Recap of L17 (P+B 5.4–5.5)

* N-identical particle states w/proper symmetry under exchanges

$$\boxed{|\vec{k}_1 \vec{k}_2 \cdots\rangle_\eta = \frac{1}{\sqrt{N! \prod_{\vec{k}} n_{\vec{k}}!}} \sum_P \eta^P |\vec{k}_{P1} \vec{k}_{P2} \cdots)}$$

$$n_{\vec{k}} = \# \text{ of particles in sp state } \vec{k} = \begin{cases} 0,1 & \text{Fermions} \\ 0,1,2,3,\dots & \text{Bosons} \end{cases}$$

$$\sum_{\vec{k}} n_{\vec{k}} = N$$

$$|\vec{k}_1 \vec{k}_2 \cdots) = |\vec{k}_1\rangle \otimes |\vec{k}_2\rangle \otimes \cdots \otimes |\vec{k}_N\rangle$$

unsymmetrized product state

* Completeness relations for N-particles:

① $$\sum_{\vec{k}_1 \cdots \vec{k}_N} |\vec{k}_1 \vec{k}_2 \cdots)(\vec{k}_1 \vec{k}_2 \cdots | = \mathbb{1}$$ distinguishable particles

② $$\sum_{\vec{k}_1 \cdots \vec{k}_N}{}' |\vec{k}_1 \vec{k}_2 \cdots \rangle_\eta \, {}_\eta\langle \vec{k}_1 \vec{k}_2 \cdots | = \mathbb{1}$$ identical particles

restricted to physically distinct N-particle states

or unrestricted sum w/ correction factor

$$\mathbb{1} = \sum_{\vec{k}_1 \cdots \vec{k}_N} \left(\frac{\prod_{\vec{k}} n_{\vec{k}}!}{N!} \right) |\vec{k}_1 \vec{k}_2 \cdots \rangle_\eta \, {}_\eta\langle \vec{k}_1 \vec{k}_2 \cdots |$$

* used this to derive canonical ensemble density matrix

$$\hat{\rho} = \frac{e^{-\beta \hat{H}}}{Z_N} = \sum_n \frac{e^{-\beta E_n}}{Z_N} |E_n\rangle\langle E_n|$$

<u>ideal gas</u>: $\hat{H} = \sum_{a=1}^{N} \frac{-\hbar^2 \nabla_a^2}{2m}$

$$\Rightarrow |E_n\rangle = |\vec{k}_1 \vec{k}_2 \cdots\rangle_\eta$$

$$E_n = \sum_a \frac{\hbar^2 k_a^2}{2m}$$

$$\vec{k}_a = \frac{2\pi}{L}\left(n_x^{(a)}, n_y^{(a)}, n_z^{(a)}\right)$$

$$\Downarrow$$

after a very tedious derivation, we find:

$$\boxed{\langle \vec{x}_1 \vec{x}_2 \cdots | \hat{\rho} | \vec{x}_1' \vec{x}_2' \cdots\rangle_\eta = \frac{1}{Z_N N! \, \ell_Q^{3N}} \sum_P \eta^P e^{-\frac{\pi}{\ell_Q^2} \sum_a \left(\vec{x}_a - \vec{x}_{Pa}'\right)^2}}$$

$$\mathrm{Tr}\,\hat{\rho} = \int \prod_a d^3x_a \langle \vec{x}_1 \vec{x}_2 \cdots | \hat{\rho} | \vec{x}_1 \vec{x}_2 \cdots\rangle_\eta = 1$$

$$\Rightarrow \boxed{Z_N = \frac{1}{N! \, \ell_Q^{3N}} \int \prod_{a=1}^{N} d^3x_a \sum_P \eta^P e^{-\frac{\pi}{\ell_Q^2} \sum_a \left(\vec{x}_a - \vec{x}_{Pa}\right)^2}}$$

$$\Rightarrow \boxed{Z_N = \frac{1}{N!\,\ell_Q^{3N}} \int \prod_{a=1}^{N} d^3x_a \sum_P \eta^P e^{-\frac{\pi}{\ell_Q^2}\sum_a (\vec{x}_a - \vec{x}_{pa})^2}}$$

(1.) $\sum\limits_P \Rightarrow$ N! different terms corresponding to the possible permutations of N objects

*explicitly separating out the simplest permutation (i.e., the identity permutation $(1,2,3,..N) \rightarrow (1,2,3,..N)$):

$$\Rightarrow Z_N = \frac{1}{N!}\left[\underbrace{\frac{1}{\ell_Q^{3N}} V^N}_{\text{Gibbs Prescription}} + \underbrace{\int \prod_a^N d^3x_a \sum_{P \neq \text{identity}} \eta^P e^{-\frac{\pi}{\ell_Q^2}\sum_a (\vec{x}_a - \vec{x}_{pa})^2}}_{\text{Corrections to Gibbs Prescription}}\right]$$

(QM exchange effects)

<u>When can we ignore QM exchange effects?</u>

$$e^{-\frac{\pi}{\ell_Q^2}(\vec{x}_i - \vec{x}_j)^2} \ll 1 \quad \text{when} \quad \frac{(\vec{x}_i - \vec{x}_j)^2}{\ell_Q^2} \gg 1$$

typical $|\vec{x}_i - \vec{x}_j| \sim \left(\frac{V}{N}\right)^{1/3} = \frac{1}{n^{1/3}}$

$\therefore$ ignore when $\frac{1}{n^{1/3}} \gg \ell_Q$ or $\boxed{n\ell_Q^3 \ll 1}$

(dilute, high T)

* We can get a better understanding by writing

$$Z_N = \frac{1}{N!\, \ell_Q^{3N}} \int \prod_{a=1}^{N} d^3x_a \sum_P \eta^P f(\vec{x}_1 - \vec{x}_{P1}) f(\vec{x}_2 - \vec{x}_{P2}) \cdots f(\vec{x}_N - \vec{x}_{PN})$$

where $f(\vec{x}_a - \vec{x}_{Pa}) = e^{-\frac{\pi}{\ell_Q^2}(\vec{x}_a - \vec{x}_{Pa})^2}$

$\therefore f(\vec{x}_i - \vec{x}_j)$ sharply peaked for high T ($\ell_Q \to 0$) at $f(0)$

$$\Downarrow$$

$\therefore$ Dominant terms are those permutations with "the most" $f(0)$'s.

e.g., $N = 3$ (6 permutations to consider)

$123 \to 123$ identity perm $\Rightarrow$ $f(0)f(0)f(0)$ Leading Order (LO)

$\left.\begin{array}{l} 123 \to 213 \\ 123 \to 132 \\ 123 \to 321 \end{array}\right\}$ terms w/ 1 pair swapped $\Rightarrow$ $f(\vec{x}_{12})f(\vec{x}_{21})f(0)$, $f(0)f(\vec{x}_{23})f(\vec{x}_{32})$, $f(\vec{x}_{13})f(0)f(\vec{x}_{31})$ NLO

$\left.\begin{array}{l} 123 \to 312 \\ 123 \to 231 \end{array}\right\}$ term w/ 2 pairs swapped $\Rightarrow$ $f(\vec{x}_{13})f(\vec{x}_{21})f(\vec{x}_{32})$, $f(\vec{x}_{12})f(\vec{x}_{23})f(\vec{x}_{31})$ NNLO

LO $\gg$ NLO $\gg$ NNLO

at high T

* By re-labelling integration variables, you can convince yourself that the permutations consisting of 1 pair swapped all contribute equally, so

$$Z_N \approx \frac{1}{N!\, \ell_\alpha^{3N}} \int \prod_{a=1}^{N} d^3x_a \left\{ 1 + \underbrace{\frac{N(N-1)}{2}}_{\substack{\text{\# of pairs} \\ \text{in } N \text{ particles}}} \eta\, e^{-\frac{2\pi}{\ell_\alpha^2}(\vec{x}_1-\vec{x}_2)^2} + \text{2 pairs swapped} + \cdots \right\}$$

$$= \frac{1}{N!}\left(\frac{V}{\ell_\alpha^3}\right)^N \left[1 + \frac{N(N-1)}{2V}\eta \int d^3r_{12}\, e^{-\frac{2\pi r_{12}^2}{\ell_\alpha^2}} + \cdots \right]$$

* From this, you can calculate corrections to the ideal gas quantities (F, P, etc..) + find

1.) $\delta P > 0$ Fermions

$\delta P < 0$ Bosons

2.) $\delta F, \delta E > 0$ Fermions

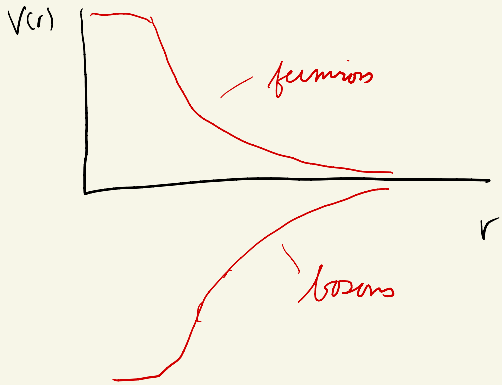
< 0 Bosons

Behaves as if there was a repulsive potential (fermions) or attractive potential (bosons) energy.

* In fact, you get the same Z, F, P, etc. if you treat the system classically (w/ Gibbs $\frac{1}{N!}$) with a potential

$$V(\vec{x}_i - \vec{x}_j) = -k_B T \log\left(1 + \eta e^{-2\pi r_{ij}^2/\ell_\alpha^2}\right)$$

$$\simeq -k_B T \eta e^{-2\pi r^2/\ell_\alpha^2}$$



* Evaluating the subsequent corrections involving more complicated permutations can be done, but it's a nightmare (see Feynman's Adv. Classics book on Stat. Mech.)

* A much easier way is to work in the Grand Canonical Ensemble (see 6.2-6.3)

* To see the way out of these complicated Canonical Ensemble calculations, note that each state

$|\vec{k}_1 \vec{k}_2 \cdots\rangle_\eta$ uniquely specified by providing a list of $\{n_{\vec{k}}\}$ for all $\vec{k}$ where $\sum_{\vec{k}} n_{\vec{k}} = N$

* More generally, for any s.p basis $|\alpha\rangle$ where $\alpha = 1, 2, \ldots M$, we uniquely specify the N-particle by a list of occupation #'s n_α $\alpha = 1, 2, \ldots M$ where $\sum_\alpha n_\alpha = N$.

"Occupation # Representation"

$$|\alpha_1 \alpha_2 \cdots\rangle_\eta \Longleftrightarrow |n_1 n_2 \cdots n_M\rangle_\eta = |\{n_\alpha\}\rangle_\eta$$

where $\sum_\alpha n_\alpha = N$

$$\mathbb{1}_N = \sum_{\vec{k}_1 \vec{k}_2 \cdots}{}' |\vec{k}_1 \vec{k}_2 \cdots\rangle_\eta \, {}_\eta\langle \vec{k}_1 \vec{k}_2 \cdots| = \sum_{\{n_{\vec{k}}\}}{}' |\{n_{\vec{k}}\}\rangle_\eta \, {}_\eta\langle\{n_{\vec{k}}\}|$$

Sum over all $n_{\vec{k}}$ values w/ constraint $\sum_{\vec{k}} n_{\vec{k}} = N$

* Now,

$$Z_N = \mathrm{Tr}\, e^{-\beta \hat{H}} = \sum_{\vec{k}_1 \vec{k}_2 \cdots}{}' e^{-\beta \sum_{a=1}^{N} \epsilon(\vec{k}_a)} = \sum_{\{n_{\vec{k}}\}}{}' e^{-\beta \sum_{\vec{k}} \epsilon(\vec{k}) n(\vec{k})}$$

Since $\sum_{a=1}^{N} \epsilon(\vec{k}_a) = \sum_{\vec{k}} \epsilon(\vec{k}) n(\vec{k})$

* In occupation # representation, we see that the canonical ensemble Z_N is complicated because we can't sum over $\{n_{\vec{k}}\}$ freely

i.e.,
$$\sum_{\{n_{\vec{k}}\}}{}' e^{-\beta \sum_{\vec{k}} \epsilon(\vec{k}) n(\vec{k})}$$
— constrained that $\sum_{\vec{k}} n_{\vec{k}} = N$

If we didn't have this constraint, the sums would be easy:

$$\sum_{\{n_{\vec{k}}\}} e^{-\beta \sum_{\vec{k}} \epsilon(\vec{k}) n(\vec{k})} = \sum_{\{n_{\vec{k}}\}} \prod_{\vec{k}} e^{-\beta \epsilon(\vec{k}) n(\vec{k})}$$

$$= \prod_{\vec{k}} \left(\sum_{n_{\vec{k}}} e^{-\beta \epsilon(\vec{k}) n(\vec{k})} \right)$$

$$= \prod_{\vec{k}} \left(1 + e^{-\beta \epsilon(\vec{k})} \right)$$ fermions since $n_{\vec{k}} = 0, 1$

$$= \prod_{\vec{k}} \frac{1}{1 - e^{-\beta \epsilon(\vec{k})}}$$ bosons since $n_{\vec{k}} = 0, 1, 2, \ldots$

But we do have this constraint (no way around it) in the Canonical Ensemble

$\Downarrow$

Suggests we go to GCE then!

N-identical particles in the GCE

* Still working w/ the ideal gas $\hat{H} = \sum_{a=1}^{N} \frac{-\hbar^2 \vec{\nabla}_a^2}{2m}$ for definiteness,

$$Z_\eta^{GCE}(T,\mu,V) = \sum_{N=0}^{\infty} \sum_{\vec{k}_1,\vec{k}_2\ldots}{}' e^{-\beta\left(\sum_{a=1}^{N} \frac{\hbar^2 k_a^2}{2m} - \mu N\right)}$$

* use

① $\sum_{\vec{k}_1,\vec{k}_2\ldots}{}' = \sum_{\{n_{\vec{k}}\}}{}'$

② $\sum_{a=1}^{N} \epsilon(\vec{k}_a) = \sum_{\vec{k}} \epsilon(\vec{k}) n_{\vec{k}}$

③ $\sum_{\vec{k}} n_{\vec{k}} = N$

$$\boxed{Z_\eta^{GCE} = \sum_{N=0}^{\infty} \sum_{\{n_{\vec{k}}\}}{}' e^{-\beta \sum_{\vec{k}} (\epsilon(\vec{k}) - \mu) n_{\vec{k}}}}$$

* Now, $\sum_{N=0}^{\infty} \sum_{\{n_{\vec{k}}\}}{}' = \sum_{\{n_{\vec{k}}\}}$

constrained to $\sum_{\vec{k}} n_{\vec{k}} = N$

unconstrained apart from

$n_{\vec{k}} = 0, 1, 2, 3, \ldots$ bosons

$n_{\vec{k}} = 0, 1$ fermions

$$\Rightarrow Z_\eta^{GCE} = \sum_{\{n_{\vec{k}}\}} e^{-\beta \sum_{\vec{k}} (\epsilon(\vec{k}) - \mu) n_{\vec{k}}}$$

$$= \sum_{\{n_k\}} \prod_{\vec{k}} e^{-\beta (\epsilon(\vec{k}) - \mu) n_{\vec{k}}}$$

$$= \prod_{\vec{k}} \left(\sum_{n_{\vec{k}}=0}^{1\,F,\ \infty\,B} e^{-\beta (\epsilon(\vec{k}) - \mu) n_{\vec{k}}} \right)$$

<u>Fermions</u>: $n_{\vec{k}} = 0, 1$ only

$$\Rightarrow \boxed{Z_F^{GCE} = \prod_{\vec{k}} \left(1 + e^{-\beta(\epsilon(\vec{k}) - \mu)} \right)}$$

<u>Bosons</u>: $n_{\vec{k}} = 0, 1, 2, \ldots \infty$

$$Z_B^{GCE} = \prod_{\vec{k}} \left(\sum_{n_{\vec{k}}=0}^{\infty} \left[e^{-\beta(\epsilon(\vec{k}) - \mu)} \right]^{n_{\vec{k}}} \right)$$

$$\boxed{Z_B^{GCE} = \prod_{\vec{k}} \left(\frac{1}{1 - e^{-\beta(\epsilon(\vec{k}) - \mu)}} \right)}$$

On combining into 1 single equation

$$\boxed{Z_\eta^{GCE} = \prod_{\vec{k}} \left(1-\eta e^{-\beta(\epsilon_{\vec{k}}-\mu)}\right)^{-\eta}}$$

* This is written for the ideal gas in momentum basis. (i.e., the s.p. states are $|\vec{k}\rangle$)

* In general, for N-noninteracting Fermions/Bosons

where $\hat{H} = \sum_{a=1}^{N} \hat{h}_a$

$$\hat{h}|\alpha\rangle = \epsilon_\alpha |\alpha\rangle$$

$$\Downarrow$$

$$E = \sum_\alpha \epsilon_\alpha n_\alpha$$

$$\Downarrow$$

$$\sum_\alpha n_\alpha = N$$

$$\therefore \boxed{Z_\eta^{GCE} = \prod_\alpha \left(1-\eta e^{-\beta(\epsilon_\alpha-\mu)}\right)^{-\eta}}$$

for general non-int. Bosons/Fermions

*Recall, in GCE

$$Z^{GCE} = e^{-\beta \Omega(T,\mu,V)} \qquad \Omega = \text{grand potential}$$

$$d\Omega = -S\,dT - P\,dV - N\,d\mu$$

$$\therefore \Omega_\eta = -\frac{1}{\beta} \log Z^{GCE}_\eta$$

$$= -\frac{1}{\beta} \log\left[\prod_{\vec{k}} \left(1 - \eta e^{-\beta(\epsilon_{\vec{k}} - \mu)}\right)^{-\eta}\right]$$

$$\boxed{\Omega_\eta = \frac{\eta}{\beta} \sum_{\vec{k}} \log\left(1 - \eta e^{-\beta(\epsilon_k - \mu)}\right)}$$

avg. particle # :

$$\langle N \rangle_\eta = -\left(\frac{\partial \Omega}{\partial \mu}\right)_{V,T}$$

$$= \frac{\cancel{-\eta}}{\cancel{\beta}} \sum_{\vec{k}} \frac{(\cancel{-\eta})(\cancel{\beta})\, e^{-\beta(\epsilon_k - \mu)}}{1 - \eta e^{-\beta(\epsilon_k - \mu)}}$$

$$\Rightarrow \boxed{\langle N\rangle_\eta = \sum_{\vec{k}} \frac{e^{-\beta(\epsilon_k-\mu)}}{1-\eta e^{-\beta(\epsilon_k-\mu)}} = \sum_{\vec{k}} \frac{1}{e^{\beta(\epsilon_k-\mu)}-\eta}}$$

<u>Note that</u>

$$\langle n_{\vec{q}}\rangle_\eta = \frac{1}{Z_\eta^{GCE}} \sum_{\{n_k\}} n_{\vec{q}}\, e^{-\beta\sum_{\vec{k}}(\epsilon_k-\mu)n_{\vec{k}}}$$

$$= \frac{1}{Z_\eta^{GCE}} \left(\frac{1}{\beta}\frac{\partial}{\partial\epsilon_{\vec{q}}}\right) \sum_{\{n_{\vec{k}}\}} e^{-\beta\sum_{\vec{k}}(\epsilon_{\vec{k}}-\mu)n_{\vec{k}}}$$

$$= \frac{1}{\beta}\frac{\partial}{\partial\epsilon_{\vec{q}}} \log Z_\eta^{GCE} = -\frac{\partial}{\partial\epsilon_{\vec{q}}}\Omega_\eta$$

$$\Downarrow$$

$$\boxed{\langle n_{\vec{q}}\rangle_\eta = \frac{1}{e^{\beta(\epsilon_q-\mu)}-\eta}}$$

$$\boxed{\therefore \langle N\rangle_\eta = \sum_{\vec{k}} \langle n_{\vec{k}}\rangle_\eta}$$

and $\langle E \rangle_\eta = \left\langle \sum_{\vec{k}} \epsilon_{\vec{k}} n_{\vec{k}} \right\rangle_\eta$

$$= \sum_{\vec{k}} \epsilon_{\vec{k}} \langle n_{\vec{k}} \rangle_\eta$$

$$\boxed{\langle E \rangle_\eta = \sum_{\vec{k}} \frac{\epsilon_{\vec{k}}}{e^{\beta(\epsilon_{\vec{k}}-\mu)} - \eta}}$$

* Generalization to other non-int fermion/boson systems

$$\mathcal{G}_\eta = \frac{\eta}{\beta} \sum_\alpha \log\left(1 - \eta\, e^{\beta(\epsilon_\alpha - \mu)}\right)$$

$$\langle N \rangle = \sum_\alpha \frac{1}{e^{\beta(\epsilon_\alpha-\mu)} - \eta}$$

$$\langle n_\alpha \rangle = \frac{1}{e^{\beta(\epsilon_\alpha-\mu)} - \eta}$$

$$\langle E \rangle = \sum_\alpha \frac{\epsilon_\alpha}{e^{\beta(\epsilon_\alpha-\mu)} - \eta}$$

$\vdots$

* Next time, will start our tour of applying these results to various fermion/boson systems.