Physics 306: Thermal Physics

Final 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:

$$\Gamma(z) \equiv \int_0^\infty x^{z-1} e^{-x} \mathrm{d}x \tag{1}$$

with specific results

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

Gaussian Integrals:

$$I_n = \frac{1}{\sqrt{2\pi}\sigma} \int_{-\infty}^{\infty} \mathrm{d}x\, e^{-x^2/2\sigma^2} x^n \tag{3}$$

with specific results

$$I_0 = 1 \quad I_2 = \sigma^2 \quad I_4 = 3\sigma^4 \quad I_6 = 15\sigma^6 \tag{4}$$

Problem 1. Quick sums

(8 points) Using techniques from the quantum harmonic oscillator, evaluate the following sums in explicit form:

$$S_0 = \sum_{n=0}^{\infty} q^n \qquad S_1 = \sum_{n=0}^{\infty} n q^n \, . \tag{5}$$

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

$$\epsilon_n = n\hbar\omega_0 \tag{6}$$

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

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

This implies

$$S_0 = 1 + q + q^2 + \ldots = \frac{1}{1-q} \tag{8}$$

i.e. the geometric series.

The mean energy of the harmonic oscillator is:

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

This implies

$$\frac{\sum_n n q^n}{\sum_n q^n} = \frac{q}{1-q} \tag{10}$$

So using the first sum we find

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

Alternate: One can also differentiate[1]:

$$q \frac{\partial S_0}{\partial q} = q \sum_n n q^{n-1} = S_1 \tag{12}$$

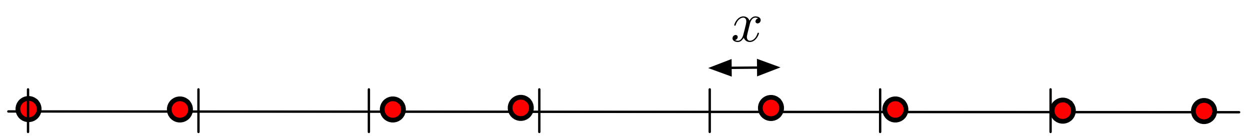
So using S_0 one has

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

[1] This 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 cite center. Here k_0 is the spring constant.



(a) (8 points) 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) (8 points) 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) (8 points) 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

$$E = \frac{p^2}{2m} + \frac{1}{2}k_0x^2 \tag{14}$$

There are two quadratic forms. Thus the mean energy is

$$U = NkT \tag{15}$$

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

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

which doubles the number of quadratic forms leading to

$$U = 2NkT \qquad C_V = 2Nk \tag{17}$$

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

$$\langle V \rangle = \left\langle \frac{1}{2}k_0x^2 \right\rangle = \frac{1}{2}k_BT \tag{18}$$

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

$$\left\langle \delta V^2 \right\rangle = \left\langle V^2 \right\rangle - \left\langle V \right\rangle^2 = \frac{1}{4}k_0^2 \left\langle x^4 \right\rangle - \left\langle V \right\rangle^2 \tag{19}$$

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

The probability of x and p is

$$\mathscr{P}_{x,p} = Ce^{-\beta(p^2/2m+V(x))}dxdp \tag{20}$$

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 $P(x,p)\,\mathrm{d}x\,\mathrm{d}p = P(p)\mathrm{d}p\,P(x)\,\mathrm{d}x$. The part that depends on x is

$$\mathscr{P}_x = P(x)\mathrm{d}x = Ce^{-\beta V(x)}\mathrm{d}x = Ce^{-\beta k_0 x^2/2} = Ce^{-x^2/2\sigma^2}\mathrm{d}x\,, \tag{21}$$

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

$$C = \frac{1}{\sqrt{2\pi\sigma^2}} \qquad \left\langle x^4 \right\rangle = 3\sigma^4\,. \tag{22}$$

So assembling the ingredients

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

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

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

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.

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

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) (8 points) Determine the probability of finding a particle with momentum (magnitude) between p and $p + \mathrm{d}p$, $P(p)\mathrm{d}p$.

(b) (5 points) Determine the mean de Broglie wavelength $\lambda \equiv h/p$ of the particles.

(c) (5 points) Determine the probability of finding a particle with de Broglie wavelength between λ and $\lambda + \mathrm{d}\lambda$?

Solution

(a) We have

$$\mathrm{d}\mathscr{P}_{\boldsymbol{p}} = Ce^{-\beta\epsilon}\,\mathrm{d}p_x\,\mathrm{d}p_y = Ce^{-\beta cp}\,\mathrm{d}p_x\,\mathrm{d}p_y \tag{26}$$

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

$$\mathrm{d}\mathscr{P}_p = Ce^{-\beta cp}\,2\pi p\,\mathrm{d}p \tag{27}$$

Normalizing

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

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

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

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

$$\mathrm{d}\mathscr{P}_p = (\beta c)^2 e^{-\beta cp}\,p\,\mathrm{d}p\,. \tag{31}$$

(b) We compute

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

$$= \int_0^\infty (\beta c)^2 e^{-\beta cp} p\,\mathrm{d}p\,\frac{h}{p} \tag{33}$$

$$= h\beta c \int_0^\infty (\beta c) e^{-\beta cp}\mathrm{d}p \tag{34}$$

$$= h\beta c \tag{35}$$

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

$$dp = \left|\frac{dp}{d\lambda}\right| \mathrm{d}\lambda = \frac{h}{\lambda^2}\mathrm{d}\lambda \tag{36}$$

we find

$$\mathrm{d}\mathscr{P}_\lambda = (h\beta c)^2\, e^{-h\beta c/\lambda}\frac{\mathrm{d}\lambda}{\lambda^3} \tag{37}$$

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.

$$E_2 = 5\Delta$$

$$E_1 = \Delta$$

$$E_0 = 0$$

(a) (8 points) Determine the partition function and mean energy of an atom as a function of temperature.

(b) (8 points not including (ii)) 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) (8 points) 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 $\Delta = 0.1\,\mathrm{eV}$, estimate the temperature (in Kelvin) when the Taylor series becomes approximately valid.

Solution

(a) We have

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

The mean energy is

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

(b) We have

$$P_1 = \frac{e^{-\beta\Delta}}{1 + e^{-\beta\Delta} + e^{-5\beta\Delta}} \qquad P_2 = \frac{e^{-5\beta\Delta}}{1 + e^{-\beta\Delta} + e^{-5\beta\Delta}} \tag{40}$$

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

$$P_1 \to \frac{1}{1+1+1} = \frac{1}{3} \qquad P_2 \to \frac{1}{1+1+1} = \frac{1}{3} \tag{41}$$

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 energy[2] and thus the same probabilities. Your graphs should transition between 0 and 1/3.

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

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

$$\simeq \frac{1-5x}{3-6x} \tag{43}$$

We should now factor out the leading result

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

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

$$3x \ll 1 \tag{45}$$

So the series would begin to work for

$$x = \frac{\Delta}{kT} \sim \frac{1}{3} \tag{46}$$

So roughly when

$$T \sim \frac{3\Delta}{k_B} \simeq \frac{0.3\,\mathrm{eV}}{0.025\mathrm{eV}/300^\circ\mathrm{K}} \sim 3600\,^\circ\mathrm{K} \tag{47}$$

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

[2] Take 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 $0, 10^{-6}, 5\times10^{-6} \simeq 0, 0, 0$.