PHYS 427 - Thermal and Statistical Physics - Discussion 04 - Solutions

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1. **Geometric series**: Repeatedly in statistical mechanics one encounters the sum:

$$S = \sum_{n=0}^{N} x^n. \tag{1}$$

[For instance, you'll encounter this sum on the upcoming homework!]

(a) Show that for $x \neq 1$:

$$\sum_{n=0}^{N} x^n = \frac{1 - x^{N+1}}{1 - x} \tag{2}$$

[Hint: explicitly write out the following sum: $(1-x)S$. You should notice that many terms cancel.]

(b) By taking a derivative of this result, show that for $x \neq 1$:

$$\sum_{n=0}^{N} n x^n = \frac{x}{(1-x)^2}\left[1 - (N+1)x^N + N x^{N+1}\right] \tag{3}$$

As an aside, it is very common to encounter this sum with $N \to \infty$ and $|x| < 1$. In this case $\lim_{N\to\infty} x^N = 0$ and the results above simplify considerably:

$$\sum_{n=0}^{\infty} x^n = \frac{1}{1-x} \quad , \quad \text{if } |x| < 1 \tag{4}$$

$$\sum_{n=0}^{\infty} n x^n = \frac{x}{(1-x)^2} \quad , \quad \text{if } |x| < 1 \tag{5}$$

(a) Following the hint:

$$\begin{aligned}
(1-x)S &= S - xS && (6)\\
&= (1 + \cancel{x + x^2 + \cdots + x^N}) - (\cancel{x + x^2 + \cdots + x^N} + x^{N+1}) && (7)\\
&= 1 - x^{N+1} && (8)
\end{aligned}$$

Therefore

$$S = \frac{1 - x^{N+1}}{1 - x} \tag{9}$$

(b) Differentiating this result with respect to x gives:

$$\frac{\partial}{\partial x}\left(\sum_{n=0}^{N} x^n\right) = \frac{\partial}{\partial x}\left(\frac{1-x^{N+1}}{1-x}\right) \tag{10}$$

$$\sum_{n=0}^{N} \frac{\partial}{\partial x} x^n = \frac{-(N+1)x^N}{1-x} + \frac{1-x^{N+1}}{(1-x)^2} \tag{11}$$

$$\sum_{n=0}^{N} n x^{n-1} = \frac{-(N+1)x^N(1-x) + 1 - x^{N+1}}{(1-x)^2} \tag{12}$$

$$= \frac{1-(N+1)x^N + N x^{N+1}}{(1-x)^2} \tag{13}$$

where we applied the product rule on the right hand side and then collected terms by using $(1-x)^2$ as a common denominator. Multiplying both sides by x gives the final result:

$$\sum_{n=0}^{N} n x^n = \frac{x}{(1-x)^2}\left[1-(N+1)x^N + N x^{N+1}\right] \tag{14}$$

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2. **2D non-interacting ultra-relativistic gas**: Consider a gas of N highly-relativistic particles confined to a square of area $A = L^2$. The particles have energy $\varepsilon_{\vec{p}} = |\vec{p}|c$ where the momentum is $\vec{p} = \hbar\vec{k}$ and the wavevectors are quantized as $\vec{k} = \pi\vec{n}/L$ with $n_x, n_y = 1, 2, \ldots, \infty$.

   (a) Show that as $L \to \infty$ we can approximate a momentum sum by an integral:

   $$\sum_{\vec{p}} F(\varepsilon_{\vec{p}}) \sim \frac{L^2}{(\pi\hbar)^2} \int_0^\infty dp_x \int_0^\infty dp_y F(\varepsilon_{\vec{p}}) \tag{15}$$

   where $F(\varepsilon_{\vec{p}})$ is an arbitrary function of the dispersion $\varepsilon_{\vec{p}}$.

   (b) Write the integral in polar coordinates (p, θ); then make a change of variables to show that:

   $$\sum_{\vec{p}} F(\varepsilon_{\vec{p}}) \sim \frac{L^2}{2\pi(\hbar c)^2} \int_0^\infty d\varepsilon\, \varepsilon\, F(\varepsilon) \tag{16}$$

   hence, we can approximate momentum sums by energy integrals!

   (c) Compute the partition function of a single particle, Z_1.

   (d) Compute the partition function of N indistinguishable particles, Z_N.

   (e) Assuming the N particle system is in thermal equilibrium with a reservoir, compute its energy. You should find that

   $$U = 2Nk_BT \tag{17}$$

(a) Here a sum over momentum states $\vec{p} = \pi\hbar\vec{n}/L$ is a sum over the positive integers $n_x = 1, 2, \ldots, \infty$ and $n_y = 1, 2, \ldots, \infty$.

$$\sum_{\vec{p}} = \sum_{n_x=1}^{\infty} \sum_{n_y=1}^{\infty} \tag{18}$$

As the length approaches infinity, the spacing between two consecutive momentum levels becomes infinitesimal: $\Delta p_x = \pi\hbar/L \to 0$ and $\Delta p_y = \pi\hbar/L \to 0$ as L blows up! Hence, the momentum approaches a <u>continuous variable</u>. In this case, the error in approximating a sum over positive integers by the following integral is minimal:

$$\sum_{\vec{p}} = \sum_{n_x=1}^{\infty} \sum_{n_y=1}^{\infty} \approx \int_1^\infty dn_x \int_1^\infty dn_y \quad \text{, as } L \to \infty \tag{19}$$

Since $\vec{p} = \pi\hbar\vec{n}/L$ (or rearranging $\vec{n} = \vec{p}L/\pi\hbar$) the integral becomes

$$\sum_{\vec{p}} \approx \frac{L^2}{(\pi\hbar)^2} \int_0^\infty dp_x \int_0^\infty dp_y \quad \text{, as } L \to \infty \tag{20}$$

An alternative way to see this is to realize that $1 = \Delta p_x L/\pi\hbar$ and $1 = \Delta p_y L/\pi\hbar$. Hence

$$\sum_{p_x} \sum_{p_y} = \frac{L^2}{(\pi\hbar)^2} \sum_{p_x} \Delta p_x \sum_{p_y} \Delta p_y \sim \frac{L^2}{(\pi\hbar)^2} \int_0^\infty dp_x \int_0^\infty dp_y \quad \text{, as } L \to \infty \tag{21}$$

(b) We're interested in applying this result to functions of the dispersion $\varepsilon_{\vec{p}} = |\vec{p}|c$.

$$\sum_{\vec{p}} F(\varepsilon_{\vec{p}}) \sim \frac{L^2}{(\pi\hbar)^2} \int_0^\infty dp_x \int_0^\infty dp_y F(\varepsilon_{\vec{p}}) \tag{22}$$

Notice this dispersion is **isotropic**, i.e. it only depends on the magnitude of the momentum and not on its orientation. Writing the integral in polar coordinates, $p_x = p\cos\theta$ and $p_y = p\sin\theta$, gives

$$\frac{L^2}{(\pi\hbar)^2} \int_0^\infty dp_x \int_0^\infty dp_y F(\varepsilon_{\vec{p}}) = \frac{L^2}{(\pi\hbar)^2} \int_0^\infty dp \int_0^{\pi/2} d\theta\, pF(pc) \tag{23}$$

$$= \frac{L^2}{(\pi\hbar)^2} \frac{\pi}{2} \int_0^\infty dp\, pF(pc) \tag{24}$$

We now make the change of variables $\varepsilon = pc$ which gives the desired result

$$\sum_{\vec{p}} F(\varepsilon_{\vec{p}}) \sim \frac{L^2}{(\pi\hbar)^2} \int_0^\infty dp_x \int_0^\infty dp_y F(\varepsilon_{\vec{p}}) = \frac{L^2}{2\pi(\hbar c)^2} \int_0^\infty d\varepsilon\, \varepsilon\, F(\varepsilon) \tag{25}$$

(c) The single-particle partition function is

$$Z_1 = \sum_{\vec{p}} e^{-\beta\varepsilon_{\vec{p}}} \tag{26}$$

$$\sim \frac{L^2}{2\pi(\hbar c)^2} \int_0^\infty d\varepsilon\, \varepsilon\, e^{-\beta\varepsilon} \quad , \text{ let } x = \beta\varepsilon \tag{27}$$

$$= \frac{L^2}{2\pi(\hbar c)^2} (k_B T)^2 \int_0^\infty dx\, x\, e^{-x} \tag{28}$$

Notice that the remaining integral is just an **unimportant** dimensionless constant! We don't actually need to evaluate it — all the physics is contained in the fact that Z_1 scales with the length squared and temperature squared.

Nevertheless, this is an example of a standard integral known as the gamma function:

$$\Gamma(\nu) = \int_0^\infty dx\, x^{\nu-1}\, e^{-x} \quad , \ \mathrm{Re}(\nu) > 0 \tag{29}$$

Thus, our integral is $\Gamma(2) = 1! = 1$ (you could quickly evaluate this integral by using integration by parts also). Therefore

$$Z_1 = \frac{L^2}{2\pi(\hbar c)^2} (k_B T)^2 \tag{30}$$

(d) The partition function of N indistinguishable particles with this dispersion is given by

$$Z_N = \frac{1}{N!}(Z_1)^N = \frac{1}{N!}\left(\frac{L^2}{2\pi(\hbar c)^2}(k_B T)^2\right)^N \tag{31}$$

(e) The energy of the gas is given by

$$U = -\frac{\partial \ln Z}{\partial \beta} = -\frac{1}{Z}\frac{\partial Z}{\partial \beta} \tag{32}$$

$$= -\frac{1}{\cancel{\frac{1}{N!}\left(\frac{L^2}{2\pi(\hbar c)^2}\right)^N}(k_BT)^{2N}} \cancel{\frac{1}{N!}\left(\frac{L^2}{2\pi(\hbar c)^2}\right)^N} \frac{\partial \beta^{-2N}}{\partial \beta} \tag{33}$$

$$= -\frac{1}{(k_BT)^{2N}}(-2N)(k_BT)^{2N+1} \tag{34}$$

$$= 2Nk_BT \tag{35}$$