Problem 1:

Before implementing anything, we need to think about what we want to do and how to do it.

We want to obtain U:

$$U = \frac{-\frac{\partial}{\partial\beta} \sum_n e^{-\beta \varepsilon_n}}{\sum_n e^{-\beta \varepsilon_n}} = -\frac{\partial}{\partial\beta} \log(Q(N,T))$$

According to Eq. (1) of the paper:

$$\underbrace{Q(N,T)}_{} = \frac{1}{N} \sum_{k=1}^{N} (\pm 1)^{k+1} S(k)\, Q(N-k,T)$$

note, the paper uses Z to denote the partition function

for the assignment: use the plus sign (we're dealing with bosons)

$\rightarrow$ to get $Q(2,T)$, we need to know $Q(1,T)$ and $Q(0,T)$;

to get $Q(3,T)$, we need to know $Q(2,T)$, $Q(1,T)$, $Q(0,T)$.

...

$Q(0,T) = 1$ by definition

to get $Q(1,T)$, we need to know

$\underbrace{S(1)}$ and $\underbrace{Q(0,T)}_{\text{by def.} = 1}$

$S(k)$ is defined in Eq. (2) of the paper

Strategy:

- work out analytical expression for $S(k)$; $k = 1, 2, \ldots$
- then calculate $Q(1,T), Q(2,T), \ldots, Q(N,T)$
- then calculate U/N for $N=10$

$$U = -\frac{\partial}{\partial \beta}\left(\log Q(N,T)\right)$$

$$= -\frac{\partial}{\partial(\beta \hbar\omega)}\left(\log Q(N,T)\right) \cdot \hbar\omega$$

$$\Rightarrow \underbrace{\frac{U}{N\hbar\omega}} = -\frac{1}{N}\frac{\partial}{\partial(\beta\hbar\omega)}\left(\log(Q(N,T))\right)$$

dimensionless internal energy per particle

Note: my Mathematica code takes the derivative with respect to $\beta\hbar\omega$.

As a warm-up exercise, let's look at $S(1)$:

$$S(1) = \sum_j e^{-\beta \varepsilon_j}$$

$k=1$

Sum over all single-particle states

For 3D HO: $\varepsilon_j \to \varepsilon_{n_x n_y n_z} = \left(n_x + n_y + n_z + \frac{3}{2}\right)\hbar\omega$

$$\Rightarrow S(1) = \left(\sum_{n_x=0}^{\infty} e^{-\beta\hbar\omega\left(n_x+\frac{1}{2}\right)}\right)^3$$

$$= e^{-\frac{3}{2}\beta\hbar\omega}\left(\underbrace{\sum_{n_x=0}^{\infty} e^{-n_x\beta\hbar\omega}}_{\sum_{n_x=0}^{\infty} x^{n_x}}\right)^3$$

$$\underbrace{\sum_{n_x=0}^{\infty} x^{n_x}}_{\frac{1}{1-x}} \qquad \text{where } x = e^{-\beta\hbar\omega}$$

$$= e^{-\frac{3}{2}\beta\hbar\omega}\left(\frac{1}{1-e^{-\beta\hbar\omega}}\right)^3$$

$$= e^{-\frac{3}{2}\beta\hbar\omega}\,\frac{e^{3\beta\hbar\omega}}{\left(e^{\beta\hbar\omega}-1\right)^3}$$

$$= \frac{e^{\frac{3}{2}\beta\hbar\omega}}{\left(e^{\beta\hbar\omega}-1\right)^3}$$

The premise (hope?) is that we can calculate / evaluate $S(k)$ in an analogous manner:

$$S(k) = \sum_j e^{-\beta k \varepsilon_j}$$

k is a fixed integer

$$= \sum_{n_x n_y n_z} e^{-\beta k \hbar\omega (n_x + n_y + n_z + \frac{3}{2})}$$

3D HO

$$= e^{-\frac{3}{2}\beta k \hbar\omega} \left(\sum_{n_x=0}^{\infty} e^{-\beta k \hbar\omega n_x} \right)^3$$

$$\sum_{n_x=0}^{\infty} x^{n_x} \quad \text{where } n_x = e^{-\beta k \hbar\omega}$$

$$= e^{-\frac{3}{2}\beta k \hbar\omega} \left(\frac{1}{1 - e^{-\beta k \hbar\omega}} \right)^3$$

$$S(k) = \frac{e^{\frac{3}{2}\beta k \hbar\omega}}{\left(e^{\beta k \hbar\omega} - 1\right)^3}$$

Define $\tilde{S}(k, \tilde{T}_{inv}) = \dfrac{e^{\frac{3}{2} k \tilde{T}_{inv}}}{\left(e^{k \tilde{T}_{inv}} - 1\right)^3}$, where $\tilde{T}_{inv} = \beta \hbar\omega$

In the Mathematica notebook:

$\tilde{S}(k, \tilde{T}_{inv}) \longrightarrow$ Stilde[k, Tinvscale]

$\tilde{T}_{inv} \longrightarrow$ Tinvscale

$Q(N, T) \longrightarrow$ Q[N, Tinvscale]

Uscale

↳ stands for $\frac{U}{\hbar\omega}$

To check the results, it is useful to remember:

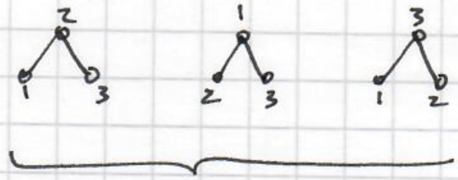
$$\frac{U}{N\hbar\omega} \longrightarrow \frac{3}{2} \quad \text{for } T \to 0$$

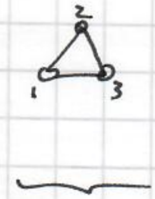
$$\frac{U}{N\hbar\omega} \longrightarrow \underbrace{3\beta\hbar\omega}_{\text{classical limit}} \quad \text{for } T \to \infty$$

My Mathematica notebook compares the results with both limits

Homework 8, Problem 2:

For three particles, we had two "classes" of configuration integrals





3 topologically equivalent "graphs"

3 particles, 2 lines

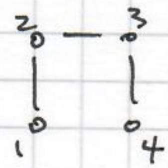
1 topologically equivalent graph

3 particles, 3 lines

How many graphs and classes do we have for four particles? 4 particles → require 3 lines

but can have 4 lines, 5 lines, or six lines

Start w/ 3 lines:

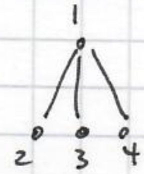


there are 12 graphs of this type

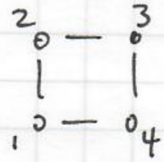
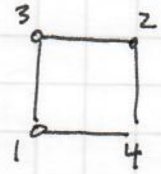
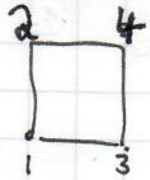
let's keep 1 and 4 but switch 2 and 3

then, we can 12, 13, 23, 24, 34 instead of 14 at the open ends

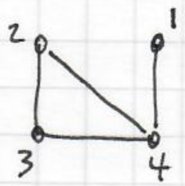
16 total



4 graphs

4 lines:   

<u>3</u> graphs

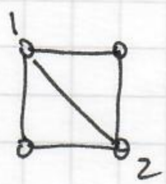


we can put 2 where 4 is and we can put 3 where for is → without moving 1, we have 3 graphs. but 1 can be replaced by 2, 3, 4.

⇒ <u>12</u> graphs

15 total

5 lines:



<u>6</u> graphs (can connect 12, 13, 14, 23, 24, 34)

6 total

6 lines  <u>1</u> graph

1 total

altogether: 16 + 15 + 6 + 1 = 38 graphs!

6 topologically different classes!

Homework 8 , Problem 3:

We want to calculate b_2 for the hard wall potential and for the square well potential ($a_2 = -b_2$):

$$a_2 = \frac{2\pi}{\lambda^3} \int_0^\infty \left(1 - e^{-\beta v(r)} \right) r^2 \, dr$$

(a)

$$v(r) = \begin{cases} \infty & \text{for } r < \sigma \\ 0 & \text{for } r > \sigma \end{cases}$$

$$\exp\left(-\beta v(r)\right) = \begin{cases} 0 & \text{for } r < \sigma \\ 1 & \text{for } r > \sigma \end{cases}$$

$$\Rightarrow \quad a_2 = \frac{2\pi}{\lambda^3} \int_0^\sigma r^2 \, dr$$

$$= + \frac{2\pi}{\lambda^3} \frac{1}{3} \sigma^3$$

$$= + \frac{2\pi \sigma^3}{3\lambda^3}$$

(b)

$$v(r) = \begin{cases} \infty & \text{for } r < \sigma \\ -\varepsilon & \text{for } \sigma < r < \alpha\sigma \\ 0 & \text{for } r > \alpha\sigma \end{cases} \qquad (\alpha \geq 1)$$

$$\exp\left(-\beta v(r)\right) = \begin{cases} 0 & r < \sigma \\ \exp(+\beta\varepsilon) & \sigma < r < \alpha\sigma \\ 1 & r > \alpha\sigma \end{cases}$$

$$\Rightarrow \quad a_2 = \frac{2\pi}{\lambda^3}\left[\int_0^{\sigma} r^2 dr + \int_{\sigma}^{\alpha\sigma}\left(1-e^{\beta\varepsilon}\right) r^2 dr\right]$$

$$= +\frac{2\pi}{\lambda^3}\left[\frac{1}{3}\sigma^3 - \frac{\sigma^3}{3}e^{\beta\varepsilon}\left(\alpha^3-1\right) + \frac{\sigma^3}{3}\left(\alpha^3-1\right)\right]$$

$$= +\frac{2\pi\sigma^3}{3\lambda^3}\left(1+\left(1-e^{\beta\varepsilon}\right)\left(\alpha^3-1\right)\right)$$

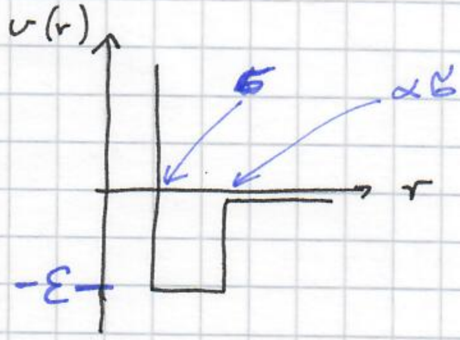
$$\Rightarrow \quad a_2^{SW} = a_2^{HS} \times \left(1 + \left(1-e^{\beta\varepsilon}\right)\left(\alpha^3-1\right)\right)$$

result
from part (a)

(c) Realistic parameters?

$$\sigma \approx \text{a few } \mathring{A} \qquad \alpha \approx 1.5 - 2$$

$$\varepsilon/k \approx \text{a few } 100\ K$$



We expect the description to work for temperatures around a few hundret Kelvin.

Homework 8, Problem 4:

We know $a_2, a_3, \dots$ $\quad x = t + a_2 t^2 + a_3 t^3 + a_4 t^4 + \dots$

(***)

We know $b_2, b_3, \dots$ $\quad y = t + b_2 t^2 + b_3 t^3 + b_4 t^4 + \dots$

(**)

We want to find A_2, A_3, A_4:

$$y = x + A_2 x^2 + A_3 x^3 + A_4 x^4 + \dots$$

(*)

Start with (*) and insert (**) on l.h.s. and (***) on r.h.s.:

$$t + b_2 t^2 + b_3 t^3 + b_4 t^4 + \dots$$

$$= t + a_2 t^2 + a_3 t^3 + a_4 t^4 + \dots$$

$$+ A_2 (t + a_2 t^2 + a_3 t^3 + a_4 t^4 + \dots)^2$$

$$+ A_3 (t + a_2 t^2 + a_3 t^3 + a_4 t^4 + \dots)^3$$

$$+ A_4 (t + a_2 t^2 + a_3 t^3 + a_4 t^4 + \dots)^4$$

$$+ \dots$$

Collect terms that have the same power of t:

$$(-b_2 + a_2 + A_2)\,t^2$$

$$+ (-b_3 + a_3 + 2a_2 A_2 + A_3)\,t^3$$

$$+ (-b_4 + a_4 + a_2^2 A_2 + 2a_3 A_2 + 3a_2 A_3 + A_4)\,t^4$$

$$+ (\ldots)\,t^5 + \ldots = 0$$

Each of the prefactors needs to vanish.

$$\Rightarrow \quad -b_2 + a_2 + A_2 = 0 \quad \rightarrow \boxed{A_2 = b_2 - a_2} \quad (1)$$

$$-b_3 + a_3 + 2a_2 A_2 + A_3 = 0$$

$$\rightarrow A_3 = b_3 - a_3 - 2a_2 A_2$$

$$\text{insert}(1) \rightarrow \; = b_3 - a_3 - 2a_2 (b_2 - a_2)$$

$$\boxed{A_3 = b_3 - a_3 - 2a_2 b_2 + 2a_2^2} \quad (2)$$

$$-b_4 + a_4 + a_2^2 A_2 + 2a_3 A_2 + 3a_2 A_3 + A_4 = 0$$

$$\rightarrow A_4 = b_4 - a_4 - a_2^2 A_2 - 2a_3 A_2 - 3a_2 A_3$$

insert ① and ②

$$= b_4 - a_4 - a_2^2(b_2 - a_2) - 2a_3(b_2 - a_2)$$

$$- 3a_2(b_3 - a_3 - 2a_2 b_2 + 2a_2^2)$$

$$= \underline{b_4} \; \underline{-a_4} \; - \underline{a_2^2 b_2} + \underline{a_2^3} - 2\underline{a_3} b_2 + 2\underline{a_2} a_3$$

$$- 3a_2 b_3 + 3\underline{a_2} a_3 + 6\underline{a_2^2} b_2 - 6\underline{a_2^3}$$

$$\boxed{\begin{aligned} A_4 = b_4 - a_4 + 5a_2^2 b_2 - 5a_2^3 - 2a_3 b_2 \\ + 5a_2 a_3 - 3a_2 b_3 \end{aligned}}$$