Recap from L19

Ideal Gas for fermionic/bosonic systems in GCE

* $$Z_\eta = \prod_{\vec{k}, m_s} \left(1 - \eta e^{-\beta(\epsilon_k - \mu)}\right)^{-\eta} = e^{-\beta \Omega(T,\mu,V)}$$

* basic TD $$\Omega(T,\mu,V) = -PV = -\frac{1}{\beta} \log Z_\eta$$

$$\Downarrow$$

$$\frac{PV}{k_B T} = -\eta \sum_{\vec{k}, m_s} \log\left(1 - \eta e^{-\beta(\epsilon_k - \mu)}\right) = -\eta g \sum_{\vec{k}} \log(\quad)$$

* taking $\sum_{\vec{k}} \to V \int \frac{d^3k}{(2\pi)^3}$ etc + changing variables $x = \beta \frac{\hbar^2 k^2}{2m}$

$$\Downarrow$$

$$\therefore \quad \boxed{\begin{aligned} \beta P_\eta &= \frac{g}{\ell_Q^3} \cdot \frac{4}{3\sqrt{\pi}} \int_0^\infty \frac{dx\, x^{3/2}}{z^{-1} e^x - \eta} \\ n_\eta &= \frac{g}{\ell_Q^3} \cdot \frac{2}{\sqrt{\pi}} \int_0^\infty \frac{dx\, x^{1/2}}{z^{-1} e^x - \eta} \\ \beta \mathcal{E}_\eta &= \frac{g}{\ell_Q^3} \frac{2}{\sqrt{\pi}} \int_0^\infty \frac{dx\, x^{3/2}}{z^{-1} e^x - \eta} \end{aligned}}$$

$\Rightarrow$ suggests defining

$$\boxed{\begin{aligned} f_m^\eta(z) &\equiv \frac{1}{\Gamma(m)} \int_0^\infty \frac{dx\, x^{m-1}}{z^{-1} e^x - \eta} \\ \Gamma(m+1) &= m! \end{aligned}}$$

$$\Gamma(m) = \int dx\, x^{m-1} e^{-x}$$

$$\Gamma\left(\tfrac{3}{2}\right) = \frac{\sqrt{\pi}}{2} \qquad \text{etc...}$$

$$\Gamma\left(\tfrac{5}{2}\right) = \frac{3}{2} \frac{\sqrt{\pi}}{2}$$

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

$g = 2s+1$

etc...

$$\boxed{\begin{aligned} \beta P_\eta &= \frac{g}{\ell_Q^3} f_{5/2}^\eta(z) \qquad \mathcal{E}_\eta = \frac{3}{2} P_\eta \\ n_\eta &= \frac{g}{\ell_Q^3} f_{3/2}^\eta(z) \end{aligned}}$$

Low density/high T limit ($z \ll 1$)

$$\boxed{f_m^\eta(z \ll 1) = z + \eta \frac{z^2}{2^m} + \frac{z^3}{3^m} + \eta \frac{z^4}{4^m} + \cdots}$$

$\Downarrow$

Use to invert $n_\eta = \frac{g}{l_\alpha^3} f_{3/2}^\eta(z)$

$$\therefore \frac{n_\eta l_\alpha^3}{g} = f_{3/2}^\eta(z) \simeq z + \eta \frac{z^2}{2^{3/2}} + \frac{z^3}{3^{3/2}} + \cdots \qquad (A)$$

$$\frac{\beta P_\eta l_\alpha^3}{g} = f_{5/2}^\eta(z) \simeq z + \eta \frac{z^2}{2^{5/2}} + \frac{z^3}{3^{5/2}} + \cdots \qquad (B)$$

From (A), $z \simeq \frac{n_\eta l_\alpha^3}{g} - \eta \frac{z^2}{2^{3/2}} - \frac{z^3}{3^{3/2}} \cdots$

Can be solved iteratively/perturbatively since $z \ll 1$, then so is the "driving term $\frac{n_\eta l_\alpha^3}{g}$

$$\Rightarrow \quad e^{\beta\mu} = z \simeq \frac{n_\eta l_\alpha^3}{g} - \frac{\eta}{2^{3/2}} \left(\frac{n_\eta l_\alpha^3}{g}\right)^2 + \cdots$$

$\therefore$ substituting this expression for z $\Rightarrow$

$$\beta P_\eta = n_\eta \left[1 - \frac{\eta}{2^{5/2}} \left(\frac{n_\eta l_\alpha^3}{g} \right) + O\left(\frac{n_q l_\alpha^3}{g} \right)^2 \cdots \right]$$

Natural expansion parameter $= \dfrac{n_\eta l_\alpha^3}{g}$

* As in our CE treatment, $\dfrac{n l_\alpha^3}{g}$ tells us whether QM effects are important ($\dfrac{n l_\alpha^3}{g} \gtrsim 1$) or not ($\lesssim 1$)

* Unlike our CE treatment, the derivation of HOT is straightforward

Single Particle Density of States (DOS)

* It's useful to be able to convert sums over discrete QM sp states to integrals. We've already done this many times using $\frac{1}{V}\sum_{\vec{k}} \longrightarrow \int \frac{d^3\vec{k}}{(2\pi)^3}$ etc.

* Here though we want a more general formulation not just limited to $\vec{k}$-modes

e.g: $$\log Z_\eta = -\eta \sum_\alpha \log\left(1-\eta e^{-\beta(\epsilon_\alpha-\mu)}\right)$$

Sum over distinct QM s.p. states α

$$= -\eta \sum_\epsilon \Omega(\epsilon) \log\left(1-\eta e^{-\beta(\epsilon-\mu)}\right)$$

Sum over distinct QM energy levels ϵ w/ degeneracy $\Omega(\epsilon)$

* let $\Sigma(\epsilon) = \sum_\alpha \Theta(\epsilon-\epsilon_\alpha)$ = # of s.p. levels w/ energy $\leq \epsilon$

$$\therefore \Omega(\epsilon) = \lim_{\Delta\epsilon \ll \epsilon}\left[\Sigma(\epsilon+\Delta\epsilon) - \Sigma(\epsilon-\Delta\epsilon)\right]$$

$$\simeq \frac{d\Sigma(\epsilon)}{d\epsilon}\Delta\epsilon \quad + \mathcal{O}(\Delta\epsilon^2)$$

$$\equiv g(\epsilon)\,\Delta\epsilon \qquad g(\epsilon) = \frac{d\Sigma(\epsilon)}{d\epsilon} \quad \text{"Density of States"}$$

$$\therefore \log Z_\eta = -\eta \sum_\epsilon g(\epsilon)\,\Delta\epsilon \,\log\left(1-\eta e^{-\beta(\epsilon-\mu)}\right)$$

$\Delta\epsilon \to 0$

$$\boxed{\log Z_\eta = -\eta \int d\epsilon\, g(\epsilon) \log\left(1-\eta e^{-\beta(\epsilon-\mu)}\right) \qquad g(\epsilon) = \frac{d\Sigma(\epsilon)}{d\epsilon} \quad \text{s.p. DOS}}$$

More generally, $\displaystyle\sum_{\alpha}^{\text{sp. QM states}} f(\epsilon_\alpha) \longrightarrow \int_{\epsilon_{min}}^{\epsilon_{max}} d\epsilon\, g(\epsilon) f(\epsilon)$

(usually $\epsilon_{min}=0$, $\epsilon_{max}=\infty$)

Example: sp DOS for a D-dimensional free gas of spin s particles

quantized $\vec{k}_{\vec{n}} = \frac{2\pi}{L}(n_1, n_2, \ldots n_D)$

$$\epsilon(\vec{k}_{\vec{n}}; m_s) = \hbar^2\left(\frac{2\pi}{L}\right)^2 (n_1^2+n_2^2+\ldots+n_D^2)$$

$$\Sigma(\epsilon) = \sum_{n_1\ldots n_D}\sum_{m_s} \Theta\left(\epsilon - \epsilon(n_1,n_2,\ldots n_D; m_s)\right)$$

as before, $\displaystyle\sum_{n_i} \longrightarrow \frac{L}{2\pi}\int_{-\infty}^{\infty} dk_i = \frac{L}{2\pi\hbar}\int_{-\infty}^{\infty} dp_i$

$$\therefore \Sigma(\epsilon) \to \left(\frac{L}{2\pi\hbar}\right)^D \sum_{m_s} \int d^D p \; \Theta(\epsilon - \epsilon(\vec{p}; m_s))$$

* for $\epsilon(\vec{p}; m_s) = \epsilon(\vec{p})$ (degenerate wrt m_s)

$$\boxed{\Sigma(\epsilon) = g\left(\frac{L}{2\pi\hbar}\right)^D \int d^D\vec{p} \; \Theta(\epsilon - \epsilon(\vec{p})) \qquad g = 2S+1}$$

$$\therefore g(\epsilon) = \frac{d\Sigma(\epsilon)}{d\epsilon} = g\left(\frac{L}{2\pi\hbar}\right)^D \int d^D p \; \frac{d\Theta(\epsilon - \epsilon(p))}{d\epsilon}$$

*Use $\frac{d\Theta(x)}{dx} = \delta(x)$

$$\Rightarrow \boxed{g(\epsilon) = g\left(\frac{L}{2\pi\hbar}\right)^D \int d^D p \; \delta(\epsilon - \epsilon(p))}$$

Now use $\delta(f(x)) = \sum_i \frac{\delta(x - x_i)}{\left| \frac{\partial f}{\partial x}\Big|_{x_i} \right|}$

where $f(x_i) = 0$

$$\Rightarrow \delta(\epsilon - \epsilon(p)) = \sum_i \frac{\delta(p-p_i)}{\left|\frac{\partial \epsilon}{\partial p}\Big|_{p_i}\right|}$$ where $\epsilon(p_i) = \epsilon$ for all $p_i \geq 0$

(for $\epsilon(p) = \frac{p^2}{2m}$ or pc or $\sqrt{p^2+m^2}$, there is only 1 root ≥ 0 so $\delta(\epsilon - \epsilon(p)) = \frac{\delta(p-p_0)}{\left|\frac{\partial \epsilon}{\partial p}\Big|_{p_0}\right|}$)

* Moreover, $\epsilon(\vec{p}) = \epsilon(p)$ for the cases we care about so we can do the $\measuredangle$ integral

$$\therefore \boxed{\begin{aligned} g(\epsilon) &= g\left(\frac{L}{2\pi\hbar}\right)^D \oint d\Omega_D \int p^{D-1} dp \, \frac{\delta(p-p_0)}{\left|\frac{\partial \epsilon}{\partial p}\Big|_{p_0}\right|} \\ &= g\left(\frac{L}{2\pi\hbar}\right)^D \oint d\Omega_D \, \frac{p_0^{D-1}}{\frac{\partial \epsilon}{\partial p}\Big|_{p_0}} \end{aligned}}$$

ex: NR gas $\epsilon(p) = \frac{p^2}{2m}$, $\frac{\partial \epsilon}{\partial p} = \frac{p}{m}$

and p_0 is the positive root of $\frac{p_0^2}{2m} = \epsilon$

$\Rightarrow p_0 = \sqrt{2m\epsilon}$

$$\boxed{\therefore g_{NR,D}(\epsilon) = g\left(\frac{L}{2\pi\hbar}\right)^D \oint d\Omega_D \, p_0^{D-2} \, m}$$

$$\boxed{\therefore\; g_{NR,D}(E) = g\left(\frac{L}{2\pi\hbar}\right)^D \oint d\Omega_D \; p_0^{D-2}\, m}$$

$p_0 = \sqrt{2mE}$

$D=3$: $\oint d\Omega_D = 4\pi$

$$\therefore\; g_{NR,D=3}(E) = g\left(\frac{L}{2\pi\hbar}\right)^3 \cdot 4\pi \sqrt{2}\, m^{3/2}\sqrt{E}$$

$$\boxed{g_{NR,D=3}(E) = \frac{(2s+1)V}{\sqrt{2}\,\pi^2\hbar^3}\, m^{3/2}\sqrt{E}}$$

$D=2$: $\oint d\Omega_2 = 2\pi$

$$g_{NR,2}(E) = \frac{(2s+1)A}{(2\pi\hbar)^2}\cdot 2\pi m$$

$$\boxed{g_{NR,2}(E) = \frac{(2s+1)A}{2\pi\hbar^2}\, m}$$

e.g.: ultra relativistic $D = 3$ $\qquad \epsilon(p) = pc$

$$g(\epsilon) = g\left(\frac{L}{2\pi\hbar}\right)^D \oint d\Omega_D \, \frac{p_0^{D-1}}{\left.\frac{\partial \epsilon}{\partial p}\right|_{p_0}}$$

$$= (2s+1)\left(\frac{L}{2\pi\hbar}\right)^3 \cdot 4\pi \, \frac{p_0^2}{c} \qquad p_0 = \frac{\epsilon}{c}$$

$$\therefore \boxed{g_{\substack{\text{ultra}\\ \text{Rel}, D=3}}(\epsilon) = \frac{(2s+1)V}{2\pi^2(\hbar c)^3}\,\epsilon^2}$$

* anyhow, these DOS formulae allow us to rapidly generalize the expressions we used for $D=3$ NR case for the ideal gas,

e.g., $$n_\eta = \frac{g}{\ell_Q^3} f^\eta_{3/2}(z)$$

$$\Downarrow \; D=3 \text{ ultra rel.}$$

$$n_\eta = \frac{g\,(k_B T)^3}{\pi^2(\hbar c)^3} f^\eta_3(z)$$

* & they also let us generalize to other systems (e.g., particles in a harmonic trap)

Degenerate Fermi Gases (low T / high density limit)

* For the low density / high T limit studied last time, we were able to treat fermionic / bosonic systems at the same time.

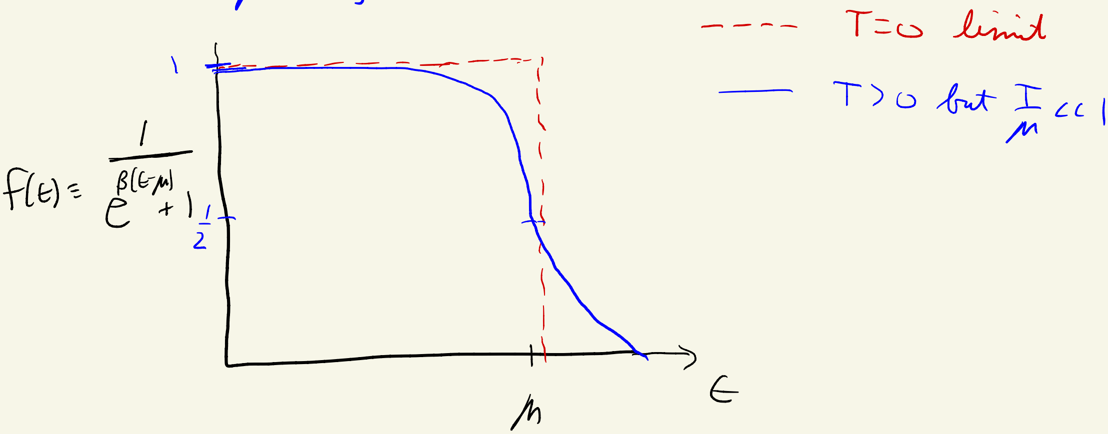
* This is because in this limit, ($z = e^{\beta\mu} \ll 1$), the FD/BE factors

$$\langle n(\epsilon)\rangle_\eta = \frac{1}{z^{-1}e^{\beta\epsilon} - \eta} \longrightarrow e^{-\beta(\epsilon-\mu)} = z e^{-\beta\epsilon} \ll 1$$

(i.e., they both approach the classical Maxwell-Boltzmann factors)

* In contrast, they behave wildly different in the opposite limit $z \gg 1$, which is where QM effects dominate

* Because of this, we have to treat Fermionic/Bosonic cases separately

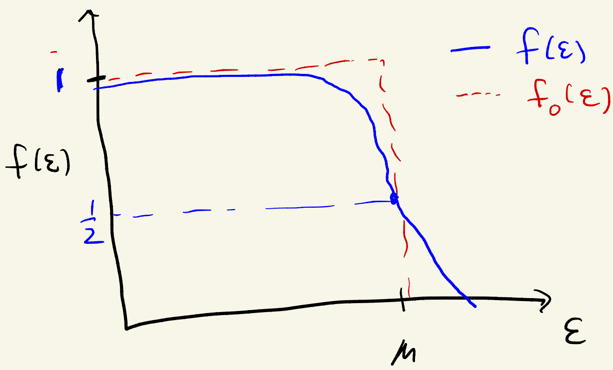


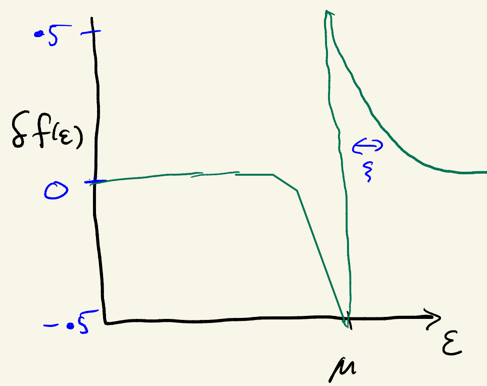
* let $f(\varepsilon) = \dfrac{1}{e^{\beta(\epsilon-\mu)}+1}$

$$f(\varepsilon) \underset{\substack{T\to 0 \\ (\beta\to\infty)}}{=} \Theta(\mu-\varepsilon) \equiv f_0$$

<u>Sommerfeld Expansion</u>: Idea is to write

$$f(\varepsilon) = f_0(\varepsilon) + \delta f(\varepsilon)$$





⇒ expand various quantities in $\delta f(\epsilon)$ to give corrections in powers of T/μ.

$$\delta f = \frac{1}{e^{\beta\xi}+1} - 1 \qquad \text{for } \xi = \epsilon - \mu < 0$$

$$= \frac{-e^{\beta\xi}}{e^{\beta\xi}+1} = -\frac{1}{1+e^{-\beta\xi}}$$

and $\delta f = \dfrac{1}{e^{\beta\xi}+1}$ for $\xi > 0$

$$\therefore n(\mu,T) = \frac{1}{V}\int_0^\infty d\epsilon\, g(\epsilon)\, f(\varepsilon)$$

$$= \frac{1}{V}\int_0^\infty d\varepsilon\, g(\epsilon)\left[f_0(\epsilon) + \delta f(\varepsilon)\right]$$

$$= \frac{1}{V}\int_0^\mu d\varepsilon\, g(\varepsilon) + \frac{1}{V}\int_0^\infty d\varepsilon\, g(\varepsilon)\,\delta f(\varepsilon)$$

let $\xi = \epsilon - \mu$

$$= n(\mu,0) + \frac{1}{V}\int_{-\mu}^{\infty} d\xi\, g(\mu+\xi)\,\delta f(\xi)$$

* Since $\delta f(\xi)$ sharply peaked near $\xi = 0$, extend the integral to $-\infty, \infty$

$$\Rightarrow n(\mu,T) \cong n(\mu,0) + \frac{1}{V}\int_{-\infty}^{\infty} d\xi \left(g(\mu) + \xi \left.\frac{dg}{d\epsilon}\right|_{\epsilon=\mu}\right)\delta f(\xi)$$

<u>Note</u>: $\delta f(\xi) = -\delta f(-\xi)$ (odd in ξ)

$\therefore$ Only need to keep even terms overall

$$\Rightarrow \delta n(\mu,T) = n(\mu,T) - n(\mu,0)$$

$$= \frac{1}{V}\int_{-\infty}^{\infty} d\xi \left[g(\mu) + \xi \frac{dg}{d\epsilon}\Big|_{\mu} \right] \delta f(\xi)$$

$$= \frac{1}{V}\int_{-\infty}^{\infty} d\xi\, \cancel{g(\mu)\,\delta f(\xi)} + \frac{1}{V}\int d\xi\, \xi \left(\frac{dg}{d\epsilon}\right)_{\mu} \delta f(\xi)$$

0 since δf odd

$$= \frac{2}{V} \frac{dg}{d\epsilon}\Big|_{\epsilon=\mu} I(\mu,T)$$

where $I(\mu,T) = \displaystyle\int_0^{\infty} d\xi\, \xi \frac{e^{-\beta\xi}}{1+e^{-\beta\xi}}$ let $x = \beta\xi$, $dx = \beta\, d\xi$

$$\boxed{I(\mu,T) = (k_B T)^2 \int_0^{\infty} dx\, \frac{x\, e^{-x}}{1+e^{-x}} = (k_B T)^2 \frac{\pi^2}{12}}$$

$$\therefore \boxed{\delta n(\mu,T) = \frac{\pi^2 (k_B T)^2}{6V} \left.\frac{dg}{d\epsilon}\right|_{\epsilon=\mu}}$$

Likewise for other quantities like energy/volume:

$$E = \int_0^\infty d\epsilon\, \epsilon g(\epsilon) f(\epsilon) \equiv \int_0^\infty d\epsilon\, \phi(\epsilon) f(\epsilon)$$

$$= \int_0^\infty d\epsilon\, \phi(\epsilon)\left(f_0(\epsilon) + \delta f(\epsilon)\right)$$

$$= \int_0^\mu d\epsilon\, \phi(\epsilon) + \int_0^\infty d\epsilon\, \phi(\epsilon)\, \delta f(\epsilon)$$

Same steps as before, use

1.) δf sharply peaked at $\epsilon \sim \mu$

2.) $\delta f(\xi) = -\delta f(-\xi)$ for $\xi = \epsilon - \mu$

⋮

$$\frac{E}{V} = \frac{E(T=0)}{V} + \mu\, \delta n + \frac{\pi^2 (k_B T)^2}{6V} g(\mu)$$

$$\Rightarrow \boxed{\frac{\delta E}{V} = \mu \frac{\pi^2 (k_B T)^2}{6V} \left.\frac{dg}{d\epsilon}\right|_{\mu} + \frac{\pi^2 (k_B T)^2}{6V} g(\mu)}$$