1,

Electrons in solids

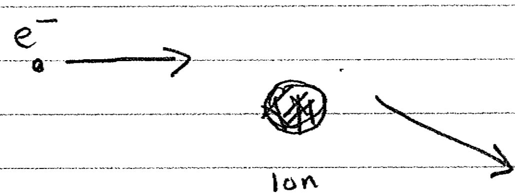
We have focussed so far on lattice

- lattice structure
  description of
  x ray scattering
- lattice vibrations

Turn now to electrons

An amazing thing is that a lot of properties of e^- in solid can be explained by ignoring lattice!

How is it possible electrons don't scatter off ions?!



Recall QM

$$\psi(\vec{r},0) \longrightarrow \psi(\vec{r},t) \quad \text{How?}$$

Solve

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right]\phi_n(\vec{r}) = E_n\phi_n(\vec{r})$$

Hermitian

complete set & orthogonal

Expand

$$\psi(\vec{r},0) = \sum_n c_n \phi_n(\vec{r})$$

$$c_n = \int d^3\vec{r}\, \psi(\vec{r},0)\, \phi_n^*(r)$$

$$\psi(\vec{r}\,t) = \sum_n c_n \phi_n(\vec{r})\, e^{-iE_n t/\hbar}$$

Sometimes eliminate c_n and write in fancy way

$$\psi(\vec{r}\,t) = \int d^3r' \underbrace{\left[\sum_n \phi_n^*(r')\,\phi_n(r)\,e^{-iE_n t/\hbar}\right]}_{G(\vec{r},\vec{r}',t)} \psi(\vec{r}'\,0)$$

$G(\vec{r},\vec{r}',t)$ "Greens function" or "propagator"

But point to emphasize is that if you have e^- in one of eigenstates initially $\psi(\vec{r},0) = \phi_e(\vec{r})$

It never scatters out of it $\psi(\vec{r},t) = \phi_e(r)\,e^{-iE_e t/\hbar}$

[Analogous in a way to classical normal modes]

One has found special states (by "absorbing" effect of ions into appropriate $\phi_n(\vec{r})$) ~~where~~

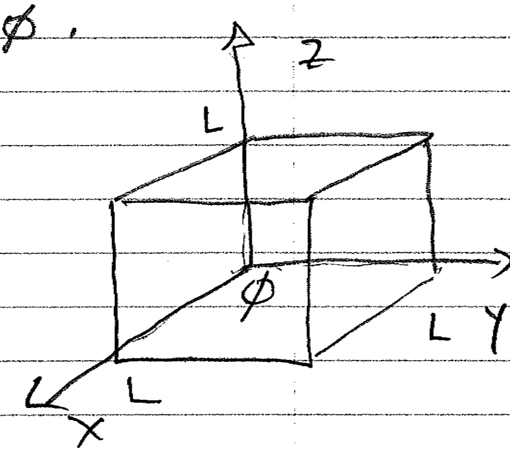
"LANDAU FERMI LIQUID THEORY"

Perhaps most famous principle of CM physics

e^- in solid can be understood as free electrons (with perhaps renormalized $m \to m_*$)

We will see other ways to understand this better in the coming weeks.

For now let's see what comes out of a description of e^- in a solid as just particles in a box with no ionic potential $V(\vec{r}) = \phi$.



$$-\frac{\hbar^2}{2m}\nabla^2 \phi_n = E_n \phi_n$$

$$\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

Solns are

$$\phi_n(x\,y\,z) = \sin\frac{n_x \pi x}{L} \sin\frac{n_y \pi y}{L} \sin\frac{n_z \pi z}{L}$$

$n_x\, n_y\, n_z$

Can easily check this obeys Sch Eqn with

$$E_n = \frac{\hbar^2}{2m}\frac{\pi^2}{L^2}\left(n_x^2 + n_y^2 + n_z^2\right)$$

$$k_x = \frac{\pi n_x}{L} \quad k_y = \frac{\pi n_y}{L} \quad k_z = \frac{\pi n_z}{L}$$

As $L \to \infty$ $\quad k_x, k_y, k_z$ continuous.

Pauli Principle: For Fermions each QM state can be occupied by at most 1 particle. (or 2 if one includes spin ↑ ↓ as additional quantum number like n_x n_y n_z)

If you put 14 e^- in box at lowest total Energy

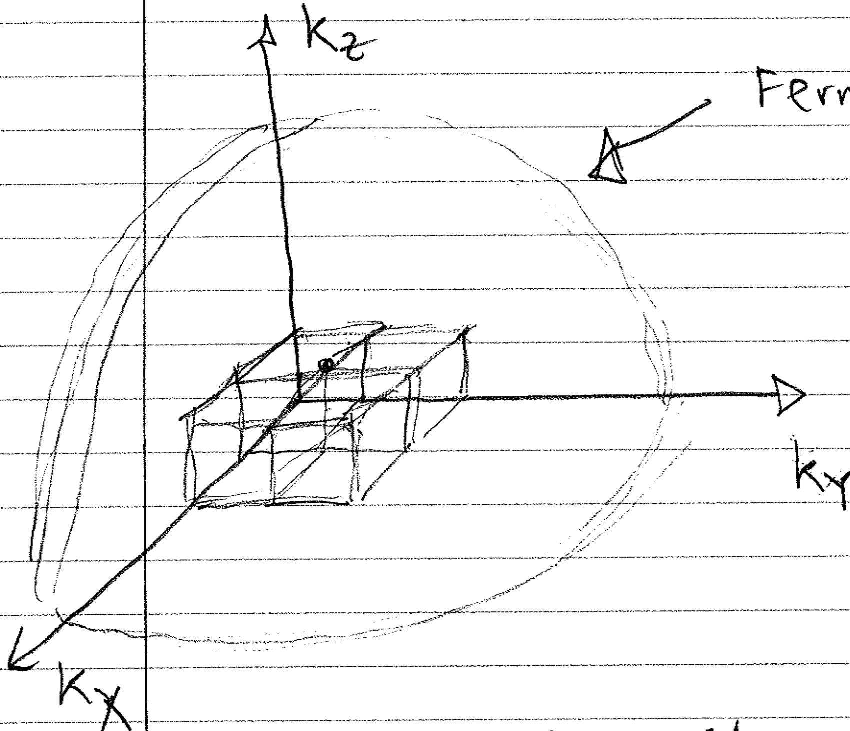
E		n_x	n_y	n_z		$\lvert\vec{k}\rvert$
$\frac{\hbar^2}{2m}\frac{\pi^2}{L^2}$	3 →	1	1	1	↑↓	$\frac{\pi}{L}\sqrt{3}$
		1	1	2	↑↓	
$\frac{\hbar^2}{2m}\frac{\pi^2}{L^2}$	6	1	2	1	↓↑	$\frac{\pi}{L}\sqrt{6}$
		2	1	1	↑↓	
		2	2	1	↑↓	$\frac{\pi}{L}\sqrt{9}$
$\frac{\hbar^2}{2m}\frac{\pi^2}{L^2}$	9	2	1	2	↑↓	↑ FILLED
		1	2	2	↑↓	
Fermi Energy E_F						k_F ← Fermi wave vector
$\frac{\hbar^2}{2m}\frac{\pi^2}{L^2}$	11	3	1	1		↓ EMPTY
$\frac{\hbar^2}{2m}\frac{\pi^2}{L^2}$	12	2	2	2		

⋮

$$E_F = \frac{\hbar^2}{2m} k_F^2$$

5.

There is a $\vec{k}$ point in every $\left(\frac{2\pi}{L}\right)^3$ of $\vec{k}$ space



\# points inside

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

$\therefore$ # electrons N is related to k_F, E_F by

$$N = \underset{\uparrow}{2} \frac{\frac{4}{3}\pi k_F^3}{\left(\frac{2\pi}{L}\right)^3} = \frac{k_F^3}{3\pi^2} \underset{\substack{\uparrow \\ V}}{L^3}$$

For spin

$$\frac{N}{V} = \boxed{n = \frac{k_F^3}{3\pi^2}}$$

$$E_F = \frac{\hbar^2}{2m} k_F^2 = \frac{\hbar^2}{2m}\left(3\pi^2 n\right)^{2/3}$$

6.

E_F is a typical kinetic energy of e^- in a metal. In fact, you can show

$$\langle KE \rangle = \frac{3}{5} E_F \qquad \leftarrow \text{good exercise}$$

$$\langle KE \rangle = \frac{1}{N} \overset{\text{spin}}{2} \int_0^{k_F} 4\pi k^2 \, dk \left(\frac{L}{2\pi}\right)^3 \frac{\hbar^2 k^2}{2m}$$

$$= \underbrace{\frac{1}{N}\left(\frac{L}{2\pi}\right)^3 8\pi}_{\frac{L^3}{N}\frac{1}{\pi^2}} \underbrace{\frac{\hbar^2}{2m} \frac{k_F^5}{5}}_{\frac{1}{5} E_F \underbrace{k_F^3}_{3\pi^2 \frac{N}{L^3}}}$$

$$= \frac{3}{5} E_F$$

How big is E_F? Any guesses?

What is KE of air molecule?

$$\frac{3}{2} k_B T = \frac{3}{2}\left(1.38 \cdot 10^{-23} \frac{J}{°K}\right)(300°K)$$

$$= 6.21 \cdot 10^{-21} J$$

7.

Velocity $\frac{1}{2} m v^2 = 6.21 \cdot 10^{-21}$ J

$32(1.67 \cdot 10^{-27})$ kg

$v = 4.82 \cdot 10^2$ m/s

Fermi Energy

$$E_F = \frac{\hbar^2}{2m}\left(3\pi^2 n\right)^{2/3}$$

$$= \frac{(1.055 \cdot 10^{-34})^2}{2(9.11 \cdot 10^{-31})}\left(3\pi^2 \frac{6}{23} 10^{29}\right)^{2/3}$$

$$\frac{6 \cdot 10^{23}}{23 \cdot 10^{-6}}$$ ← mole

$cm^3 \to m^3$

Na 23

density 1

$$= \frac{(1.055)^2}{2(9.11)}\left(\frac{3\pi^2 600}{23}\right)^{2/3}$$

$10^{-68}\, 10^{31}\, 10^{18}$

$= 5.1 \quad 10^{-19}$ J ← MAIN POINT IS 100 x AS BIG AS KE OF AIR MOLECULE

$= 3$ eV

Another impt application is astrophysical...

prevents collapse of neutron star: gravity favors smaller radius but if n increases so does KE cost

Neutron star $\quad N$ neutrons

$$PE \sim -\frac{Gm^2}{r} N^2 \sim -Gm^2 N^2 V^{-1/3}$$

N^2: # pairs

r: typical separation $\sim V^{1/3}$

$$KE \sim +N E_F = N \frac{\hbar^2}{2m}\left(3\pi^2 \frac{N}{V}\right)^{2/3}$$

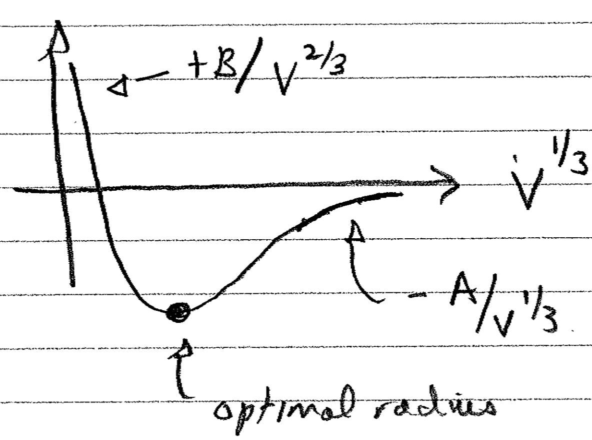
$$\sim \frac{\hbar^2}{2m}\left(3\pi^2\right)^{2/3} N^{5/3} V^{-2/3}$$

If $V \to V/8$ $\quad$ PE increases by $\times 2$

KE increases by $\times 4$

Balance between 2 $\to$ neutron star radius

Need to know N, typical # of neutrons



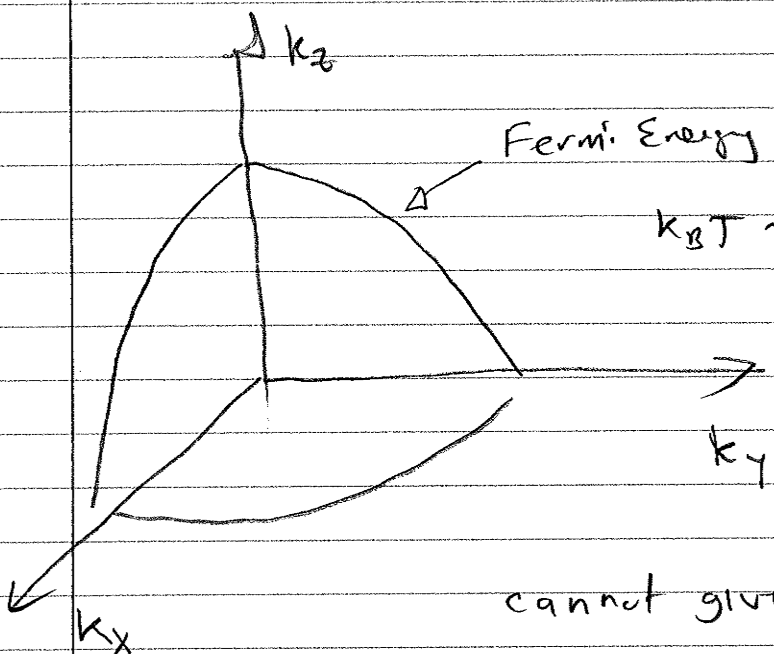
seen before where?

9.

Specific heat of solid

$$C(T) = \gamma T + AT^3$$

Crude argument



cannot give Energy to electrons (deep) inside Fermi sphere because all neighboring states filled (Pauli Blocked)

Only states within $k_B T$ of E_F can absorb energy (respond to increase in T)

$$C \sim N k_B \frac{k_B T}{E_F} \quad \therefore \quad C \sim \gamma T$$

classical ideal gas answer

Pauli Blocking reduction