Recap from L16 (see 5.4–5.5 of P+B)

Quantum Stat. Mech. $\langle O \rangle = \mathrm{Tr}\,\hat{\rho}\,\hat{O}$ $\quad \hat{\rho} = \hat{\rho}[\hat{H}]$ for equilibrium

$$[\hat{\rho}(\hat{H}), \hat{H}] = 0 \Rightarrow \hat{\rho} = \sum_n w_n |E_n\rangle\langle E_n|$$

$\Rightarrow$ "Correct" treatment of N identical particle systems, since we know that QM wf's have to be either totally symmetric (bosons) or anti-symmetric (fermions) under exchange of particle labels

i.e, $\hat{P}\,|\Psi(1,2,\ldots N)\rangle = |\Psi(P1,P2,\ldots PN)\rangle = \eta^P\,|\Psi(1,2,\ldots N)\rangle$

some permutation of $(1\,2\,3 \ldots N) \rightarrow (P1\,P2 \ldots PN)$

$$\eta = \begin{cases} +1 & \text{bosons} \\ -1 & \text{fermions} \end{cases}$$

P = # of pairwise exchanges to make $(1\,2\,3 \ldots N) \rightarrow (P1\,P2 \ldots PN)$

("even or odd" permutation)

1

3 2

e.g: $\hat{P}\,|\Psi(1,2,3)\rangle = \eta^P\,|\Psi(3,1,2)\rangle$

here $P=2$ since $123 \rightarrow 312$

in 2 pairwise exchanges

$123 \rightarrow 321 \rightarrow 312$

N non-interacting particles

$$\hat{H} = \sum_{a=1}^{N} \frac{-\hbar^2 \vec{\nabla}_a^2}{2m}$$

* If these are distinguishable, then

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

Notation: curved bra|ket to denote simple product state

$$\hat{H}\,|\vec{k}_1 \vec{k}_2 \cdots \vec{k}_N) = \left(\sum_{a=1}^{N} \frac{\hbar^2 k_a^2}{2m} \right) |\vec{k}_1 \vec{k}_2 \cdots \vec{k}_N)$$

* For identical particles, need to symmetrize (bosons) or antisymmetrize

$$|\vec{k}_1 \vec{k}_2 \cdots\rangle_- = \frac{1}{\sqrt{N!}} \sum_P (-1)^P \hat{P} |\vec{k}_1 \vec{k}_2 \cdots) \qquad \text{Fermions}$$

$$|\vec{k}_1 \vec{k}_2 \cdots\rangle_+ = \frac{1}{\sqrt{N! \prod_{\vec{k}} n_{\vec{k}}!}} \sum_P \hat{P} |\vec{k}_1 \vec{k}_2 \cdots) \qquad \text{Bosons}$$

$n_{\vec{k}}$ = # of particles in sp state $\vec{k}$

"Occupation #'s"

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

* Using $n_{\vec{k}} = 0, 1$ for fermions, and $0! = 1! = 1$, we can combine the 2 cases to

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

ex: $N=2$

$$|\vec{k}_1 \vec{k}_2\rangle_- = \frac{1}{\sqrt{2!}} \left(|\vec{k}_1 \vec{k}_2) - |\vec{k}_2 \vec{k}_1) \right) \qquad \vec{k}_1 \neq \vec{k}_2$$

$$|\vec{k}_1 \vec{k}_2\rangle_+ = \frac{1}{\sqrt{2!}} \left(|\vec{k}_1 \vec{k}_2) + |\vec{k}_2 \vec{k}_1) \right) \qquad \vec{k}_1 \neq \vec{k}_2$$

$$|\vec{k} \vec{k}\rangle_+ = \frac{1}{\sqrt{2!\,2!}} \left(|\vec{k} \vec{k}) + |\vec{k} \vec{k}) \right) = |\vec{k} \vec{k}) \qquad \vec{k}_1 = \vec{k}_2 = \vec{k}$$

Completeness relations

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

N distinguishable particles

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

N identical fermions or bosons

the Σ' means only sum over physically distinct states

e.g., for $N=2$, $\quad |\vec{k}_1 \vec{k}_2\rangle_\eta = \eta |\vec{k}_2 \vec{k}_1\rangle_\eta$

$\therefore$ $|\vec{k}_1 \vec{k}_2\rangle_\eta$ & $|\vec{k}_2 \vec{k}_1\rangle_\eta$ represent the same physical state (they only differ by a phase η), and so shouldn't be counted twice

$$\therefore \quad \mathbb{1}_{\text{2-fermions}} = \sum_{\vec{k}_1 \vec{k}_2}{}' |\vec{k}_1 \vec{k}_2\rangle_- \, {}_-\langle \vec{k}_1 \vec{k}_2|$$

$$= \sum_{\vec{k}_1 < \vec{k}_2} |\vec{k}_1 \vec{k}_2\rangle_- \, {}_-\langle \vec{k}_1 \vec{k}_2|$$

$$\mathbb{1}_{\text{2-bosons}} = \sum_{\vec{k}_1 \vec{k}_2}{}' |\vec{k}_1 \vec{k}_2\rangle_+ \, {}_+\langle \vec{k}_1 \vec{k}_2|$$

$$= \sum_{\vec{k}_1 < \vec{k}_2} |\vec{k}_1 \vec{k}_2\rangle_+ \, {}_+\langle \vec{k}_1 \vec{k}_2| + \sum_{\vec{k}} |\vec{k}\vec{k}\rangle_+ \, {}_+\langle \vec{k}\vec{k}|$$

* alternatively, we can use unrestricted completeness sums provided we insert a numerical factor that corrects for the overcounting of states that merely differ by permutation of labels

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

$$= \underbrace{\sum_{\vec{k}_1\vec{k}_2\cdots}}_{\text{unrestricted sums}} \underbrace{\left(\frac{\prod_{\vec{k}} n_{\vec{k}}!}{N!}\right)}_{\text{overcounting correction factor}} |\vec{k}_1\vec{k}_2\cdots\rangle_\eta \, {}_\eta\langle\vec{k}_1\vec{k}_2\cdots|$$

* See ch. 7 of Kardar for more details

* Now let's use this to derive $\hat{\rho}$ + Z_N for ideal gas of N-identical particles:

$$\hat{\rho} = \sum_{\{\vec{k}\}}{}' \frac{e^{-\beta\sum_{a=1}^{N}\epsilon(\vec{k}_a)}}{Z_N} |\vec{k}_1\vec{k}_2\cdots\rangle_\eta \, {}_\eta\langle\vec{k}_1\vec{k}_2\cdots|$$

$$= \sum_{\{\vec{k}\}}{}' \sum_{PP'} \frac{e^{-\beta\sum_a \epsilon(\vec{k}_a)}}{Z_N} \frac{\eta^P\eta^{P'}}{N!\prod_k n_{\vec{k}}!} |\vec{k}_{P_1}\vec{k}_{P_2}\cdots)(\vec{k}_{P'_1}\vec{k}_{P'_2}\cdots|$$

* Now taking matrix elements in $\vec{x}$-basis + going to an unrestricted sum $\sum_{\{k\}}{}' \to \sum_{\{\vec{k}\}} \frac{\prod_k n_k!}{N!}$

$$\Rightarrow \langle \vec{x}_1'\vec{x}_2'\cdots|\hat{\rho}|\vec{x}_1\vec{x}_2\cdots\rangle_\eta =$$

$$\sum_{\{\vec{k}\}} \frac{\cancel{\prod_{\vec{k}}} n_{\vec{k}}!}{N!} \sum_{P,P'} \frac{e^{-\beta\sum_a \epsilon(k_a)}}{Z_N} \frac{\eta^P\eta^{P'}}{N!\cancel{\prod_{\vec{k}} n_{\vec{k}}!}} \langle \vec{x}_1'\vec{x}_2'\cdots|\vec{k}_{P1}\vec{k}_{P2}\cdots\rangle\langle\vec{k}_{P'1}\vec{k}_{P'2}\cdots|\vec{x}_1\vec{x}_2\cdots\rangle$$

$$= \frac{1}{(N!)^2 Z_N}\sum_{\{\vec{k}\}}\sum_{P,P'} e^{-\beta\sum_{a=1}^{N}\epsilon(\vec{k}_a)}\eta^P\eta^{P'}\frac{1}{V^N}e^{-i\sum_{a=1}^{N}(\vec{k}_{P'a}\cdot\vec{x}_a-\vec{k}_{Pa}\cdot\vec{x}_a')}$$

use $\frac{1}{V}\sum_{\vec{k}} \longrightarrow \int\frac{d^3k}{(2\pi)^3}$

$$\Rightarrow \langle \vec{x}_1'\vec{x}_2'\cdots|\hat{\rho}|\vec{x}_1\vec{x}_2\cdots\rangle_\eta =$$

$$\frac{1}{(N!)^2 Z_N}\sum_{P,P'}\eta^P\eta^{P'}\int\left(\prod_{a=1}^{N}\frac{d^3\vec{k}_a}{(2\pi)^3}\right)e^{-\beta\sum_a\epsilon(\vec{k}_a)}\,e^{-i\sum_a(\vec{k}_{P'a}\cdot\vec{x}_a-\vec{k}_{Pa}\cdot\vec{x}_a')}$$

$$\sum_a \vec{k}_{P'a}\cdot\vec{x}_a = \sum_b \vec{k}_b\cdot\vec{x}_{P'^{-1}b}$$

let $P'a = b$

$a = P'^{-1}b$

and

$$\sum_a \vec{k}_{Pa}\cdot\vec{x}_a' = \sum_b \vec{k}_b\cdot\vec{x}'_{P^{-1}b}$$

$\therefore \langle \vec{x}_1' \vec{x}_2' \ldots | \hat{\rho} | \vec{x}_1 \vec{x}_2 \ldots \rangle =$

$$\frac{1}{(N!)^2 Z_N} \sum_{P,P'} \eta^P \eta^{P'} \int \left(\prod_{a=1}^{N} \frac{d^3 k_a}{(2\pi)^3} \right) e^{-\beta \sum_a \frac{\hbar^2 k_a^2}{2m}} e^{-i \sum_a \vec{k}_a \cdot (\vec{x}_{P'^{-1}a} - \vec{x}'_{P^{-1}a})}$$

* Now we see we can factor this N-fold integral into a product of N single integrals:

$$= \frac{1}{(N!)^2 Z_N} \sum_{P,P'} \eta^P \eta^{P'} \prod_{a=1}^{N} \left[\underbrace{\int \frac{d^3 k_a}{(2\pi)^3} e^{-\beta \frac{\hbar^2 k_a^2}{2m}} \cdot e^{-i \vec{k}_a \cdot (\vec{x}_{P'^{-1}a} - \vec{x}'_{P^{-1}a})}}_{} \right]$$

We did this integral in our N=1 calculation!

$$\parallel$$

$$\frac{1}{\ell_Q^3} e^{-\frac{\pi}{\ell_Q^2} \left(\vec{x}_{P'^{-1}a} - \vec{x}'_{P^{-1}a} \right)^2}$$

$$\ell_Q = \sqrt{\frac{2\pi\hbar^2}{m k_B T}}$$

* let $P'^{-1} a = b$

$$= \frac{1}{\ell_Q^{3N}} \frac{1}{(N!)^2 Z_N} \sum_{P,P'} \eta^P \eta^{P'} e^{-\frac{\pi}{\ell_Q^2} \sum_{b=1}^{N} \left(\vec{x}_b - \vec{x}'_{P^{-1}P'b} \right)^2}$$

let $P^{-1} P' = Q$ + use

1.) $\eta^P = \eta^{P^{-1}}$

2.) $\eta^P \eta^{P'} = \eta^{P^{-1}} \eta^{P'} = \eta^{P^{-1}P'} = \eta^Q$

3.) $\sum_{P,P'} \eta^P \eta^{P'} \ldots \longrightarrow \sum_{PQ} \eta^Q \ldots$

* whew! Running out of steam, but fortunately we are basically at the end:

$$\langle \vec{x}_1' \vec{x}_2' \ldots | \hat{\rho} | \vec{x}_1 \vec{x}_2 \ldots \rangle_\eta = \frac{1}{\ell_Q^{3N}} \frac{1}{Z_N (N!)^2} \sum_{P,Q} \eta^Q e^{-\frac{\pi}{\ell_Q^2} \sum_b (\vec{x}_b - \vec{x}_{Qb}')^2}$$

no P-dependence, so $\sum_P$ gives $N!$

$$\boxed{\langle \vec{x}_1' \vec{x}_2' \ldots | \hat{\rho} | \vec{x}_1 \vec{x}_2 \ldots \rangle_\eta = \frac{1}{\ell_Q^{3N} Z_N N!} \sum_Q \eta^Q e^{-\frac{\pi}{\ell_Q^2} \sum_b (\vec{x}_b - \vec{x}_{Qb}')^2}}$$

* get Z_N from $\mathrm{Tr}\,\hat{\rho} = 1 \Rightarrow$

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

as advertised last class.

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

$\Rightarrow$ The identity permutation $Qa = a$

$$\Rightarrow Z_N = \frac{1}{N!} \left[\frac{1}{\ell_Q^{3N}} V + \int \prod_{a=1}^N d^3x_a \sum_{Q \neq \text{identity}} \eta^Q e^{-\frac{\pi}{\ell_Q^2} \sum_a (\vec{x}_a - \vec{x}_{Qa})^2} \right]$$

$\Rightarrow$ We see the Gibbs ad-hoc prescription corresponds to throwing away the $(N!-1)$ terms in $\sum_\alpha \eta^\alpha \cdots$ that are not the identity permutation

* We can get a better understanding by writing

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

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

* for high T, $l_Q \to 0$, so the f's are sharply peaked at $f(0)$ + decay rapidly.

* estimate of when $f(\vec{x}_i-\vec{x}_j)$ small $\quad |\vec{x}_i-\vec{x}_j| \sim \left(\frac{V}{N}\right)^{1/3} = \frac{1}{n^{1/3}}$

$\Rightarrow$ so QM exchange effects NOT important when $\frac{1}{n^{1/3}} \gg l_Q \Rightarrow \boxed{n l_Q^3 \ll 1}$

$\therefore$ Dominant high T terms are those permutations with "the most" $f(0)$'s.

e.g., $N=3$

at high T:

leading order (LO)

$123 \to 123$ identity perm $\Rightarrow f(0)f(0)f(0)$

next-to-leading order (NLO)

$123 \to 213$
$123 \to 132$
$123 \to 321$
} terms w/ 1 pair swapped
$\Rightarrow f(\vec{x}_1-\vec{x}_2) f(\vec{x}_2-\vec{x}_1) f(0)$
$\Rightarrow f(0) f(\vec{x}_2-\vec{x}_3) f(\vec{x}_3-\vec{x}_2)$
$\Rightarrow f(\vec{x}_1-\vec{x}_3) f(0) f(\vec{x}_3-\vec{x}_1)$

$123 \to 312$
$123 \to 231$
} term w/ 2 pairs swapped
$\Rightarrow f(\vec{x}_1-\vec{x}_3) f(\vec{x}_2-\vec{x}_1) f(\vec{x}_3-\vec{x}_2)$
$\Rightarrow f(\vec{x}_1-\vec{x}_2) f(\vec{x}_2-\vec{x}_3) f(\vec{x}_3-\vec{x}_1)$

NNLO

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

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

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

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

1.) $\delta P > 0$ Fermions
$\delta P < 0$ Bosons

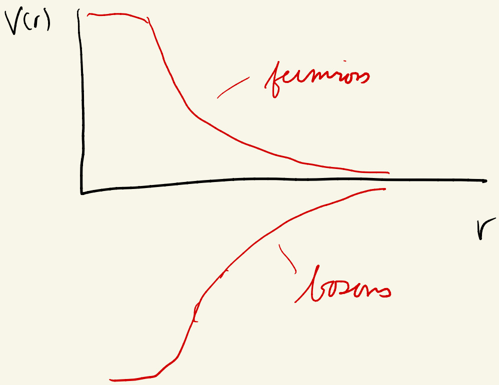
2.) $\delta F, \delta E > 0$ Fermions
< 0 Bosons

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 Lectures on SM)

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