PHYS 4410

Quantum Mechanics 2

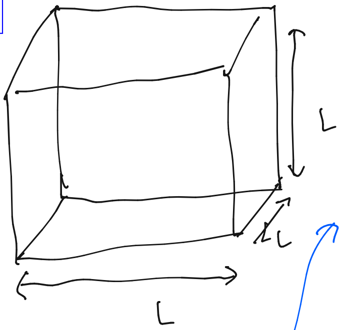
Spring 2023

Lecture 9

The Fermi gas

February 8

$\boxed{1}$



Consider $N \gg 1$ spin-$1/2$ fermions (electrons) in box.

$n_{x,y,z} = 1, 2, 3, \ldots$

"infinite square well"

$$H = \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{p_z^2}{2m} + V$$

$$H = \underbrace{H_x + H_y + H_z}_{\text{3 non-interacting particles}}$$

$$V = \begin{cases} 0 & \text{in box} \\ \infty & \text{outside} \end{cases}$$

in box: $0 \leq x, y, z \leq L$.

Single particle energy levels?

SoV: $$-\frac{\hbar^2}{2m}\left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right]\psi = E\psi$$

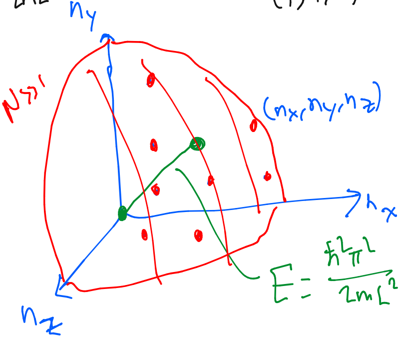
glue together 3 1d-square well:

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

$$\psi_{n_x n_y n_z} = \left(\frac{2}{L}\right)^{3/2} \sin\left(\frac{n_x \pi x}{L}\right) \sin\left(\frac{n_y \pi y}{L}\right) \sin\left(\frac{n_z \pi z}{L}\right)$$

$\boxed{2}$ Find ground state w/ $N \gg 1$ noninteracting electrons.

E	(n_x, n_y, n_z)	
$\frac{\hbar^2\pi^2}{2mL^2}(1+1+1)$	$(1,1,1)$	$\uparrow\downarrow$
	$(2,1,1)$	$\uparrow\downarrow$
$\frac{\hbar^2\pi^2}{2mL^2}(1+1+2^2)$	$(1,2,1)$	$\uparrow\downarrow$
	$(1,1,2)$	$\uparrow\downarrow$ $(N=8)$

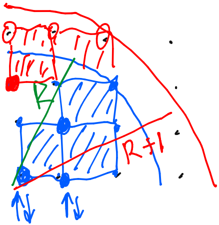


States inside sphere lowest energy.

$$E = \frac{\hbar^2\pi^2}{2mL^2}\underbrace{\left[n_x^2 + n_y^2 + n_z^2\right]}_{\text{dist}^2 \text{ from origin}}$$

$\boxed{3}$ Approx # of lattice points inside sphere.

radius $R=\sqrt{n_x^2+n_y^2+n_z^2}$



$\frac{N}{2}$ = # of points $\approx$ volume of $\frac{1}{8}$ sphere

$$= \frac{1}{8}\left(\frac{4\pi}{3}R^3\right) \rightsquigarrow R \approx \left(\frac{3N_{est}}{\pi}\right)^{1/3}$$

overcount:

exact # of points $\leq$

$$\frac{N_{over}}{2} = \frac{1}{8}\,\frac{4\pi}{3}(R+1)^3 = \frac{\pi}{6}\left[R^3+3R^2+\cancel{3R}+\cancel{1}\right]$$

$$= \frac{N_{est}}{2} + \frac{\pi}{2}R^2 = \frac{N_{est}}{2} + \underbrace{\frac{\pi}{2}\left(\frac{3N_{est}}{\pi}\right)^{2/3}}_{\text{small}}$$

relative error: $\dfrac{N_{est}^{2/3}}{N_{est}} \sim \dfrac{1}{N_{est}^{1/3}}$

4 single particle states:

$E < E_F$ occupied

$E > E_F$ unoccupied

Fermi energy

$$E_F = \frac{\hbar^2 \pi^2}{2mL^2} \underbrace{R^2}_{n_x^2 + n_y^2 + n_z^2} = \frac{\hbar^2 \pi^2}{2mL^2} \left(\frac{3N}{\pi} \right)^{2/3}$$

Total energy: $\uparrow\downarrow$

$$E_{tot} = \sum_{\substack{n_x, n_y, n_z \\ \text{occupied}}} 2 \cdot E_{n_x n_y n_z} \approx \int_0^R 2 \underbrace{dN_{\text{lattice}}}_{r \text{ to } r+dr} \overbrace{E(r)}^{\frac{\hbar^2}{2m} \frac{\pi^2}{L^2} \cdot r^2}$$

$\frac{1}{8}(4\pi r^2 dr)$

$$= \frac{\hbar^2 \pi^3}{mL^2} \frac{R^5}{10}$$

$\boxed{5}$ Re express in terms of density:

$$\underbrace{n = N/L^3}_{\frac{\#\text{ of } e^-}{\text{volume}}} \qquad \underbrace{\varepsilon = \frac{E_{tot}}{L^3}}_{\text{energy density.}}$$

Goal: ε depends only on n (not N or L)

$$\varepsilon = \frac{\frac{\hbar^2\pi^3}{10mL^2}R^5}{L^3} = \frac{\hbar^2\pi^3}{10mL^5}\left(\frac{3N}{\pi}\right)^{5/3} = \frac{\hbar^2\pi^3}{10m}\left(\frac{3}{\pi}\frac{N}{L^3}\right)^{5/3}$$

$$= \frac{\hbar^2\pi^3}{10m}\left(\frac{3n}{\pi}\right)^{5/3}$$

Fermi energy: $E_F = \frac{\hbar^2}{2m}\frac{\pi^2}{L^2}R^2 = \frac{\hbar^2\pi^2}{2m}\left(\frac{3n}{\pi}\right)^{2/3}$

"typical kin energy"

6

Copper: mass density $10^4\ kg/m^3$

$$m_{Cu} \sim 10^{-25}\ kg.$$

Each Cu atom contributes 1 mobile electron:

So $n \approx \dfrac{10^4\ kg/m^3}{10^{-25}\ kg} = 10^{29}\ e^-/m^3$

$E_F = ?$ $\hbar \sim 10^{-34}\ J\cdot s$, $m_{el} \sim 10^{-30}\ kg$

$$E_F \sim 10^{-18} - 10^{-19}\ J$$

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

room $T \sim 300\ K$

$$k_B T \sim 4 \times 10^{-21}\ J$$

$$\frac{E_F}{T} \sim 100 - 1000$$

$$\text{speed} \sim \sqrt{\frac{E_F}{m}} \sim \frac{c}{100 - 1000}$$