33-765 Homework 12

Nathaniel D. Hoffman

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42. Occupation Number Fluctuations in the Free Ideal Fermi/Bose-Gas

The occupation number n_α of a single-particle energy eigenstate α is a random number. Its expectation value is the Fermi/Bose-distribution, $\langle n_\alpha \rangle = (e^{\beta(\epsilon_\alpha - \mu)} \pm 1)^{-1}$. Prove that its variance is given by $\sigma^2_{n_\alpha} = \langle n_\alpha \rangle (1 \mp \langle n_\alpha \rangle)$.

$$\begin{aligned}
\langle n_\alpha^2 \rangle &= \frac{1}{\mathcal{Z}} \left(\prod_{\alpha'} \sum_{n_{\alpha'}} n_\alpha^2 e^{-\beta(\epsilon_\alpha - \mu) n_{\alpha'}} \right) \\
&= \frac{1}{\mathcal{Z}} \left(\prod \sum \left(\frac{1}{\beta^2} \partial^2_{\epsilon_\alpha} \right) e^{-\beta(\epsilon_\alpha - \mu) n_{\alpha'}} \right) \\
&= \frac{1}{\beta^2} \frac{1}{\mathcal{Z}} \partial^2_{\epsilon_\alpha} \mathcal{Z} \\
&= \frac{1}{\beta^2} \left(\partial_{\epsilon_\alpha} \ln(\mathcal{Z}) + \frac{1}{\mathcal{Z}^2} (\partial_{\epsilon_\alpha} \mathcal{Z})^2 \right) \\
&= -\frac{1}{\beta} \partial^2_{\epsilon_\alpha} \Omega - (\partial_{\epsilon_\alpha} \Omega)^2 \\
&= -\left(\frac{1}{\beta} \partial^2_{\epsilon_\alpha} \Omega + \langle n_\alpha \rangle^2 \right) \\
&= -\left(\frac{1}{\beta} \partial^2_{\epsilon_\alpha} \left[\mp \frac{1}{\beta} \sum_{\alpha'} \ln\left(1 \pm e^{-\beta(\epsilon_{\alpha'} - \mu)}\right) \right] + \langle n_\alpha \rangle^2 \right) \\
&= \left(\mp \langle n_\alpha \rangle^2 + \langle n_\alpha \rangle - \langle n_\alpha \rangle^2 \right)
\end{aligned}$$

so

$$\sigma^2_{n_\alpha} = \langle n_\alpha^2 \rangle - \langle n_\alpha \rangle^2 = \mp \langle n_\alpha \rangle^2 + \langle n_\alpha \rangle - \langle n_\alpha \rangle^2 - \langle n_\alpha \rangle^2 = \langle n_\alpha \rangle (1 \mp \langle n_\alpha \rangle)$$

43. Bose-Einstein Condensation in a Harmonic Trap

Consider bosonic atoms in an optically generated harmonic trap: $V(x,y,z) = \frac{1}{2} m(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2)$.

1. What are the single-particle energy eigenstates of this system? Write down the energy spectrum of the single-particle Hamiltonian and subtract away the irrelevant ground-state energy.

The eigenstates of a 3D anisotropic harmonic oscillator can be written as a tensor product of three eigenstates of 1D oscillators:

$$|n\rangle = |n_x\rangle |n_y\rangle |n_z\rangle$$

with

$$|n_{x_\mu}\rangle = \frac{1}{\sqrt{2^n n!}} \left(\frac{m\omega_\mu}{\pi\hbar}\right)^{1/4} e^{-m\omega_\mu x_\mu/2\hbar} H_n\left(\sqrt{\frac{m\omega_\mu}{\hbar}} x_\mu\right)$$

where $H_n(x)$ are the Hermite polynomials. The energy spectrum is therefore a sum of the energy spectra for each 1D oscillator:

$$E = E_x + E_y + E_z = \sum_\mu \hbar\omega_\mu \left(n_\mu + \frac{1}{2}\right) = \frac{\hbar}{2}(\sum_\mu \omega_\mu + 2n_{\mu\omega_\mu})$$

If we consider the ground-state energy to be where $n_\mu = 0$,

$$E_0 = \frac{\hbar}{2}(\sum_\mu \omega_\mu)$$

and

$$E = E_0 + \hbar(\omega_x n_x + \omega_y n_y + \omega_z n_z)$$

2. As a useful result, prove that $\frac{1}{e^x-1} = \sum_{k=1}^\infty e^{-kx}$ as long as $x > 0$.

We can rewrite $\frac{1}{e^x-1} = \frac{e^{-x}}{1-e^{-x}}$. This is a geometric series if $x > 0$ (since we need e^{-x} to be less than 1):

$$\frac{a}{1-r} = \sum_{k=0}^\infty ar^k$$

so with $a = e^{-x}$ and $r = e^{-x}$, we have

$$\frac{1}{e^x - 1} = \sum_{k=0}^\infty e^{-x}(e^{-x})^k = \sum_{k=1}^\infty e^{-kx}$$

3. Bose-Einstein condensation happens if the total number N' of particles contained in all excited states is bounded from above. Without using a continuum approximation, find an expression for N' and look for an upper bound by focusing on the "best-case scenario" $\mu = 0$. Why is this "best case"? You will end up with an unwieldy looking sum.

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

We choose $\mu = 0$ because $\mu > 0$ would make $e^{\beta(\epsilon-\mu)}$ smaller making N' bigger, so $\mu = 0$ gives the smallest upper bound.

4. Rewrite the sum using the identity you proved in part (2), swap the two sums, sum up the inner one, and expand it for large temperatures. Now show that the leading order is

$$N' = \zeta(3)\left(\frac{k_B T}{\hbar\bar{\omega}}\right)^3 + \mathcal{O}(T^2) \qquad \text{with } \bar{\omega} = (\omega_x\omega_y\omega_z)^{1/3}.$$

$$N' = \sum_{\alpha=1}^\infty \left(\sum_{k=1}^\infty e^{-\beta k \epsilon_\alpha}\right)$$

$$
\begin{aligned}
&= \sum_{k=1}^{\infty}\sum_{\alpha=1}^{\infty} e^{-\beta k \epsilon_\alpha} \\
&= \sum_{k=1}^{\infty}\left(\underbrace{\sum_{n_x}^{\infty}\sum_{n_y}^{\infty}\sum_{n_z}^{\infty}}_{n_x+n_y+n_z\geq 1} e^{-k\beta\hbar\omega_x n_x} e^{-k\beta\hbar\omega_y n_y} e^{-k\beta\hbar\omega_z n_z}\right) \\
&= \sum_{k=1}^{\infty}\sum_{n_x=0}^{\infty}\sum_{n_y=0}^{\infty}\sum_{n_z=0}^{\infty}\left(e^{-k\beta\hbar\omega_x n_x} e^{-k\beta\hbar\omega_y n_y} e^{-k\beta\hbar\omega_z n_z}\right) - 1 \\
&= \sum_{k=1}^{\infty}\prod_{\mu}(-e^{-k\beta\hbar\omega_\mu x_\mu} + 1) \\
&= \sum_{k=1}^{\infty}\frac{1}{\omega_x\omega_y\omega_z}\left(\frac{k_B T}{k\hbar}\right)^3 + \frac{\omega_x+\omega_y+\omega_z}{2\omega_x\omega_y\omega_z}\left(\frac{k_B T}{k\hbar}\right)^2 + \mathcal{O}(T) \\
&= \sum_{k=1}^{\infty}\frac{1}{k^3}\left(\frac{k_B T}{\hbar\bar{\omega}}\right) + \mathcal{O}(T^2) \\
&= \zeta(3)\left(\frac{k_B T}{\hbar\bar{\omega}}\right)^3 + \mathcal{O}(T^2)
\end{aligned}
$$

5. What is the Einstein temperature T_E for this case? How is it different from what we found for the gas-in-a-box?

The Einstein temperature occurs when $N = N'$ or

$$N = \zeta(3)\left(\frac{k_B T_E}{\hbar\bar{\omega}}\right)^3$$

so

$$T_E = \frac{\hbar\bar{\omega}}{k_B}\left(\frac{N}{\zeta(3)}\right)^{1/3}$$

For the gas-in-a-box, we found

$$T_E = \frac{h^2}{2\pi m k_B}\left((2s+1)\frac{V}{N}\gamma\left(\frac{3}{2}\right)\right)^{-2/3}$$

We have already included the degeneracy of the energy states in our derivation, and interestingly the mass doesn't seem to explicitly factor int, but the dependence on N is different:

$$N_E^{\text{SHO}} \propto N^{1/3} \qquad T_E^{\text{Box}} \propto N^{2/3}$$

6. For $\omega_x = 4681\text{Hz}$, $\omega_y = 1477\text{Hz}$, and $\omega_z = 2576\text{Hz}$, how many atoms should be trapped in a BEC at 2mK?

With these numbers, we get $\bar{\omega} = 2611.49\text{Hz}$. Plugging in values for everything, we find that

$$N \approx 1.21163 \times 10^6$$

44. Bose-Einstein Condensation in a Harmonic Trap—Finite Size Corrections

Let us look a bit more closely at a simplified version of the previous problem, namely the isotropic case $\omega_x = \omega_y = \omega_z \equiv \omega$.

1. Show that continuing the series expansion that led to the answer for problem 43.4 leads to

$$N' = \zeta(3)\left(\frac{k_B T}{\hbar\omega}\right)^3 + \frac{3}{2}\zeta(2)\left(\frac{k_B T}{\hbar\omega}\right)^2 + \zeta(1)\left(\frac{k_B T}{\hbar\omega}\right) + \cdots$$

   But alas, this high temperature series expansion should strike you as a terrible disappointment. Why?

In the isotropic case, we can write

$$\begin{aligned}
N' &= \sum_{k=1}^{\infty}\prod_{\mu}\left(-e^{-k\beta\hbar\omega x_\mu}+1\right) \\
&= \sum_{k=1}^{\infty}\frac{1}{k^3}\left(\frac{k_B T}{\hbar\omega}\right)^3 + \frac{3}{2}\frac{1}{k^2}\left(\frac{k_B T}{\hbar\omega}\right)^2 + \frac{1}{k\left(\frac{k_B T}{\hbar\omega}\right)} + \frac{3}{8} + \mathcal{O}(T^{-1}) \\
&= \zeta(3)\left(\frac{k_B T}{\hbar\omega}\right)^3 + \frac{3}{2}\zeta(2)\left(\frac{k_B T}{\hbar\omega}\right)^2 + \zeta(1)\left(\frac{k_B T}{\hbar\omega}\right) + \cdots
\end{aligned}$$

Unfortunately, $\gamma(1) = \tilde{\infty}$, so this series is really an asymptotic expansion which fails miserably at the third term.

2. Boldly ignoring your perfectly reasonable anxieties, and taking only the first two terms from the previous equation, show that they predict a slight downward shift of the Bose-Einstein transition temperature that vanishes in the limit $N \to \infty$ and is given by

$$\frac{T_{\text{transition}} - T_E}{T_E} = -\frac{\alpha}{N^{1/3}} \qquad \text{with } \alpha = \frac{\zeta(2)}{2\zeta(3)^{2/3}} \approx 0.7275.$$

First, we can write the Einstein temperature for the leading-order as

$$T_E = \frac{\hbar\omega}{k_B}\left(\frac{N}{\zeta(3)}\right)^{1/3}$$

so

$$\frac{k_B}{\hbar\omega} = \frac{1}{T_E}\left(\frac{N}{\zeta(3)}\right)^{1/3}$$

We can now write the expression with the next-order in terms of $\frac{T_T}{T_E}$ with $T_T \equiv T_{\text{transition}}$ for brevity and later $x \equiv \frac{T_T}{T_E}$:

$$N\left(\frac{T_T}{T_E}\right) = \zeta(3)\left(\frac{N}{\zeta(3)}\right)\left(\frac{T_T}{T_E}\right)^3 + \frac{3}{2}\zeta(2)\left(\frac{N}{\zeta(3)}\right)^{2/3}\left(\frac{T_T}{T_E}\right)^2$$

For $N \to \infty$, the downward shift vanishes, so $\frac{T_T}{T_E} \to 1$. We can think of the downward shift as a linear perturbation in $\frac{T_T - T_E}{T_E} = \epsilon$ for $\frac{T_T}{T_E} \to 1+\epsilon$, where we will ignore all ϵ^2 and higher orders. Note that this makes $\epsilon \propto N^{-1/3}$ so we will also ignore terms of order $N^{-1/3}\epsilon$ (this is important in the final step of the derivation):

$$\begin{aligned}
N &= Nx^3 + 3\alpha N^{2/3}x^2 \\
&= N(1 + 3\epsilon + 3\epsilon^2 + \epsilon^3) + 3\alpha N^{2/3}(1 - 2\epsilon + \epsilon^2) \\
1 &= 1 + 3\epsilon + 3\frac{\alpha}{N^{1/3}}(1 + 2\epsilon) \\
1 &= 1 + 3\epsilon + 3\frac{\alpha}{N^{1/3}}
\end{aligned}$$

$$\implies \epsilon = \frac{T_T - T_E}{T_E} = -\frac{\alpha}{N^{1/3}}$$