfrac{\hbar^2 k^2}{2m}$

Can put two electrons in each state
(& these electrons are in spin singlet)

So if we have a lot of electrons, we'll
need a lot of states
∴ lots of states at high energy

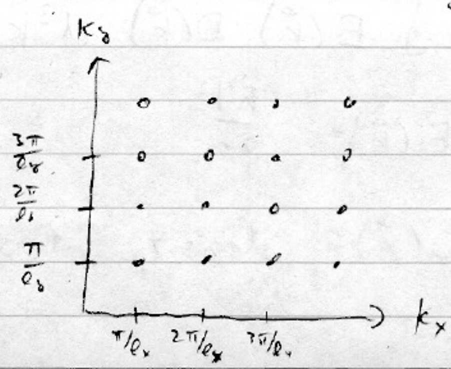
Calculate total energy of gas

Say Nq electrons: N atoms, each donates q electrons

Use geometrical construction

Allowed wave vectors $\vec{k}$ form grid in "k-space"

2D picture:



We will occupy $\frac{N_q}{2}$ points

Lowest energy configuration = sphere

Actually $1/8$ of sphere, since n's > 0

Say sphere radius $k_F \equiv$ "k-Fermi"

Then volume is $\frac{1}{8} \times \frac{4}{3}\pi k_f^3 = \frac{\pi}{6} k_f^3$

Each point occupies volume $(\Delta k)^3 = \frac{\pi^3}{l_x l_y l_z} = \frac{\pi^3}{V}$

So number of states in sphere is

$$\frac{\frac{\pi}{6} k_f^3}{\pi^3/V} = \frac{1}{6\pi^2} k_f^3 V$$

$$= \frac{N_q}{2}$$

$$\text{Solve for } k_F = \left(3\pi^2 \frac{N_q}{V}\right)^{1/3}$$

$$= \left(3\pi^2 \rho\right)^{1/3} \qquad \rho = \frac{N_q}{V}$$

= density of e^-'s

Ground state is

all states with $|\vec{k}| < k_F$ filled

all states with $|\vec{k}| > k_F$ empty

Then get ground state energy:

$$E_{TOT} = \int E(\vec{k})\, D(\vec{k})\, d^3k$$

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

$D(\vec{k})$ = density of states = $\frac{\#\text{ of states}}{\text{volume in k-space}}$

$$D(\vec{k}) = \frac{2}{(\Delta k)^3} = \frac{2V}{\pi^3}$$

So $$E_{TOT} = \int_0^{k_F} \frac{\hbar^2 k^2}{2m} \frac{2V}{\pi^3} \frac{1}{8} \times 4\pi k^2 dk$$

only $\frac{1}{8}$ of sphere

$$= \frac{V}{2\pi^2} \frac{\hbar^2}{m} \int_0^{k_F} k^4 dk$$

$$= \frac{V}{2\pi^2} \frac{\hbar^2}{m} \frac{k_F^5}{5}$$

So $$\boxed{E_{TOT} = \frac{V}{10\pi^2} \frac{\hbar^2}{m} (3\pi^2 \rho)^{5/3}}$$

For instance, if $\rho = \frac{1 \text{ electron}}{(10^{-10} m)^3}$, $k_F = 3 \times 10^{10} m^{-1}$

Energy density $\frac{E}{V} = 3.5 \times 10^{12} \frac{J}{m^3}$

Then $(10 \text{ cm})^3$ chunk of metal contains 3×10^9 J worth of electron energy

Hope that helps illustrate the significance of exchange force

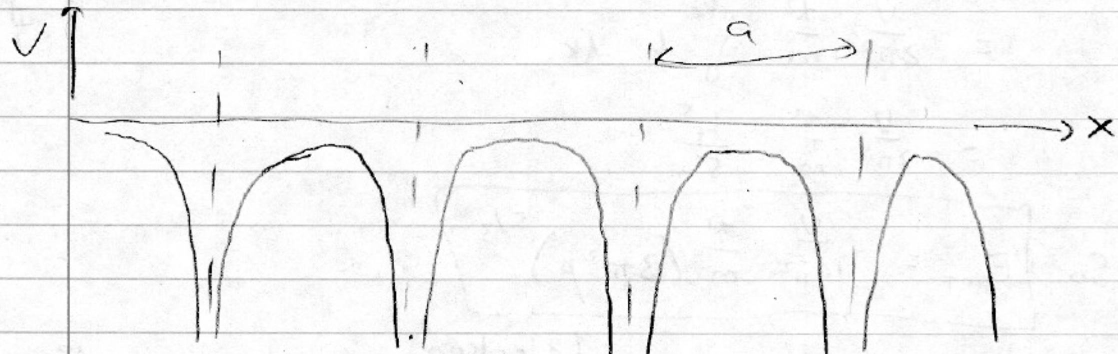
Not a great model for a solid, though.
Turns out that neglecting $e^- - e^-$ interactions is not so bad
- Because here exchange forces are much bigger

But neglecting interaction with positive ions isn't so good
- Crystal lattice of ions changes single particle states; exchange doesn't matter

Can introduce idea of how ions affects things

In crystal lattice, have regular array of ions:

Electrons see periodic potential:



[Note most solids are crystalline on microscopic level... only glasses are not. They are more complicated.]

Want to find single particle states

Key tool: Bloch's theorem:

If $V(x+a) = U(x)$, then the energy eigenstates have form

$$\psi_K(x) \text{ with } \psi_K(x+a) = e^{iKa}\psi(x)$$

K = real

Prove if time:

$D\psi = \lambda\psi$

$\lambda = e^{iKa}$

K real so ψ remains bounded

Book has proof... not here!

I'll ~~try~~ to give intuitive motivation

- Certainly want $|\psi(x+a)|^2 = |\psi(x)|^2$, observables should be periodic

But that allows $\psi(x+a) = e^{i\phi(x,a)}\psi(x)$

Bloch's theorem says ϕ indep of x