Physics 614 Homework 3

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1. **Bose-Einstein condensation in 2D**

Recall that the average number of particles in a Bose gas is given by

$$N = \sum_r \frac{1}{e^{\beta(E_r - \mu)} - 1} \tag{1}$$

which we can rewrite for the 2D case using the density of states, $g(\epsilon) = \frac{L^2 m}{2\pi\hbar^2}$, and rearrange to find the density. With $z = e^{\beta\mu}$, the fugacity, we have

$$\begin{aligned}
N &= \int_0^\infty d\epsilon \frac{g(\epsilon)}{z^{-1}e^{\beta\epsilon} - 1} \\
N &= \frac{L^2 m}{2\pi\hbar^2} \int_0^\infty d\epsilon \frac{1}{z^{-1}e^{\beta\epsilon} - 1} \\
N &= \frac{L^2 m k_B T}{2\pi\hbar^2} \int_0^\infty dy \frac{1}{z^{-1}e^{y} - 1} \\
\rho &= \frac{m k_B T}{2\pi\hbar^2} g_1(z) \\
\rho &= \frac{1}{\lambda^2} g_1(z)
\end{aligned} \tag{2}$$

where $g_\alpha(z) = \frac{1}{(\alpha-1)!} \int_0^\infty dy \frac{y^{\alpha-1}}{z^{-1}e^y - 1}$ are the Bose functions. Suppose there exists T_c such that the continuum approximation in (2) breaks down. That is, suppose there is T_c such that

$$\rho \frac{2\pi\hbar^2}{m k_B T_c} = g_1(1) \tag{3}$$

Then we would have

$$\rho \frac{2\pi\hbar^2}{m k_B T_c} = \zeta(1) = \sum_{n=1}^\infty \frac{1}{n} = \infty \tag{4}$$

but then T_c must be zero. So there is no Bose-Einstein condensation transition in two dimensions.

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2. **Two-state Bose-Einstein condensation**
Consider an ideal Bose gas consisting of molecules with two internal states, the ground state with energy $\epsilon_0 = 0$ and an excited state with energy $\epsilon_1 > 0$.

 i. We can write the grand canonical partition function as

$$\begin{aligned} \mathcal{Q} &= \prod_\alpha \mathcal{Z}_\alpha \\ \mathcal{Q} &= \prod_\alpha \frac{1}{1 - e^{-\beta(\epsilon_\alpha - \mu)}} \end{aligned} \tag{5}$$

where α indexes the many-particle eigenstates of the Hamiltonian, $\mathcal{H}$. We can divide these states into two categories: one with energy $\epsilon_{\boldsymbol{k}}$, for each allowed $\boldsymbol{k}$ value, and the other with energy $\epsilon_{\boldsymbol{k}} + \epsilon_1$, in which the internal degree of freedom is excited. In this case the grand partition function becomes

$$\mathcal{Q} = \prod_{\boldsymbol{k}} \frac{1}{\left[1 - e^{-\beta(\epsilon_{\boldsymbol{k}} - \mu)}\right]\left[1 - e^{-\beta(\epsilon_{\boldsymbol{k}} + \epsilon_1 - \mu)}\right]} \tag{6}$$

 ii. Recall that the average number of particles N can be written in terms of $\mathcal{Q}$ as $N = \frac{1}{\beta}\frac{\partial \ln \mathcal{Q}}{\partial \mu}$. Using the expression for $\mathcal{Q}$ found in (4), and setting $z_1 = e^{\beta\mu}$ and $z_2 = e^{\beta(\mu - \epsilon_1)}$, we have

$$\begin{aligned} N &= \frac{1}{\beta}\frac{\partial \ln \mathcal{Q}}{\partial \mu} \\ N &= -\frac{1}{\beta}\frac{\partial}{\partial \mu}\left(\sum_{\boldsymbol{k}} \ln\left(1 - e^{-\beta(\epsilon_{\boldsymbol{k}} - \mu)}\right) + \ln\left(1 - e^{-\beta(\epsilon_{\boldsymbol{k}} + \epsilon_1 - \mu)}\right)\right) \\ N &= \frac{1}{\beta}\left(\sum_{\boldsymbol{k}} \frac{\beta e^{-\beta(\epsilon_{\boldsymbol{k}} - \mu)}}{1 - e^{-\beta(\epsilon_{\boldsymbol{k}} - \mu)}} + \frac{\beta e^{-\beta(\epsilon_{\boldsymbol{k}} + \epsilon_1 - \mu)}}{1 - e^{-\beta(\epsilon_{\boldsymbol{k}} + \epsilon_1 - \mu)}}\right) \\ N &= \sum_{\boldsymbol{k}} \frac{z_1 e^{-\beta\epsilon_{\boldsymbol{k}}}}{1 - z_1 e^{-\beta\epsilon_{\boldsymbol{k}}}} + \sum_{\boldsymbol{k}} \frac{z_2 e^{-\beta\epsilon_{\boldsymbol{k}}}}{1 - z_2 e^{-\beta\epsilon_{\boldsymbol{k}}}} \\ N &= \sum_{\boldsymbol{k}} \frac{1}{z_1^{-1} e^{\beta\epsilon_{\boldsymbol{k}}} - 1} + \sum_{\boldsymbol{k}} \frac{1}{z_2^{-1} e^{\beta\epsilon_{\boldsymbol{k}}} - 1} \end{aligned} \tag{7}$$

Now, using the density of states $g(\epsilon) = \frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\epsilon^{1/2}$, we can rewrite the sums in (5) as integrals over ϵ

$$
\begin{aligned}
N &= \sum_{\boldsymbol{k}} \frac{1}{z_1^{-1} e^{\beta \epsilon_{\boldsymbol{k}}} - 1} + \sum_{\boldsymbol{k}} \frac{1}{z_2^{-1} e^{\beta \epsilon_{\boldsymbol{k}}} - 1} \\
N &\approx \frac{V}{4\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} \left[\int d\epsilon \frac{\epsilon^{1/2}}{z_1^{-1} e^{\beta\epsilon} - 1} + \int d\epsilon \frac{\epsilon^{1/2}}{z_2^{-1} e^{\beta\epsilon} - 1}\right] \\
N &= \frac{V}{4\pi^2} \left(\frac{2m}{\beta\hbar^2}\right)^{3/2} \left(\frac{1}{2}\right)! \left[\frac{1}{(1/2)!} \int dy \frac{y^{1/2}}{z_1^{-1} e^{y} - 1} + \frac{1}{(1/2)!} \int dy \frac{y^{1/2}}{z_2^{-1} e^{y} - 1}\right] \\
N &= \frac{V}{4\pi^2} \left(\frac{2m}{\beta\hbar^2}\right)^{3/2} \frac{\sqrt{\pi}}{2} \left(g_{3/2}(z_1) + g_{3/2}(z_2)\right) \\
\rho &= \left(\frac{m k_B T}{2\pi\hbar^2}\right)^{3/2} \left(g_{3/2}(z_1) + g_{3/2}(z_2)\right) \\
\rho &= \frac{1}{\lambda^3} \left(g_{3/2}(z_1) + g_{3/2}(z_2)\right) \\
\rho\lambda^3 &= g_{3/2}(z_1) + g_{3/2}(z_2)
\end{aligned}
\tag{8}
$$

iii. In the low temperature limit $z_1 \to 1$ while λ increases without bound. So there must be some T_c at which the approximation in (5) breaks down. Setting $z_1 = 1$, we have

$$
\begin{aligned}
\rho \left(\frac{2\pi\hbar^2}{m k_B T_c}\right)^{3/2} &= g_{3/2}(z_1) + g_{3/2}(z_2) \\
\rho \left(\frac{2\pi\hbar^2}{m k_B T_c}\right)^{3/2} &= g_{3/2}(z_1) + g_{3/2}(z_1 e^{-\beta\epsilon_1}) \\
\rho \left(\frac{2\pi\hbar^2}{m k_B T_c}\right)^{3/2} &= g_{3/2}(1) + g_{3/2}(e^{-\epsilon_1/(k_B T_c)})
\end{aligned}
\tag{9}
$$

The solution to equation (7) yields the critical temperature, T_c, for condensation in this system.
Let T_c^0 be the critical temperature for the same gas of molecules with all molecules restricted to the ground state (i.e. the solution to $(h/\sqrt{2\pi m k_B T_c^0})^3 \rho = \zeta(3/2)$).

- In the low temperature limit, if T_c^0 solves $(h/\sqrt{2\pi m k_B T_c^0})^3 \rho = \zeta(3/2)$ then T_c^0 solves (7) to a good approximation. Therefore, when $k_B T_c^0 \ll \epsilon_1$, we have

$$
\begin{aligned}
\left(\frac{T_c}{T_c^0}\right)^{3/2} &= \frac{\zeta(3/2)}{\zeta(3/2) + g_{3/2}(e^{-\epsilon_1/(k_B T_c^0)})} \\
\frac{T_c}{T_c^0} &\approx \frac{1}{\left(1 + \frac{1}{\zeta(3/2)} e^{-\epsilon_1/(k_B T_c^0)}\right)^{2/3}} \\
\frac{T_c}{T_c^0} &\approx 1 - \frac{2}{3\zeta(3/2)} e^{-\epsilon_1/(k_B T_c^0)}
\end{aligned}
\tag{10}
$$

- When $k_B T_c^0 \gg \epsilon_1$,

$$
\begin{aligned}
\frac{T_c}{T_c^0} &= \left(\frac{\zeta(3/2)}{\zeta(3/2) + g_{3/2}(e^{-\epsilon_1/(k_B T_c^0)})} \right)^{2/3} \\
\frac{T_c}{T_c^0} &= \left(\frac{1}{1 + \frac{1}{\zeta(3/2)}(\Gamma(-1/2)(\epsilon_1/(k_B T_c^0)^{1/2} + \zeta(3/2) + \mathcal{O}(\epsilon_1/(k_B T_c^0)))} \right)^{2/3} \\
\frac{T_c}{T_c^0} &= \left(\frac{1}{2 + \frac{1}{\zeta(3/2)}(-2(\pi\epsilon_1/(k_B T_c^0))^{1/2} + \zeta(3/2))} \right)^{2/3} \\
\frac{T_c}{T_c^0} &= 2^{-2/3} \left(\frac{1}{1 - \frac{1}{\zeta(3/2)}\sqrt{\pi\epsilon_1/(k_B T_c^0)}} \right)^{2/3} \\
\frac{T_c}{T_c^0} &\approx 2^{-2/3} \left(1 + \frac{2}{3\zeta(3/2)}\sqrt{\pi\epsilon_1/(k_B T_c^0)} \right)
\end{aligned}
\tag{11}
$$

where we have omitted a factor of $2^{4/3}$ due primarily to confusion.

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3. **Density of states for 1d phonons**

Consider a linear chain of N point masses m confined to move in one dimension, and connected to their nearest neighbors with harmonic bonds of spring constant κ and rest length a. The standard harmonic analysis of classical mechanics shows that a complete basis to describe the displacements of the masses at positions $x = ia$, $i \in (0, 1, \ldots, N-1)$ is provided by plane-wave-like normal modes

$$
u(x) = \frac{1}{\sqrt{L}} e^{ikx} \tag{12}
$$

where $k = \frac{2\pi}{L} n$, $n = 0, \pm 1, \pm 2, \ldots, \pm(N-1)/2$. In contrast to the continuous medium, the lattice constant imposes a finite range to the momenta, $-\pi/a < k < \pi/a$ in the limit of large N. Classically, each mode has a momentum-dependent oscillation frequency, $\omega_k = \omega_0 |\sin(ka/2)|$, where $\omega_0 = 2\sqrt{\kappa/m}$.

i. For a sum over k of a function $F(\omega_k)$, we have $\sum_k F(\omega_k) \approx \frac{L}{2\pi} \int_{-\pi/a}^{\pi/a} dk F(\omega_k) = \frac{L}{\pi} \int_0^{\pi/a} dk F(\omega_k)$ since ω_k is even on the interval $-\pi/a < k < \pi/a$. We can rewrite the differential dk as follows

$$\begin{aligned}
\omega_k &= \omega_0 \left|\sin\left(\frac{ka}{2}\right)\right| \\
\omega_k &= \omega_0 \sin\left(\frac{ka}{2}\right), \text{ for } \ k < \pi/a \\
\frac{\mathrm{d}\omega_k}{\mathrm{d}k} &= \frac{\omega_0 a}{2} \cos\left(\frac{ka}{2}\right) \\
d\omega_k &= \frac{\omega_0 a}{2} \sqrt{1 - \left(\frac{\omega_k}{\omega_0}\right)^2} dk \\
dk &= \frac{2}{\omega_0 a} \frac{d\omega_k}{\sqrt{1 - \left(\frac{\omega_k}{\omega_0}\right)^2}}
\end{aligned} \tag{13}$$

With the prefactors from the integration, we have

$$g(\omega) = \frac{2L}{\pi a \omega_0} \frac{1}{\sqrt{1 - \left(\frac{\omega}{\omega_0}\right)^2}} \tag{14}$$

ii. .

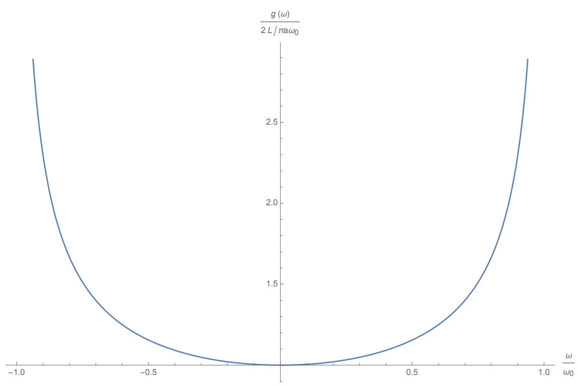

Figure 1: Plot of the density of states as a function of ω/ω_0. Sorry this plot is so small.

The singularity in this plot is due to the fact that, at large N, we have $\omega/\omega_0 = 1$.

iii. As $k \to 0$, $\omega_k \to vk$, where $v = \omega_0 a/2$. In this limit, $\frac{1}{v} d\omega_k = dk$. So $g(\omega) = \frac{L}{v\pi}$.

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