

Physics 306: Thermal Physics

Midterm Exam

Stony Brook University

Spring 2024

General Instructions:

You may use one page (front and back) of handwritten notes and a calculator. Graphing calculators are allowed. **No other materials may be used.**

1 Integrals

Gamma Function:

$$\Gamma(z) \equiv \int_0^\infty x^{z-1} e^{-x} dx \quad (1)$$

with specific results

$$\Gamma(z+1) = z\Gamma(z) \quad \Gamma(n) = (n-1)! \quad \Gamma(\tfrac{1}{2}) = \sqrt{\pi} \quad (2)$$

Gaussian Integrals:

$$I_n = \frac{1}{\sqrt{2\pi}\sigma} \int_{-\infty}^\infty dx e^{-x^2/2\sigma^2} x^n \quad (3)$$

with specific results

$$I_0 = 1 \quad I_2 = \sigma^2 \quad I_4 = 3\sigma^4 \quad I_6 = 15\sigma^6 \quad (4)$$

Problem 1. Quick sums

Using techniques from the quantum harmonic oscillator, evaluate the following sums in explicit form:

$$S_0 = \sum_{n=0}^{\infty} q^n \quad S_1 = \sum_{n=0}^{\infty} nq^n. \quad (5)$$

Here q is a real number that is less than unity and greater than 0.

Solution

The partition function of the harmonic oscillator are these sums. In the harmonic oscillator the energy levels are

$$\epsilon_n = n\hbar\omega_0 \quad (6)$$

Thus partition function is the geometric series with $q \equiv e^{-\beta\hbar\omega_0}$:

$$Z = \sum_n e^{-n\beta\hbar\omega_0} = 1 + (e^{-\beta\hbar\omega_0}) + (e^{-\beta\hbar\omega_0})^2 + \dots = \frac{1}{1 - e^{-\beta\hbar\omega_0}} \quad (7)$$

This implies

$$S_0 = 1 + q + q^2 + \dots = \frac{1}{1 - q} \quad (8)$$

i.e. the geometric series.

The mean energy of the harmonic oscillator is:

$$\frac{\langle \epsilon \rangle}{\hbar\omega_0} = \frac{1}{Z} \sum_n n e^{-n\beta\hbar\omega_0} = \frac{e^{-\beta\hbar\omega_0}}{1 - e^{-\beta\hbar\omega_0}} \quad (9)$$

This implies

$$\frac{\sum_n nq^n}{\sum_n q^n} = \frac{q}{1 - q} \quad (10)$$

So using the first sum we find

$$\sum_n nq^n = \frac{q}{(1 - q)^2} \quad (11)$$

Alternate: One can also differentiate¹:

$$q \frac{\partial S_0}{\partial q} = q \sum_n nq^{n-1} = S_1 \quad (12)$$

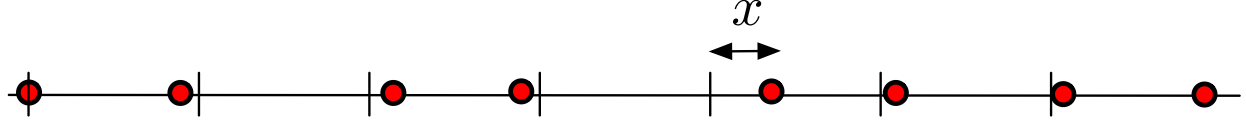
So using S_0 one has

$$S_1 = q \frac{\partial}{\partial q} \left(\frac{1}{1 - q} \right) = \frac{q}{(1 - q)^2} \quad (13)$$

¹This step is essentially the same as differentiating the partition function with respect to β in the statistical mechanics problem

Problem 2. Vibrations of a chain of atoms

A one dimensional wire at temperature T , consists of N independent atoms of mass m “living” at separate sites as shown below. The atoms oscillate harmonically around their individual site centers with vibrational potential energy of $V(x) = \frac{1}{2}k_0x^2$ for an atom displaced from by x from the site center. Here k_0 is the spring constant.



- (a) Treat the harmonic oscillators as independent and classical, and assume that the motion is only in the x direction. What is the energy and specific heat of the substance? How would your result change if the atoms could move in both the x and y directions?
- (b) Consider a single classical oscillator of part (a) with the motion only in the x direction. What is the mean and standard deviation of the vibrational potential energy of the oscillator?
- (c) Now, imagine that the oscillators are quantum as opposed to classical.
 - (i) What is the probability that an atom is vibrating with at least two units of vibrational quanta $2\hbar\omega_0$?

Solution

- (a) We use the equipartition theorem. Each oscillator has Hamiltonian

$$E = \frac{p^2}{2m} + \frac{1}{2}k_0x^2 \quad (14)$$

There are two quadratic forms. Thus the mean energy is

$$U = NkT \quad (15)$$

where N is the number of particles. The specific heat is $C_V = \partial U / \partial T = Nk$. In two dimensions one would have

$$E = \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{1}{2}k_0(x^2 + y^2) \quad (16)$$

which doubles the number of quadratic forms leading to

$$U = 2NkT \quad C_V = 2Nk \quad (17)$$

- (b) The potential energy is $V \equiv \frac{1}{2}k_0x^2$. The mean potential energy is given again by the equipartition theorem

$$\langle V \rangle = \left\langle \frac{1}{2}k_0x^2 \right\rangle = \frac{1}{2}k_B T \quad (18)$$

Indeed, the equipartition theorem says that the average of *each* quadratic form in the energy function (Hamiltonian) is $\frac{1}{2}k_B T$. Then variance is

$$\langle \delta V^2 \rangle = \langle V^2 \rangle - \langle V \rangle^2 = \frac{1}{4}k_0^2 \langle x^4 \rangle - \langle V \rangle^2 \quad (19)$$

So we need to compute $\langle x^4 \rangle$.

The probability of x and p is

$$\mathcal{P}_{x,p} = C e^{-\beta(p^2/2m + V(x))} dx dp \quad (20)$$

Since the energy is a sum of a part that depends on momentum plus a part that depends only on space, $V(x)$, the probability distribution will also factorize $P(x, p) dx dp = P(p) dp P(x) dx$. The part that depends on x is

$$\mathcal{P}_x = P(x) dx = C e^{-\beta V(x)} dx = C e^{-\beta k_0 x^2/2} = C e^{-x^2/2\sigma^2} dx, \quad (21)$$

where we defined $\sigma^2 \equiv 1/\beta k_0$. The probability distribution is Gaussian, which we studied in detail. Then using the Gaussian integrals provided at the front of the exam

$$C = \frac{1}{\sqrt{2\pi\sigma^2}} \quad \langle x^4 \rangle = 3\sigma^4. \quad (22)$$

So assembling the ingredients

$$\langle V^2 \rangle - \langle V \rangle^2 = \left[\left(\frac{1}{4}k_0^2 \right) 3 \left(\frac{1}{\beta k_0} \right)^2 \right] - \left[\frac{1}{2}k_B T \right]^2 = \frac{1}{2}(k_B T)^2 \quad (23)$$

(c) For the quantum harmonic oscillator, the probability of having n quanta of energy is

$$P_n = \frac{e^{-n\beta\hbar\omega_0}}{Z} = e^{-n\hbar\omega_0} (1 - e^{-\hbar\omega_0}) \quad (24)$$

To find the probability of having at least two quanta, i.e. *not* $n = 0$ or $n = 1$, we subtract from unity the probability of having $n = 0$ and $n = 1$, i.e.

$$P_{n \geq 2} = 1 - P_0 - P_1 = 1 - (1 + e^{-\hbar\omega_0})(1 - e^{-\hbar\omega_0}) = e^{-2\hbar\omega_0} \quad (25)$$

Problem 3. Relativistic particles

Consider a classical mono-atomic ideal gas in two dimensions at temperature T . Note however, that these particles have zero mass and move at the speed of light, c . Compared to the non-relativistic case, the difference is that the energy of a massless particle is related to its momentum via $\varepsilon(p) = cp$ instead of $\varepsilon(p) = p^2/2m$. Otherwise, statistical mechanics and notions of phase space are unchanged.

- (a) Determine the probability of finding a particle with momentum (magnitude) between p and $p + dp$, $P(p)dp$.
- (b) Determine the mean de Broglie wavelength $\lambda \equiv h/p$ of the particles.
- (c) Determine the probability of finding a particle with de Broglie wavelength between λ and $\lambda + d\lambda$?

Solution

- (a) We have

$$d\mathcal{P}_{\mathbf{p}} = Ce^{-\beta\varepsilon} dp_x dp_y = Ce^{-\beta cp} dp_x dp_y \quad (26)$$

Since we are asking about the magnitude we integrate over the angle as done in homework

$$d\mathcal{P}_p = Ce^{-\beta cp} 2\pi p dp \quad (27)$$

Normalizing

$$1 = 2\pi C \int_0^\infty e^{-\beta cp} p dp \quad (28)$$

$$= 2\pi C \frac{1}{(\beta c)^2} \int_0^\infty e^{-u} u du \quad (29)$$

$$= 2\pi C \frac{1}{(\beta c)^2} \Gamma(2) \quad (30)$$

Using that $\Gamma(2) = 1$ we have finally $C = (\beta c)^2/2\pi$ and thus

$$d\mathcal{P}_p = (\beta c)^2 e^{-\beta cp} p dp. \quad (31)$$

- (b) We compute

$$\langle \lambda \rangle = \int_0^\infty P(p) dp \frac{h}{p} \quad (32)$$

$$= \int_0^\infty (\beta c)^2 e^{-\beta cp} p dp \frac{h}{p} \quad (33)$$

$$= h\beta c \int_0^\infty (\beta c) e^{-\beta cp} dp \quad (34)$$

$$= h\beta c \quad (35)$$

(c) Changing variables $p = h/\lambda$, using

$$dp = \left| \frac{dp}{d\lambda} \right| d\lambda = \frac{h}{\lambda^2} d\lambda \quad (36)$$

we find

$$d\mathcal{P}_\lambda = (h\beta c)^2 e^{-h\beta c/\lambda} \frac{d\lambda}{\lambda^3} \quad (37)$$

Problem 4. Partition function of three level system

Consider an ensemble at temperature T of N independent “atoms”, each of which have the three energy levels shown below.

$$\text{—————} E_2 = 5\Delta$$

$$\text{—————} E_1 = \Delta$$

$$\text{—————} E_0 = 0$$

- (a) Determine the partition function and mean energy of an atom as a function of temperature.
- (b) Determine the probabilities to be in the first excited and second excited states, P_1 and P_2 , and qualitatively sketch these probabilities versus temperature on the same graph, from very low to very high temperatures:
 - (i) Explain the qualitative features of your graph by pointing to specific terms in your equations.
 - (ii) Determine a Taylor series expansion for the probability P_2 at high temperature, including the leading and first subleading terms. Explain the value of the leading term physically. Taking $\Delta = 0.1 \text{ eV}$, estimate the temperature (in Kelvin) when the Taylor series becomes approximately valid.

Solution

- (a) We have

$$Z = \sum_n e^{-\beta \epsilon_n} = 1 + e^{-\beta \Delta} + e^{-5\beta \Delta} \quad (38)$$

The mean energy is

$$\langle \epsilon \rangle = \frac{-1}{Z} \frac{\partial Z}{\partial \beta} = \frac{\Delta e^{-\beta \Delta} + 5\Delta e^{-5\beta \Delta}}{1 + e^{-\beta \Delta} + e^{-5\beta \Delta}} \quad (39)$$

- (b) We have

$$P_1 = \frac{e^{-\beta \Delta}}{1 + e^{-\beta \Delta} + e^{-5\beta \Delta}} \quad P_2 = \frac{e^{-5\beta \Delta}}{1 + e^{-\beta \Delta} + e^{-5\beta \Delta}} \quad (40)$$

- (i) At low temperatures, $e^{-\beta \Delta} \rightarrow 0$, and thus $P_1 \rightarrow 0$ and $P_2 \rightarrow 0$. At high temperatures we have $e^{-\beta \Delta} \rightarrow 1$ thus at high temperatures we have

$$P_1 \rightarrow \frac{1}{1 + 1 + 1} = \frac{1}{3} \quad P_2 \rightarrow \frac{1}{1 + 1 + 1} = \frac{1}{3} \quad (41)$$

This is the expected result. At high temperatures the spacing between the levels $\sim \Delta$ is negligible compared to kT . Thus in the high temperature limit it is as if all the levels have the same energy² and thus the same probabilities. Your graphs should transition between 0 and 1/3.

(ii) We call $x = \beta\Delta \ll 1$ and have

$$P_2 = \frac{e^{-5x}}{1 + e^{-x} + e^{-5x}} \simeq \frac{1 - 5x}{1 + (1 - x) + (1 - 5x)} \quad (42)$$

$$\simeq \frac{1 - 5x}{3 - 6x} \quad (43)$$

We should now factor out the leading result

$$P_2 \simeq \frac{1}{3} \frac{1 - 5x}{1 - 2x} \simeq \frac{1}{3} (1 - 5x)(1 + 2x) \simeq \frac{1}{3} (1 - 3x + \mathcal{O}(x^2)) \quad (44)$$

Based on the first term in the series expansion we require that

$$3x \ll 1 \quad (45)$$

So the series would begin to work for

$$x = \frac{\Delta}{kT} \sim \frac{1}{3} \quad (46)$$

So roughly when

$$T \sim \frac{3\Delta}{k_B} \simeq \frac{0.3 \text{ eV}}{0.025 \text{ eV}/300^\circ\text{K}} \sim 3600^\circ\text{K} \quad (47)$$

Though any rough estimate of a couple thousand degrees would have been acceptable.

²Take for instance $\Delta = 10^{-6}$ in some units and $kT = 1$ in the same units. Then all levels are essentially at energy zero i.e. the energy levels are $0, 10^{-6}, 5 \times 10^{-6} \simeq 0, 0, 0$.