Wed. Sept. 19

- Today we continue our discussion of electrons in conductors + degeneracy pressure

- we found two electrons, as fermions, cannot occupy the same quantum state

- let's see the consequences of this

- assume we have a rectangular solid of dimensions (l_x, l_y, l_z)

- if electrons experience no forces within the solid (free electron gas)

$$V(x,y,z) = \begin{cases} 0 & ; \quad 0 < x < l_x, \ldots \\ \infty & ; \quad \text{elsewise} \end{cases}$$

- we solve $\frac{-\hbar^2}{2m}\nabla^2\psi = E\psi$ (ind. of time)

- by separation of variables

$$\psi(x,y,z) = X(x)\,Y(y)\,Z(z)$$

$$-\frac{\hbar^2}{2m}\frac{d^2X}{dx^2} = E_x X$$, same for other two

& $E = E_x + E_y + E_z$

let $k_x \equiv \frac{\sqrt{2mE_x}}{\hbar}$, . . . , $k_z \equiv \frac{\sqrt{2mE_z}}{\hbar}$

& get $X(x) = A_x \sin(k_x x) + B_x \cos(k_x x)$

$Y(y) = \ldots$; $Z(z) = \ldots$ (same form)

- using boundary conditions of $V(x)$

$$\psi_{n_x n_y n_z} = \sqrt{\frac{8}{l_x l_y l_z}} \sin\left(\frac{n_x \pi}{l_x}x\right) \sin\left(\frac{n_y \pi}{l_y}y\right) \sin\left(\frac{n_z \pi}{l_z}z\right)$$

with energy

$$E_{n_x n_y n_z} = \frac{\hbar^2 \pi^2}{2m}\left(\frac{n_x^2}{l_x^2} + \frac{n_y^2}{l_y^2} + \frac{n_z^3}{l_z^2}\right) = \frac{\hbar^2 k^2}{2m}$$

where $k^2 = |\vec{k}|^2$, & $\vec{k} \equiv (k_x, k_y, k_z)$

- note n_x, n_y, n_z are positive integers

- if we imagine a 3D k-space with planes @

$$k_x = \frac{\pi}{l_x}, \frac{2\pi}{l_x}, \ldots$$

$$k_y = \frac{\pi}{l_y}, \ldots \quad ; \quad k_z = \ldots$$

each intersection represents a stationary state, (k_x, k_y, k_z)

- each block of the grid takes up a volume (in k-space) of

$$\frac{\pi^3}{l_x l_y l_z} = \frac{\pi^3}{V}$$

where V is the volume of the solid

- because electrons are fermions, each additional atom gives say 1 electron each of which must have its own unique $\bar{k}$ in k-space

- again N is huge, so spacing between volumes is small (quasi-cont.)

- we recognize we are only operating in one octant of k-space! Why?

- the highest value of k, is k_F, F stands for "Fermi"

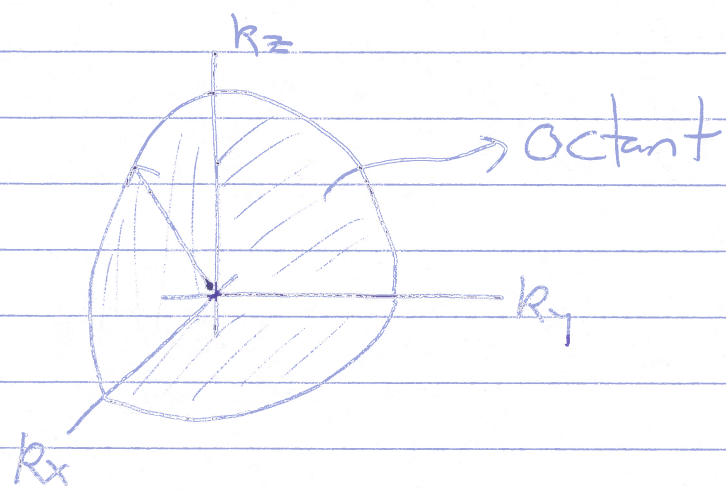
$$\frac{1}{8}\left(\frac{4}{3}\pi k_F^3\right) = \frac{Nq}{2}\left(\frac{\pi}{V}\right)^3$$

volume each state occupies

pairs of electrons (spin up + down)

$q \rightarrow$ # electrons/atom

$N \rightarrow$ # atoms



- think of k's as standing waves as in 1D box ((+) energy states)

$$\Rightarrow \quad k_F = (3\rho\pi^2)^{1/3}, \quad \rho \equiv \frac{Nq}{V}$$

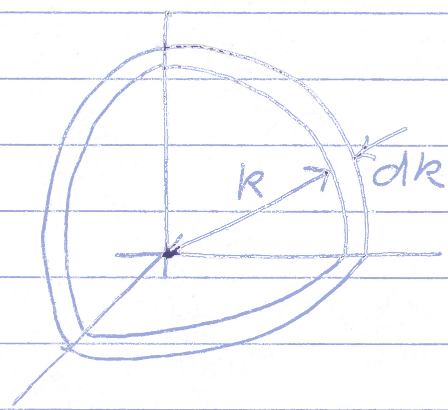
$\rho \rightarrow$ free electron density

- the boundary of sphere @ $k = k_F$ is called the Fermi surface

+ the Fermi energy

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

- How do we determine the total energy?
- one octant of a shell in k-space



- Volume of shell: $\frac{1}{8}\left(4\pi k^2\right)dk = dV$
- We know $\frac{N_q}{2}\left(\frac{\pi^3}{V}\right) = \frac{1}{8}\, 4\pi k^2 dk$

$$\Rightarrow N_q = \frac{V}{\pi^2} k^2 dk \longrightarrow$$

- each state in shell has energy (each with $\hbar^2 k^2/2m$)

$$dE = \underbrace{\frac{\hbar^2 k^2}{2m}}_{\substack{\text{energy}\\ \text{per } e^-}} \underbrace{\frac{V}{\pi^2} k^2 dk}_{\#\text{ in shell } (N_q)}$$

- so $E_{tot} = \frac{\hbar^2 V}{2m} \int_0^{k_F} k^4 dk = \frac{\hbar^2 k_F^5 V}{10\pi^2 m}$

$k_F = (3\pi^2 N_q / V)$

or $$E_{tot} = \frac{\hbar^2 (3\pi^2 N_q)^{5/3}}{10\pi^2 m} V^{-2/3}$$

- let's assume the box expands by dV

$$dE_{tot} = -\frac{2}{3} \frac{\hbar^2 (3\pi^2 N_q)^{5/3}}{10\pi^2 m} V^{-5/3}$$

- energy drops, + $dE_{tot} = \frac{-2}{3} E_{tot} \frac{dV}{V}$

$-dE_{tot} = +\frac{2}{3} E_{tot} \frac{dV}{V} = P\,dV$

- work done $dW = P\,dV$ by pressure

($PV = \frac{2}{3} U$ monatomic gas)

$$P = \frac{2}{3} \frac{E_{tot}}{V} = \frac{(3\pi^2)^{2/3} \hbar^2}{5m} \rho^{5/3}$$ "quantum pressure"