Name: Huan Q. Bui

Course 8.333 Stat Mech 1

Prof Kardar

Test Final Exam

Date Wed 15 Dec 2021
9:00 am – 12:00pm

1. FREE FERMIONS

(a) Joint probability, fermions $\Rightarrow \eta = -1$

$$P(\{n_\ell\}) = \frac{1}{Q_{-1}} \prod_{\ell} \exp\left[-\beta\left(\varepsilon(\ell) - \mu\right) n_\ell\right]$$

$$= \frac{\prod_\ell \exp\left[-\beta\left(\varepsilon(\ell) - \mu\right) n_\ell\right]}{\prod_\ell \text{txp}\left[1 + \exp\left(\beta\mu - \beta\varepsilon(\ell)\right)\right]}$$

$$= \prod_\ell \exp\left[-\beta\left(\varepsilon(\ell) - \mu\right) n_\ell\right]\left[1 + \exp\left(\beta\mu - \beta\varepsilon(\ell)\right)\right]^{-1}$$

(b) Average occupation number

$$\langle n_\ell \rangle_{-1} = \frac{-\partial \ln Q_{-1}}{\partial(\beta \varepsilon(\ell))} = \frac{1}{z^{-1} e^{\beta \varepsilon(\ell)} + 1}$$

$$= \frac{1}{e^{\beta \varepsilon(\ell)} e^{-\beta\mu} + 1} = \frac{1}{e^{\beta(\varepsilon(\ell) - \mu)} + 1}$$

~~Answer in part (a); for a fixed ℓ~~

From here, can solve ...

$$\boxed{e^{\beta(\varepsilon(\ell)-\mu)} = \frac{1}{\langle n_\ell \rangle_{-1}} - 1} \Rightarrow e^{-\beta(\varepsilon(\ell)-\mu)} = \frac{\langle n_\ell \rangle_-}{1 - \langle n_\ell \rangle_-}$$

So

$$P(\{n_\ell\}_{-1}) = \prod_\ell \frac{e^{-\beta(\varepsilon(\ell)-\mu)n_\ell}}{1 + e^{\beta(\mu - \varepsilon(\ell))}} = \prod_\ell \frac{\left(\frac{\langle n_\ell \rangle_-}{1 - \langle n_\ell \rangle_-}\right)^{n_\ell}}{1 + \frac{\langle n_\ell \rangle_-}{1 - \langle n_\ell \rangle_-}}$$

$\hookrightarrow$ next page

$$\ldots = \prod_\ell \frac{\left[\langle n_\ell \rangle_- / (1 - \langle n_\ell \rangle_-)\right]^{n_\ell}}{1 + \dfrac{\langle n_\ell \rangle_-}{1 - \langle n_\ell \rangle_-}}$$

$$= \prod_\ell \frac{\left(\langle n_\ell \rangle_- / (1 - \langle n_\ell \rangle_-)\right)^{n_\ell}}{\dfrac{1}{1 - \langle n_\ell \rangle_-}}$$

$$= \boxed{\prod_\ell (1 - \langle n_\ell \rangle_-) \cdot \left[\frac{\langle n_\ell \rangle_-}{1 - \langle n_\ell \rangle_-}\right]^{n_\ell}}$$

or

$$= \boxed{\prod_\ell \langle n_\ell \rangle_-^{n_\ell} \left(1 - \langle n_\ell \rangle_-\right)^{+1 - n_\ell}}$$

(c) Entropy for dist? Max entropy?

Entropy is

$$\boxed{S = -k_B \sum_{n=1}^{M} p_n \ln p_n}$$

Max entropy is obtained when $p_n = 1/M$

$$\rightarrow \quad \boxed{S_{max} = k_B \ln M}$$

(d) Entropy for $P(\{n_\ell\}_-)$, zero temp limit

$\cancel{S = -k_B \sum_\ell}$

Occupation numbers of different one-particle states are independent, so the corresponding entropies are additive ...

$$\boxed{S = -k_B \sum_\ell \left\{ \langle n_\ell \rangle_- \ln \langle n_\ell \rangle_- + (1-\langle n_\ell \rangle_-) \ln (1-\langle n_\ell \rangle_-) \right\}}$$

This is just $-k_B \sum_\ell p_\ell \ln p_\ell + (1-p_\ell)\ln(1-p_\ell)$

since $n_\ell = 0$ or 1 ...

- in the zero-temperature limit,

all occupation numbers are either 0 (excited) ~~or 0~~ or 1 (ground)

So if $n_\ell = 1$, then

$$S = -k_B \sum_\ell 0 = 0$$

if $n_\ell = 0$ then

$$S = -k_B \sum_\ell 0 = 0$$

So in either case contribution to entropy is zero,

$\Rightarrow$ system at $T = 0$ has $\boxed{S = 0}$.

(e) Variance in total # of particles

& T = 0 behavior?

(For a fixed l have to calculate $\langle e^{ikn_l}\rangle$

$$\langle e^{ikn_l}\rangle = \underbrace{\frac{e^{-\beta(\varepsilon(l)-\mu)}}{1+e^{-\beta(\varepsilon(l)-\mu)}}\cdot e^{ik} + \frac{1}{1+e^{-\beta(\varepsilon(l)-\mu)}}}_{n_l=0}$$

$$= \frac{1+e^{-\beta(\varepsilon(l)-\mu)+ik}}{1+e^{-\beta(\varepsilon(l)-\mu)}}$$

→ now get cumulants ...

$$\ln\langle e^{ikn_l}\rangle = (ik)\frac{1}{1+e^{\beta(\varepsilon(l)-\mu)}} - \frac{k^2}{2}\boxed{\frac{e^{\beta(\varepsilon(l)-\mu)}}{(1+e^{\beta(\varepsilon(l)-\mu)})^2}} + \ldots$$

so $$\langle n_l^2\rangle_c = \frac{e^{\beta(\varepsilon(l)-\mu)}}{(1+e^{\beta(\varepsilon(l)-\mu)})^2}$$

$$\to \boxed{\langle N^2\rangle_c = \sum_l \langle n_l^2\rangle_c = \sum_l \frac{e^{\beta(\varepsilon(l)-\mu)}}{(1+e^{\beta(\varepsilon(l)-\mu)})^2}}$$

zero temp $\rightarrow$ $\beta \to \infty$

and $\varepsilon(\ell) < \mu = \varepsilon_F$

So

$$\langle N^2 \rangle_c \sim \sum_\ell \frac{e^{-\beta X}}{\left(1 + e^{-\beta X}\right)^2} \to \boxed{0}$$

So all fluctuations in total particle number vanishes at zero temprature.

2. NON DEGENERATE QUANTUM GAS

$n = N/V$, g , $\mathcal{H} = \sum_i p_i^2/2m$, also 3D

$n\lambda^3/g \ll 1 \Rightarrow$ non degenerate

$$\lambda = \frac{h}{\sqrt{2\pi m k_B T}}$$

(a) Density

$z = e^{\beta\mu}$

$$\boxed{n_\eta \equiv \frac{N_\eta}{V} = \frac{g}{\lambda^3} f_{3/2}^{\eta}(z)}$$

Pressure

$$\boxed{P_\eta = \frac{1}{\beta}\frac{g}{\lambda^3} f_{5/2}^{\eta}(z)}$$

(b) Find $P(n,T)$

To do this, follow procedure from textbook...

- First, we use the identity

$$f_m^\eta(z) \simeq \sum_{\alpha=1}^{\infty} \eta^{\alpha+1} \frac{z^\alpha}{\alpha^m} \quad \text{@ nondegenerate regime}$$

$$\Rightarrow \begin{cases} \dfrac{n_\eta \lambda^3}{g} = f_{3/2}^\eta(z) = z + \eta\, z^2/2^{3/2} + \dfrac{z^3}{3^{3/2}} + \eta \dfrac{z^4}{4^{3/2}} \\ \beta P_\eta \lambda^3/g = f_{5/2}^\eta(z) \simeq z + \eta\, z^2/2^{5/2} + \dfrac{z^3}{3^{5/2}} + \eta \dfrac{z^4}{4^{5/2}} \end{cases}$$

→ get z in terms of $n\lambda^3$...

$$z = \left(\frac{n_\eta \lambda^3}{g}\right) - \frac{\eta}{2^{3/2}}\left(\frac{n_\eta \lambda^3}{g}\right)^2 + \left(\frac{1}{4} - \frac{1}{3^{3/2}}\right)\left(\frac{n_\eta \lambda^3}{g}\right)^3$$

Put this back into P_η to find

$$\frac{\beta P_\eta \lambda^3}{g} = \left(\frac{n_\eta \lambda^3}{g}\right) - \frac{\eta}{2^{3/2}}\left(\frac{n_\eta \lambda^3}{g}\right)^2 + \left(\frac{1}{4} - \frac{1}{3^{3/2}}\right)\left(\frac{n_\eta \lambda^3}{g}\right)^3$$
$$+ \frac{\eta}{2^{5/2}}\left(\frac{n_\eta \lambda^3}{g}\right)^2 - \frac{1}{8}\left(\frac{n_\eta \lambda^3}{g}\right)^3 + \frac{1}{3^{5/2}}\left(\frac{n\lambda^3}{g}\right)^3 + \cdots$$

Ultimately we'll have

$$\boxed{P_\eta = n_\eta k_B T \left[1 \underbrace{- \frac{\eta}{2^{5/2}}\left(\frac{n_\eta \lambda^3}{g}\right)}_{\text{2nd virial coeff.}} + \left(\frac{1}{8} - \frac{2}{3^{5/2}}\right)\left(\frac{n_\eta \lambda^3}{g}\right)^2 + \cdots \right]}$$

(c) Expression for $\mathcal{E}_\eta = E/V$ up to n^2

Well ... we use the nice fact that

$$\mathcal{E}_\eta \equiv \frac{E_\eta}{V} = \frac{3}{2} P_\eta$$ to get

$$\boxed{\mathcal{E}_\eta = \cancel{\frac{3}{2}}\, n_\eta k_B T \left[\frac{3}{2} - \frac{3\eta}{2^{7/2}}\left(\frac{n_\eta \lambda^3}{g}\right) + \left(\frac{3}{16} - \frac{3}{3^{5/2}}\right)\left(\frac{n_\eta \lambda^3}{g}\right)^2 + \cdots \right]}$$

(d) <u>Heat capacity</u> C_V/N

From (c) we have

$$E = V\varepsilon_\eta = \left(\frac{N}{n_\eta}\right)\varepsilon_\eta = Nk_BT\left[\frac{3}{2} - \frac{3\eta}{2^{7/2}}\left(\frac{n\lambda^3}{g}\right) + \cdots\right]$$

so

$$\frac{C_V}{N} = \frac{1}{N}\frac{dE}{dT} = \ ?$$

$$\lambda = \frac{h}{\sqrt{2\pi m k_B T}} = \left(\frac{h}{\sqrt{2\pi m k_B}}\right)T^{-1/2} = \Omega T^{-1/2}$$

$$\Rightarrow E = Nk_BT\left(\frac{3}{2} - \frac{3\eta}{2^{7/2}}\frac{n}{g}\Omega^3 T^{-3/2} + \cdots\right).$$

$$\frac{1}{N}\frac{dE}{dT} = \frac{d}{dT}\left[k_BT\frac{3}{2} - k_B\frac{3\eta}{2^{7/2}}\frac{n}{g}\Omega^3 T^{-1/2} + \cdots\right]$$

$$= \left(\frac{3}{2}k_B\right) + \frac{k_B}{2}\frac{3\eta}{2^{7/2}}\cdot\frac{n}{g}\Omega^3 T^{-3/2} + \cdots$$

$$\boxed{\frac{C_V}{N} = \frac{3}{2}k_B + \frac{k_B}{2}\frac{3\eta}{2^{7/2}}\frac{n}{g}\underbrace{\left(\Omega^3 T^{-3/2}\right)}_{\lambda^3} + \cdots}$$

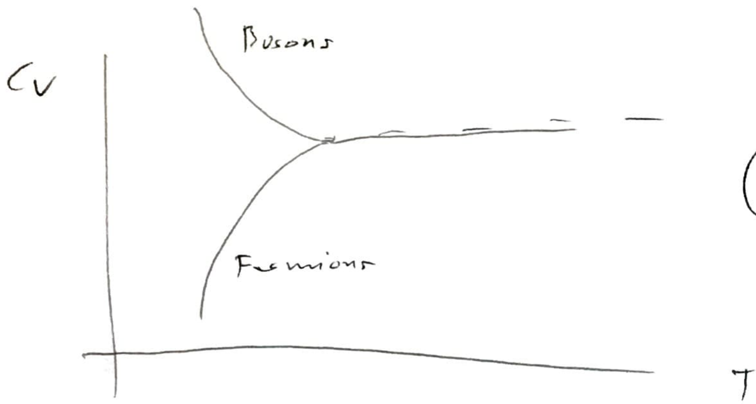
First QM correction

Since the first QM correction $\propto \eta$

we have that

$$\boxed{\frac{C_V}{N} \sim \frac{3}{2} k_B \left(1 + \frac{\eta}{2^{7/2}} \left(\frac{n\lambda^3}{g} \right) + \cdots \right)}$$

$\begin{cases} C_V \text{ increases for bosons} \\ C_V \text{ decreases for fermions} \end{cases}$



(non degenerate still)

(e) Calculate $\boxed{\alpha_p = \frac{1}{V} \frac{\partial V}{\partial T} \Big|_{P,N}}$

To do this ... use $V = N/n$ to get

$$\alpha_p = \left(\frac{n}{N} \right) \frac{\partial (N/n)}{\partial T} = n \frac{\partial (1/n)}{\partial T} = n \frac{\partial (1/n)}{\partial n} \frac{\partial n}{\partial T}$$

$$= n \cdot (-1) n^{-2} \frac{\partial n}{\partial T} = \frac{-1}{n} \frac{\partial n}{\partial T}$$

And now, we have

$n = \frac{g}{\lambda^3} f^{\eta}_{3/2}(z)$ so, ... next page

Need to find an expression for

$n(P,T)$ ...

To do this we'll need to find

z in terms of P.

$$z = \frac{\beta P \lambda^3}{g} - \eta \frac{z^2}{2^{5/2}} - \frac{z^3}{3^{5/2}}$$

$$= \left(\frac{\beta P \lambda^3}{g}\right) - \frac{\eta}{2^{5/2}}\left(\frac{\beta P \lambda^3}{g}\right)^2 - \cdots$$

Subbing this into

$$\frac{n\lambda^3}{g} = z + \eta \frac{z^2}{2^{3/2}} + \cdots$$

$$= \left(\frac{\beta P \lambda^3}{g}\right) + \frac{\eta}{\underset{\substack{\downarrow \\ 2^{5/2}}}{4\sqrt{2}}}\left(\frac{\beta P \lambda^3}{g}\right)^2$$

$$+ \left(\frac{1}{3^{5/2}} - \frac{1}{8}\right)\left(\frac{\beta P \lambda^3}{g}\right)^3 + \cdots$$

So

$$n = \beta P \left[1 + \frac{\eta}{2^{5/2}} \left(\frac{\beta P \lambda^3}{g} \right) + \left(\frac{1}{3^{5/2}} - \frac{1}{8} \right) \left(\frac{\beta P \lambda^3}{g} \right)^2 + \cdots \right]$$

$$= \frac{P}{k_B T} \left[1 + \frac{\eta}{2^{5/2}} \left(\frac{\beta P \lambda^3}{g} \right) + \cdots \right]$$

to first order correction only

Now

$$\alpha_P = -\frac{1}{n} \frac{\partial n}{\partial T} \equiv \text{(mathematica...)}$$

Let $\lambda = \dfrac{h}{\sqrt{2\pi m k_B T}} = \Omega T^{-1/2}$

Then

$$\alpha_P = \frac{-1}{n} \frac{\partial n}{\partial T}$$

I don't wanna simplify this ...

$$\boxed{\alpha_P \simeq \frac{7}{2T} - \frac{20 g k_B T^{3/2}}{8 g k_B T^{5/2} + \sqrt{2}\, \Omega^3 P \eta}}$$

(f) <u>what is C_p/N ?</u>

assuming that $C_P/C_V = \gamma = 5/3$

Then

$$\frac{C_P}{N} = \frac{5}{3}\frac{C_V}{N} = \frac{5}{2}k_B + \frac{5}{2}k_B\frac{\eta}{2^{7/2}}\frac{n}{g}\underbrace{\Omega^3 T^{-3/2}}_{\lambda^3}$$

$$= \frac{5}{2}k_B + \frac{5}{2}k_B\frac{\eta}{2^{7/2}}\left(\frac{n\lambda^3}{g}\right) + \cdots$$

$$= \frac{5}{2}k_B\left[1 + \frac{\eta}{2^{7/2}}\left(\frac{n\lambda^3}{g}\right) + \cdots\right]$$

$\uparrow$

first QM correction.

3. TRAP SITES IN A BOSE GAS

(a) Use standard Bose statistics

$$\cancel{\langle n_t \rangle = \frac{1}{\exp\left(\beta\left(\varepsilon(\vec{k})-\mu\right)\right)-1} = \frac{1}{e^{\beta\left[\frac{\hbar^2 k^2}{2m}-\mu\right]}-1}}$$

$$\boxed{\langle n_t \rangle = \frac{1}{e^{-\beta(\mu+w)}-1}}$$

trapped → not free so energy is $\varepsilon = -w$

(b) For $\langle n_g \rangle$ use standard Bose gas result ...

$$\langle n_g \rangle = \frac{g}{\lambda^3} f^+_{3/2}(z)$$

$$\boxed{\langle n_g \rangle = \frac{g\,(2\pi m k_B T)^{3/2}}{h^3} f^+_{3/2}\left(e^{\beta\mu}\right)}$$

→ $\boxed{?}$ Where does the density ρ come in???

(c) Find $n_c(T)$ for the onset of BEC

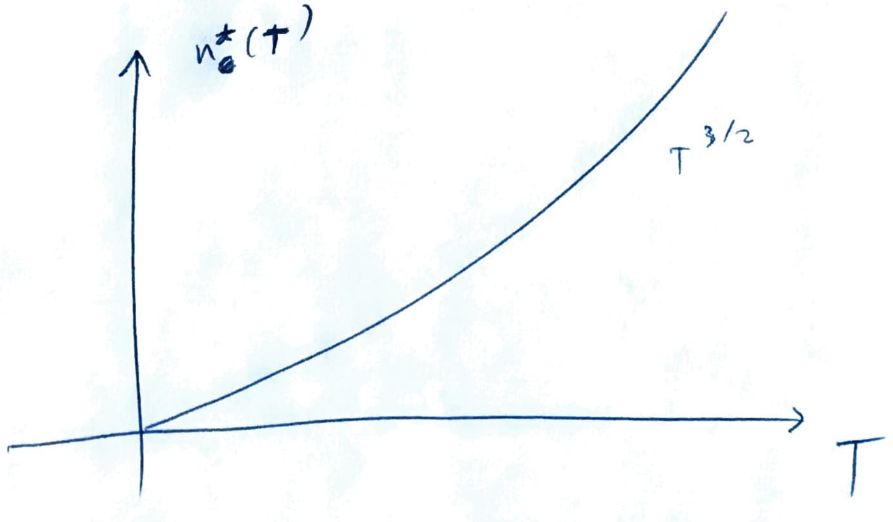
→ BEC occurs when $\mu = -\omega$ state accommodates a macroscopic fraction of particles ...

→ ~~$n_c(T)$ [illegible] by equating the [illegible] that at $\mu = -\omega$~~

$$\boxed{n_c^*(T) = \frac{g}{\lambda^3} f^+_{3/2}\big(\underbrace{e^{-\beta\omega}}_{\text{"}\beta w\text{"}}\big)}$$

For small w ... ~~same as $\beta \to 0$ ... $T \to \infty$~~

$f^+_{3/2}\big(\underbrace{e^{-\beta w}}_{\sim 1}\big) \sim \zeta_{3/2}$ so $n^*(T) \sim T^{3/2}$



(d) Total energy density in the BEC

The total energy density in the BEC comes ~~contributions~~ from the continuum states + particles in trapped states

① use usual results for energy density of an ideal Bose gas, but setting μ to its limiting value of $-w$ (continuum)

(First contribution)

$$\mathcal{E}_+ = \frac{3}{2} P_+ = \frac{3}{2\beta} \frac{g}{\lambda^3} f^+_{5/2}(z).$$

$$\boxed{\mathcal{E}_+ = \frac{3}{2\beta} \frac{g}{\lambda^3} f^+_{5/2}\left(e^{-\beta w}\right)}$$

multiply this by density of trap, ρ — basically how many trap sites there are

② Second contribution from trapped states

$$\mathcal{E}_{trap} = -\rho w \langle n_t \rangle = -\rho w \left(n - \langle n_g \rangle\right)$$

density not in ~~trap~~ continuum

$$= \boxed{-\rho w \left(n - \frac{g}{\lambda^3} f^+_{3/2}\left(e^{-\beta w}\right)\right)}$$

So, total energy density is

$$\boxed{\mathcal{E}_{tot} = -\rho w n + \frac{g}{\lambda^3}\left[\frac{3}{2\beta} f^+_{5/2}\left(e^{-\beta w}\right) + \rho w f^+_{3/2}\left(e^{-\beta w}\right)\right]}$$