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Statistical Mechanics

PHYS 5163 Homework Assignment 9

Problems: {1, 2, 3, 4}

Due: April 29, 2022 at 6:00 PM

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Problem 1:

Fill in all the steps needed to get from Eqs. (1) and (2) to Eqs. (3), (4), and (6).

Taking equation (1) and (2) from the paper we have

$$N = \sum_{i=0}^{\infty} \frac{ze^{-\beta E_i}}{1 - ze^{-\beta E_i}} \tag{*}$$

We can take this expression and express it as

$$N = \sum_{i=0}^{\infty} \frac{ze^{-\beta E_i}}{1 - ze^{-\beta E_i}} = \sum_{i=0}^{\infty} \frac{ze^{-\beta E_i}}{1 - ze^{-\beta E_i}} \frac{e^{\beta E_i}}{e^{\beta E_i}} = \sum_{i=0}^{\infty} \frac{z}{e^{\beta E_i} - z}$$

We then expand about $z=0$

$$N = e^{-\beta E_1} z + e^{-2\beta E} z^2 + e^{-3\beta E} z^3 + e^{-4\beta E} z^4 + \ldots\ldots$$

This is of course

$$\boxed{N = \sum_{i=0}^{\infty} \sum_{j=1}^{\infty} z^j \exp(-j\beta E_i)}$$

Which is equation (3) in the paper. Taking the above expression we can write the energies for a 3D isotropic simple Harmonic oscillator

$$E_i = \left(n + \frac{3}{2}\right)\hbar\omega \implies n \doteq n_x + n_y + n_z$$

This means we can write equation 3 from the paper as $(E_i \to E_n)$

$$N = \sum_{j=1}^{\infty} z^j \sum_{n=0}^{\infty} \exp(-j\beta(n + 3/2)\hbar\omega)$$

$$= \sum_{j=1}^{\infty} z^j \sum_{n=0}^{\infty} \exp(-j\beta(n_x + \tfrac{1}{2} + n_y + \tfrac{1}{2} + n_z + \tfrac{1}{2})\hbar\omega)$$

$$= \sum_{j=1}^{\infty} z^j \sum_{n=0}^{\infty} \exp(-j\beta(n_x + 1/2)\hbar\omega) \exp(-j\beta(n_y + 1/2)\hbar\omega) \exp(-j\beta(n_z + 1/2)\hbar\omega)$$

Problem 1: Continued

we can then take the last expression to say

$$N = \sum_{j=1}^{\infty} z^j \sum_{n=0}^{\infty} \exp(-j)^3 \exp(-\beta(n_x+1/2)\hbar w)\exp(-\beta(n_y+1/2)\hbar w)\exp(-\beta(n_z+1/2)\hbar w)$$

Where we make the distinction that the above can be written with the separation between states (i.e not $\hbar w/2$) but $\hbar w$. Therefore we have

$$N = \sum_{j=1}^{\infty} z^j \exp(-j)^3 \left(\sum_{n_x=0}^{\infty} \exp(-\beta n_x \hbar w)\sum_{n_y=0}^{\infty} \exp(-\beta n_y \hbar w)\sum_{n_z=0}^{\infty} \exp(-\beta n_z \hbar w)\right)$$

we can then say with $n_x, n_y, n_z \doteq n$, we can then say

$$N = \sum_{j=1}^{\infty} z^j \left(\sum_{n=0}^{\infty} \exp(-j\beta n \hbar w)\right)^3$$

we can then re-write the above as

$$\sum_{n=0}^{\infty} x^n = \frac{1}{1-x} \Rightarrow \sum_{n=0}^{\infty} x^{mn} = \frac{1}{1-x^m} \quad \therefore \quad w/\ x \doteq \exp(-\beta n \hbar w)$$

using this we can say

$$\left(\sum_{n=0}^{\infty} \exp(-j\beta n \hbar w)\right)^3 = \frac{1}{1-\exp(-j\beta n\hbar w)^3} \quad w/\ x = \exp(-\beta \hbar w)$$

we can then finally say

$$\boxed{N = \sum_{j=1}^{\infty} \frac{z^j}{(1-x^j)^3}}$$

Which is exactly equation (4) in the paper. Before you apply the High temperature expansion we re-write equation (4) as

$$N = \frac{z}{1-z} + \sum_{j=1}^{\infty} z^j \left(\frac{1}{(1-x^j)^3} - 1\right) \qquad (**)$$

Problem 1: Continued

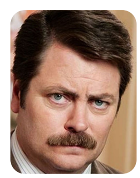
we then substitute $x = \exp(-\beta\hbar\omega)$. We then wish to expand in the high temperature limit, i.e $k_B T \gg \hbar\omega$. We can go on to say

$$1 \gg \frac{\hbar\omega}{k_B T}$$

we then begin expanding (**)

$$N\Big|_{x=\exp(-\beta\hbar\omega)} = \frac{z}{1-z} + \sum_{j=1}^{\infty} z^j \left(\frac{1}{(1-\exp(-\beta\hbar\omega)^j)^3} - 1 \right)$$

Where we make the variable substitution

Let $\beta\hbar\omega \longrightarrow$ 

Where we perform an expansion for the high temp limit

$\Big(1 / (1-\exp(-$  $)^j)^3 - 1 \Big) \longrightarrow 0$

Because in the high temperature limit we must only have the first term in (**), ∴

$= 1/(j^3$  $^3) + \frac{3}{2}\, 1/(j^2$  $^2) + \cdots$

We then substitute back in  and $\beta = 1/k_B T$

$$= \frac{1}{j^3(\beta\hbar\omega)^3} + \frac{3}{2}\frac{1}{j^2(\beta\hbar\omega)^2} + \cdots$$

This then means the above becomes equation (6) in the paper

$$\boxed{N = \frac{z}{1-z} + \sum_{j=1}^{\infty} \frac{z^j}{j^3}\left(\frac{k_B T}{\hbar\omega}\right)^3 + \frac{3}{2}\sum_{j=1}^{\infty}\frac{z^j}{j^2}\left(\frac{k_B T}{\hbar\omega}\right)}$$

Problem 1: Review

Procedure:

- – Begin by taking equations (1) and (2) from the paper and the expanding the result about $z = 0$
  – Take the previous result and then substitute in $\mathbf{n} = n_x + n_y + n_z$ to eventually get to a point when N is

$$N = \sum_{j=1}^{\infty} z^j \Big(\sum_{n=0}^{\infty} \exp\left(-j\beta n\hbar\omega\right) \Big)^3$$

  – Use

$$\sum_{n=0}^{\infty} x^{mn} = \frac{1}{1 - x^m}$$

  on the previous expression to show equation (4)
  – Proceed to apply a high temperature expansion where one expands

$$(1 - \exp\left(\xi\right)^j)^3$$

  about $\xi = 0$ and then substitute this result back into the modified expression for equation (4)
  – Using the result after the expansion one can derive equation (6)

Key Concepts:

- – The purpose of this problem is to show us how one gets specific results found in a paper
  – We use various mathematical principles to show how we can go between equations in the paper

Variations:

- – We could be given a different paper to derive the results
    * This of course is very broad but is essentially the biggest way this problem can change
  – We could be asked to derive other equations
    * This would require us to use different mathematical rules to go between equations but the same broad idea would be used

Problem 2:

What is being discussed in Eqs. (5), (7), and (8)? To address this question perform calculations as needed and provide a discussion. Be as specific as you can when converting the infinite sum to an integral.

Note that the density of state expression $\rho(E)$ given in the paper contains a typo. The units should be 1/energy; thus,

$$\rho(E) = \frac{\left(\frac{E}{\hbar\omega}\right)^2}{2\hbar\omega}. \tag{1}$$

To begin, equation (5) in the paper is discussing the critical temperature at which $N \to \infty$ and our ground state is not occupied.

Equation (7) is the 3D treatment of the Bose Einstein Condensates in a Harmonic potential.

Equation (8) can be found by integrating and evaluating equation (7) and this is done like

$$N - N_0 = \sum_{j=1}^{\infty} z^j \frac{1}{2(\hbar\omega)^3} \int_0^\infty E^2 \exp(-j\beta E)\, dE$$

Where to solve this we start integrating by parts

$$u = E^2,\ du = 2E\, du,\ dv = \exp(-j\beta E),\ v = \frac{\exp(-j\beta E)}{-j\beta}$$

$$\Rightarrow \int_0^\infty E^2 \exp(-j\beta E)\, dE = \cancel{\frac{-E^2\exp(-j\beta E)}{j\beta}}^{\,0}\Bigg|_0^\infty + \frac{2}{j\beta}\int_0^\infty E\exp(-j\beta E)\, dE$$

$$a = E,\ da = dE,\ dB = \exp(-j\beta E),\ B = \frac{\exp(-j\beta E)}{-jB}$$

$$\Rightarrow \frac{2}{j\beta}\int_0^\infty E\exp(-j\beta E)\, dE = \frac{2}{j\beta}\left(\cancel{\frac{E\exp(-j\beta E)}{-jB}}^{\,0}\Bigg|_0^\infty + \frac{1}{jB}\int_0^\infty \exp(-j\beta E)\, dE\right)$$

$$= \frac{2}{j\beta}\left(-\frac{1}{(j\beta)^2}\exp(-j\beta E)\Bigg|_0^\infty\right) = \frac{2}{(j\beta)^3}$$

We can then plug this result back into the result in the paper

Problem 2: Continued

$$\sum_{j=1}^{\infty} z^j \frac{1}{2(\hbar\omega)^3}\int_0^{\infty} E^2 \exp(-j\beta E)\, dE = \sum_{j=1}^{\infty} z^j \frac{1}{\cancel{2}(\hbar\omega)^3}\frac{\cancel{2}}{(j\beta)^3}$$

$$= \sum_{j=1}^{\infty} \frac{z^j}{j^3}\left(\frac{k_B T}{\hbar\omega}\right)^3 \quad \text{w} \quad \sum_{j=1}^{\infty}\frac{z^j}{j^3} \equiv g_3(z)$$

$$= g_3(z)\left(\frac{k_B T}{\hbar\omega}\right)^3$$

Where if we include the number of particles in the ground state (N_0), we then have

$$\boxed{N = \frac{z}{1-z} + g_3(z)\left(\frac{k_B T}{\hbar\omega}\right)^3}$$

Which is of course, equation (8). Equation (8) in this paper is the number of particles originally in the ground state with the second term being the max number of particles in excited states before they condense to the ground state.

In Equation (1) (of my assignment), I am not entirely certain how the infinite sum is converted.

Problem 2: Review

Procedure:

- - We begin by discussing the physical meaning of equations (5), (7), and (8)
  - Take equation (7) and integrate it (twice by parts) and this will reproduce equation (8)

Key Concepts:

- - The critical temperature, which is equation (5) in the paper, is for when $N \to \infty$
  - Equation (7) is the 3D treatment of the Bose Einstein Condensates in a harmonic potential
  - We then can find equation (8) by integrating equation (7) and substituting in the correct expression for N_0

Variations:

- - This problem cannot be changed without requiring us to derive a different part of the paper or looking at a new paper all together

Problem 3:

Write a little code that allows you to reproduce Figs. 1(a) and 1(b) for $N = 100$. If you use a cutoff in any of the infinite sums, you are encouraged to make sure that your results are converged with respect to the cutoff.

This can be done fairly straightforwardly in Mathematica. Before you start setting this up on the computer, write down clearly on a piece of paper what the steps are that you want to implement (unless you have a clear idea of what you want the computer to do for you, you cannot "teach" the computer to accomplish the task).

To reproduce the plots in Figure 1, we must solve for the Fugacity numerically. This is done by taking equation (4)

$$N = \sum_{j=1}^{\infty} \frac{z^j}{(1-x^j)^3}$$

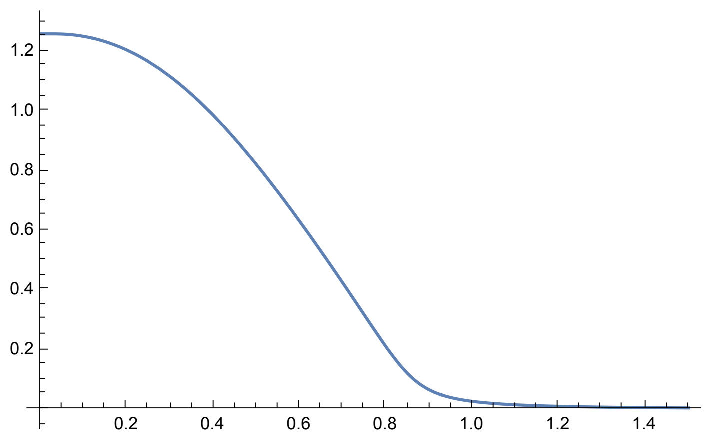
and solving for z numerically w/ $N = 100$,

$$100 = \sum_{j=1}^{\infty} \frac{z^j}{(1-\exp(-\beta\hbar\omega)^j)^3}$$

where the plots in Figures (1a) and (1b) are of N_0/N. For the check on convergence I set $j=200$ and varied the temperatures respectively

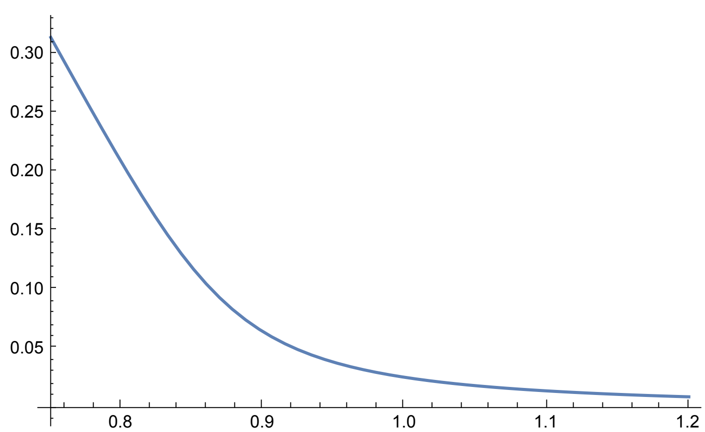
In[∘]:=
```
ClearAll["Global`"]
h = 1.05 * 10^-34;
k = 1.38 * 10^-23;
t = (100 / NSum[1^j / j^3, {j, 1, Infinity}])^(1/3) * h/k;
Quiet[Plot[((z /. NSolve[100 == Sum[z^j / (1 - Exp[-h/(k*t*x)]^j)^3, {j, 1, 200}], z, Reals][[2]]) / (1 - z /. NSolve[100 == Sum[z^j / (1 - Exp[-h/(k*t*x)]^j)^3, {j, 1, 200}], z, Reals][[2]])) / 100, {x, 0.0001, 1.5}]]
Quiet[Plot[((z /. NSolve[100 == Sum[z^j / (1 - Exp[-h/(k*t*x)]^j)^3, {j, 1, 200}], z, Reals][[2]]) / (1 - z /. NSolve[100 == Sum[z^j / (1 - Exp[-h/(k*t*x)]^j)^3, {j, 1, 200}], z, Reals][[2]])) / 100, {x, 0.75, 1.2}]]
```

Out[∘]=



→ 1(a)

Out[∘]=



→ 1(b)

Problem 3: Review

Procedure:

- – We need to solve for N_0/N numerically for $N = 100$, this is done by solving

  $$N = \sum_{j=1}^{\infty} \frac{z^j}{(1 - \exp{(-\beta\hbar\omega)^j})^3}$$

  with Mathematica
  - See Mathematica code for how this was done
    - Note: If we increase the value j, we will get more accurate graphs. This comes at the expense of time in that as the max value of j grows, the time it will take to compute this sum will as well

Key Concepts:

- – We can see that as the ratio of T/T_0 increases, the ratio of N_0/N will decrease as well

Variations:

- – The only way this can feasibly change is if the value of N changes
  - This causes us to change the value that we feed into Mathematica for N

Problem 4:

This problem builds on the tools developed in Problem 3.

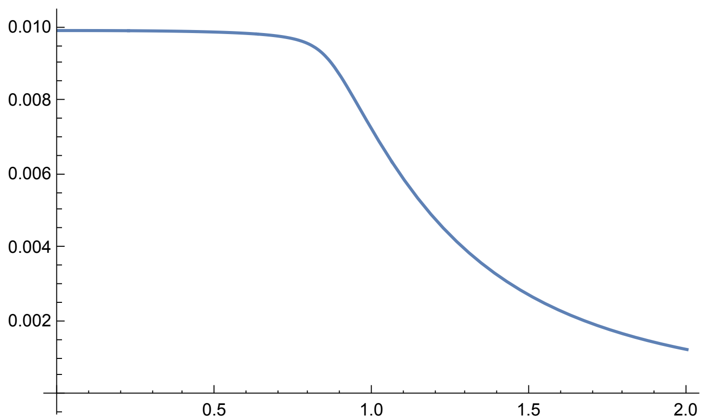
For $N = 100$, plot the fugacity and the chemical potential as a function of T/T_c^0.

The mathematica code used to produce this can be found below

$$\mu = KT\log(z)$$

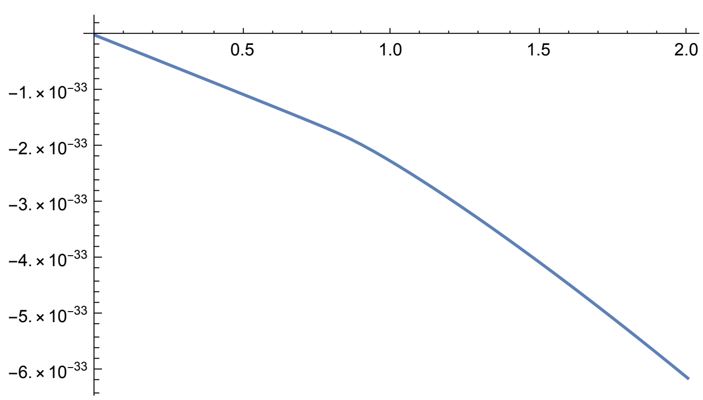
```
In[1]:= ClearAll["Global`"]
h = 1.05 * 10^-34;
k = 1.38 * 10^-23;
t = (100 / NSum[1^j / j^3, {j, 1, Infinity}])^(1/3) * h/k;
Quiet[Plot[(z /. NSolve[100 == Sum[z^j / (1 - Exp[-h/(k*t*x)]^j)^3, {j, 1, 200}], z, Reals][[2]]) / 100,
  {x, 0.0001, 2.0}]]
```

Out[5]=




```
In[8]:= Quiet[Plot[
  k * t * x * Log[(z /. NSolve[100 == Sum[z^j / (1 - Exp[-h/(k*t*x)]^j)^3, {j, 1, 200}], z, Reals][[2]]) / 100],
  {x, 0.0001, 2.0}]]
```

Out[8]=



Problem 4: Review

Procedure:

- – Numerically solve for the Fugacity (using the previous equation in problem 3) and plot this in Mathematica
  – Plot the chemical potential with
  $$\mu = KT\log(z)$$
  where we of course are solving for this in Mathematica again

Key Concepts:

- – This problem has essentially the same concepts as problem 3 but with different physical quantities
  – If we increase the value of j in our sum for solving for the Fugacity we will get more accurate graphs

Variations:

- – We could be asked to graph different quantities or for different ranges
  - ∗ We then would slightly modify our Mathematica code to accommodate for these changes