PHYS 418 Solutions Endterm Exam 2025

1) Label the states as suggested in the problem

$\{s_i\}$ where $s_i = \begin{cases} 0 & \text{site } i \text{ empty} \\ 1 & \text{one particle absorbed} \\ 2 & \text{two particles absorbed} \end{cases}$

Total number of particles in configuration $\{s_i\}$ is

$$N = \sum_i s_i$$

Define $\varepsilon(s_i) = \begin{cases} 0 & \text{site } i \text{ empty} \\ -\varepsilon_0 & \text{one particle absorbed} \\ -2\varepsilon_0+\Delta & \text{two particles absorbed} \end{cases}$

Total energy of system

$$E = \sum_i \varepsilon(s_i)$$

Grand canonical partition function is then

$$\mathcal{Z} = \sum_{\{s_i\}} e^{-\beta\left(E(\{s_i\}) - \mu N(\{s_i\})\right)}$$

$$= \sum_{\{s_i\}} e^{-\beta \sum_i \left(\varepsilon(s_i) - \mu s_i\right)}$$

$$= \sum_{s_1}\sum_{s_2}\cdots\sum_{s_{N_0}} \prod_i e^{-\beta(\varepsilon(s_i) - \mu s_i)}$$

$$\mathcal{Z} = \left[\sum_{s=0,1,2} e^{-\beta(\varepsilon(s) - \mu s)} \right]^{N_0}$$

$$= \Big[\underbrace{1}_{s=0} + \underbrace{e^{\beta(\varepsilon_0 + \mu)}}_{s=1} + \underbrace{e^{2\beta(\varepsilon_0 + \mu - \frac{\Delta}{2})}}_{s=2} \Big]^{N_0}$$

The Grand potential is then

$$\Phi = -k_B T \ln \mathcal{Z} = -k_B T N_0 \ln \left[1 + e^{\beta(\varepsilon_0+\mu)} + e^{2\beta(\varepsilon_0 + \mu - \frac{\Delta}{2})} \right].$$

Average number of particles is then

$$N = -\left(\frac{\partial \Phi}{\partial \mu}\right)_T = k_B T N_0 \frac{\left[\beta e^{\beta(\varepsilon_0+\mu)} + 2\beta e^{2\beta(\varepsilon_0+\mu-\frac{\Delta}{2})} \right]}{\left[1 + e^{\beta(\varepsilon_0+\mu)} + e^{2\beta(\varepsilon_0+\mu-\frac{\Delta}{2})} \right]}$$

$$\boxed{N = N_0 \frac{\left[e^{\beta(\varepsilon_0+\mu)} + 2 e^{2\beta(\varepsilon_0+\mu-\frac{\Delta}{2})} \right]}{\left[1 + e^{\beta(\varepsilon_0+\mu)} + e^{2\beta(\varepsilon_0+\mu-\frac{\Delta}{2})} \right]}}$$

Note: If $\Delta \to \infty$, so that the probability to have two particles absorbed on the same site $\to 0$, then we recover the result in notes 2-19.

Consider limits:

$T \to 0$ ie $\beta \to \infty$ provided $\varepsilon_0 + \mu > \frac{\Delta}{2}$ then

$e^{2\beta(\varepsilon_0+\mu-\frac{\Delta}{2})}$ dominates over $e^{\beta(\varepsilon_0+\mu)}$

$$N \to N_0 \frac{2e^{2\beta(\varepsilon_0+\mu-\frac{\Delta}{2})}}{e^{2\beta(\varepsilon_0+\mu-\frac{\Delta}{2})}} = 2N_0$$

ie all sites are doubly occupied. That is what is expected since it is the state of lowest energy.

$T \to \infty$ ie $\beta \to 0$

$$N \to N_0 \frac{[1+2]}{[1+1+1]} = N_0 \frac{3}{3} = N_0$$

That is what we expect since as $T \to \infty$, all possibilities, ie $s=0, s=1, s=2$, are equally likely. So

$$N = N_0 \sum_s p(s)\, s = N_0 \left(\frac{0+1+2}{3} \right) = N_0$$

2) a) To find the density of states $g(\varepsilon)$ we first find $G(\varepsilon)$, the number of single particle states per unit volume with energy $< \varepsilon$.

Because $\varepsilon(\vec{k})$ depends only on $|\vec{k}|$, all states with energy $< \varepsilon$ lie within a sphere of radius $k = \varepsilon/c\hbar$. Each allowed $\vec{k}$ within this sphere occupies a volume of k-space equal to $(\Delta k)^4 = (2\pi/L)^4$.
The volume of the sphere is $\frac{\pi^2}{2}k^4$.
Therefore

$$G(\varepsilon) = \frac{g_s \frac{\pi^2}{2} k^4}{V\ (2\pi/L)^4}$$ where $g_s = 2$ is the spin degeneracy

$$G(\varepsilon) = \frac{\pi^2 k^4}{(2\pi)^4} = \frac{k^4}{16\pi^2}$$

Then $$g(\varepsilon) = \frac{dG}{d\varepsilon} = \frac{dG}{dk}\frac{dk}{d\varepsilon} = \frac{4k^3}{16\pi^2}\frac{dk}{d\varepsilon}$$

$$k = \varepsilon/c\hbar \quad \text{so} \quad \frac{dk}{d\varepsilon} = \frac{1}{c\hbar}$$

$$\boxed{g(\varepsilon) = \frac{k^3}{4\pi^2 c\hbar} = \frac{\varepsilon^3}{4\pi^2 (c\hbar)^4}}$$

b) The Fermi energy is determined by

$$n = \int_0^{\varepsilon_F} d\varepsilon\, g(\varepsilon) = \frac{1}{4\pi^2 (c\hbar)^4} \int_0^{\varepsilon_F} d\varepsilon\, \varepsilon^3$$

$$= \frac{\varepsilon_F^4}{16\pi^2 (c\hbar)^4}$$

so $$\boxed{\varepsilon_F = \left[16\pi^2 (c\hbar)^4 n\right]^{1/4} = 2\sqrt{\pi}\, c\hbar\, n^{1/4}}$$

c) The total $\overbrace{\text{energy}}^{\text{at } T=0}$ per volume is given by

$$\frac{E}{V} = \int_0^{\varepsilon_F} d\varepsilon\, g(\varepsilon)\varepsilon = \frac{1}{4\pi^2 (c\hbar)^4} \int_0^{\varepsilon_F} d\varepsilon\, \varepsilon^4$$

$$\boxed{\frac{E}{V} = \frac{\varepsilon_F^5}{20\pi^2 (c\hbar)^4} = \frac{4}{5} n \varepsilon_F}$$

d) The pressure $p = -\left(\frac{\partial A}{\partial V}\right)_{T,N}$ at $T=0$ becomes

$$p = -\left(\frac{\partial E}{\partial V}\right)_{T,N}$$

since $A = E - TS$
$\to E$ as $T \to 0$

using result from (c)

$$p = -\frac{1}{20\pi^2 (c\hbar)^4} \left(\frac{\partial (V \varepsilon_F^5)}{\partial V}\right)_N$$

from (b)

$$\varepsilon_F = 2\sqrt{\pi}\, c\hbar\, m^{1/4} = 2\sqrt{\pi}\, c\hbar \left(\frac{N}{V}\right)^{1/4}$$

so

$$V \varepsilon_F^5 = (2\sqrt{\pi}\, c\hbar)^5 N^{5/4} V^{-1/4}$$

$$\left(\frac{\partial (V\varepsilon_F^5)}{\partial V}\right)_N = (2\sqrt{\pi}\, c\hbar)^5 N^{5/4} \left(-\frac{1}{4} V^{-1/4}\right) \frac{1}{V}$$

$$= -\frac{1}{4} \frac{V \varepsilon_F^5}{V} = -\frac{\varepsilon_F^5}{4}$$

so

$$p = \left(-\frac{1}{20\pi^2 (c\hbar)^4}\right)\left(-\frac{\varepsilon_F^5}{4}\right)$$

$$\boxed{p = \frac{1}{4} \frac{\varepsilon_F^5}{20\pi^2 (c\hbar)^4} = \frac{1}{4}\frac{E}{V}}$$

An easier way to get the above is:

from (c) $\frac{E}{V} = \frac{4}{5} m \varepsilon_F = \frac{4}{5}\frac{N}{V}\varepsilon_F$ so $E = \frac{4}{5} N \varepsilon_F$

$$p = -\left(\frac{\partial E}{\partial V}\right)_N = -\frac{4}{5} N \left(\frac{\partial \varepsilon_F}{\partial V}\right)_N$$

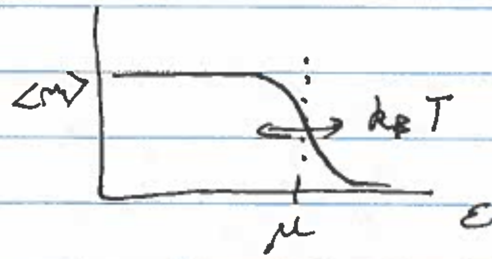
$$\varepsilon_F = 2\sqrt{\pi}\, c\hbar \left(\frac{N}{V}\right)^{1/4} \Rightarrow \left(\frac{\partial \varepsilon_F}{\partial V}\right)_N = -\frac{1}{4}\, 2\sqrt{\pi}\, c\hbar \left(\frac{N}{V}\right)^{1/4} \frac{1}{V}$$

$$= -\frac{1}{4}\frac{\varepsilon_F}{V}$$

so

$$p = \left(-\frac{4}{5} N\right)\left(-\frac{1}{4}\frac{\varepsilon_F}{V}\right) = \frac{1}{5} m \varepsilon_F = \frac{1}{4}\frac{E}{V}$$

e)



Just like for the 3D gas of fermions discussed in lecture, when a small T is turned on, only the particles within $k_B T$ of ε_F can be excited. The number of such particles per unit volume is thus

$$g(\varepsilon_F) k_B T$$

each such particle absorbs $\sim k_B T$ in energy, so the change in energy per unit volume from the ground state is

$$\Delta u \approx (g(\varepsilon_F) k_B T)(k_B T) = g(\varepsilon_F) k_B^2 T^2$$

the specific heat at constant volume, per unit volume, is then roughly

$$\boxed{c_v = \frac{C_v}{V} = \left(\frac{\partial \Delta u}{\partial T}\right)_V \approx 2 g(\varepsilon_F) k_B^2 T}$$

For our case $g(\varepsilon_F) = \dfrac{\varepsilon_F^3}{4\pi^2 (c\hbar)^4} = 4\dfrac{m}{\varepsilon_F}$

$$= \frac{\left[2\sqrt{\pi}\, c\hbar\, m^{1/4}\right]^3}{4\pi^2 (c\hbar)^4} = \frac{2}{\sqrt{\pi}} \frac{m^{3/4}}{(c\hbar)^3}$$

$$\boxed{C_V \approx \frac{4}{\sqrt{\pi}} \frac{m^{3/4}}{(c\hbar)^3} k_B^2 T = \frac{8m}{\varepsilon_F} k_B^2 T}$$

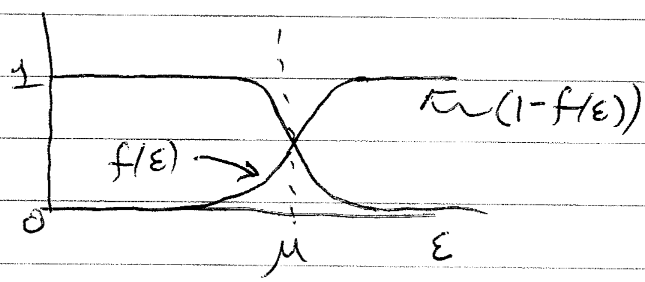
3) a) For fermions

$$\langle(\Delta N)^2\rangle = \langle N^2\rangle - \langle N\rangle^2 = \sum_i \left[\langle n_i^2\rangle - \langle n_i\rangle^2\right] = \sum_i \langle n_i\rangle(1-\langle n_i\rangle)$$

$$\langle n_i\rangle = f(\varepsilon_i) = \frac{1}{e^{\beta(\varepsilon_i-\mu)}+1}$$ Fermi occupation function

$$\Rightarrow \langle(\Delta N)^2\rangle = \sum_i \langle n_i\rangle(1-\langle n_i\rangle) = V\int_0^\infty d\varepsilon\, g(\varepsilon) f(\varepsilon)(1-f(\varepsilon))$$

$g(\varepsilon)$ is density of states



So the product $f(\varepsilon)(1-f(\varepsilon))$ is non zero only in an interval of width k_BT about chemical potential μ.

$$\Rightarrow V\int_0^\infty d\varepsilon\, g(\varepsilon) f(\varepsilon)(1-f(\varepsilon)) \approx V g(\mu) k_BT \approx V g(\varepsilon_F) k_BT$$

using $\mu \approx \varepsilon_F$ for Fermi gas at $T \ll T_F$ in degenerate limit

For free particles $g(\varepsilon_F) = \frac{3}{2}\frac{n}{\varepsilon_F}$ so

$$\langle(\Delta N)^2\rangle \simeq \frac{3}{2}\frac{V n k_BT}{\varepsilon_F} = \frac{3}{2}\frac{N k_BT}{\varepsilon_F} = \frac{3}{2}N\left(\frac{T}{T_F}\right)$$

Classically, we have $\langle (\Delta N)^2 \rangle = \langle N \rangle$

(see the solutions to problem 2 on Problem Set 6)

So for the fermion gas $\langle (\Delta N)^2 \rangle$ also $\sim N$ ~~f~~ but it is smaller than classical result by a factor (T/T_F).

Relative fluctuation is

$$\frac{\sqrt{(\Delta N)^2}}{\langle N \rangle} \simeq \frac{\sqrt{\frac{3}{2} N (T/T_F)}}{N} = \frac{\sqrt{\frac{3}{2}\frac{T}{T_F}}}{\sqrt{N}} \sim \frac{1}{\sqrt{N}}$$

$\to 0$ as $N \to \infty$ just like classically

b) For bosons at $T < T_c$ in Bose Einstein Condensed state.

$$\langle (\Delta N)^2 \rangle = \langle N^2 \rangle - \langle N \rangle^2 = \sum_i \left[\langle n_i^2 \rangle - \langle n_i \rangle^2 \right] = \sum_i \langle n_i \rangle \left(1 + \langle n_i \rangle \right)$$

$$= \langle N_0 \rangle \left(1 + \langle N_0 \rangle \right) + V \int_0^\infty d\varepsilon \, g(\varepsilon) \, h(\varepsilon) \left(1 + h(\varepsilon) \right)$$

where $h(\varepsilon) = \dfrac{1}{e^{\beta(\varepsilon - \mu)} - 1}$ is the Bose occupation function

N_0 is the occupation number of the ground state

For $T < T_c$, $z = 1$ or equivalently $\mu = 0$ and $\langle N_0 \rangle > 0$.

Look at contribution from ground state.

We have for total density $n = \frac{N}{V}$

$$n = \frac{N_0}{V} + \frac{g_{3/2}(1)}{\lambda^3}$$

$g_{3/2}(z)$ is Boson special function

T_c is when $N_0 = 0$ so $n = \dfrac{g_{3/2}(1)}{\lambda_c^3}$

$$\lambda \sim \frac{1}{\sqrt{T}} \Rightarrow n = C \, T_c^{3/2}$$

C some constant

$$\Rightarrow \frac{N_0}{V} = n - \frac{g_{3/2}(1)}{\lambda^3} = n - n\left(\frac{T}{T_c}\right)^{3/2} = n\left(1 - \left(\frac{T}{T_c}\right)^{3/2}\right)$$

$$N_0 = Vn\left(1 - \left(\frac{T}{T_c}\right)^{3/2}\right) = N\left(1 - \left(\frac{T}{T_c}\right)^{3/2}\right)$$

So the contribution to $\langle(\Delta N)^2\rangle$ from ground state is

$$\langle N_0\rangle\left(1+\langle N_0\rangle\right) = N\left(1-\left(\tfrac{T}{T_c}\right)^{3/2}\right)\left(1+N\left(1-\left(\tfrac{T}{T_c}\right)^{3/2}\right)\right)$$

to leading order in N the $\langle N_0\rangle^2$ term dominates

$$\sim N^2\left(1-\left(\tfrac{T}{T_c}\right)^{3/2}\right)^2$$

One can show that the contribution to $\langle(\Delta N)^2\rangle$ from the excited states do not grow this fast with N, so the ground state gives the leading term to $\langle(\Delta N)^2\rangle$

Relative fluctuation

$$\frac{\sqrt{\langle(\Delta N)^2\rangle}}{\langle N\rangle} \sim \frac{N\left(1-\left(\tfrac{T}{T_c}\right)^{3/2}\right)}{N} = \left(1-\left(\tfrac{T}{T_c}\right)^{3/2}\right) \sim O(1)$$

This does <u>NOT</u> vanish in the thermodynamic limit $N\to\infty$! This raises question whether or not we are justified in using the grand canonical ensemble for a bose condensed system $T<T_c$ when the total number of particles N is conserved.

See Ziff et al. Physics Reports <u>32</u>, 169 (1977)