THE UNIVERSITY OF QUEENSLAND
SCHOOL OF MATHEMATICS AND PHYSICS
PHYS3020/3920/7021 – Statistical Mechanics

Module 1 Worksheet: Microcanonical Ensembles

Module Problem Set Due Monday 15 Aug, 2 pm. Submission portal on Blackboard.

Questions 2, 4, 7 and 8 are for assessment.

1. **[PRACTICE PROBLEM] Partial derivatives**

As an illustration of why it matters which variables you hold fixed when taking partial derivatives, consider the following mathematical example. Let $w = xy$ and $x = yz$.

(a) Write w purely in terms of x and z, and then purely in terms of y and z.

(b) Compute the partial derivatives

$$\left(\frac{\partial w}{\partial x}\right)_y \text{ and } \left(\frac{\partial w}{\partial x}\right)_z,$$

and show that they are not equal. [Hint: To compute, for example, $(\partial w/\partial x)_y$, use a formula for w in terms of x and y, not z.]

(c) Compute the other four partial derivatives of w (two each with respect to y and z), and show that it matters which variable is held fixed.

2. **[FOR ASSESSMENT] Two harmonic oscillators**

The quantum states of a harmonic oscillator have the energy eigenvalues $E_q = q\hbar\omega$, where the quantum number q is a positive integer or zero, and ω is the angular frequency of the oscillator. (We omit the zero point energy $\frac{1}{2}\hbar\omega$.) The number of states is infinite, and the multiplicity of each is one.

(a) Consider a system composed of two harmonic oscillators each of natural frequency ω and each having permissible energies $E_q = q\hbar\omega$, where q is a non-negative integer. Let $U_1 = n_1\hbar\omega$ is the total energy of the system, where n_1 is a non-negative integer. How many microstates are available to the system? What is the entropy of the system as a function of U_1?

(b) Consider a second system also composed of two harmonic oscillators, each of natural frequency 2ω. The total energy of this system is $U_2 = n_2\hbar\omega$, where n_2 is an even non-negative integer. How many microstates are available to the system? What is the entropy of the system as a function of U_2?

(c) Consider now a system composed of two preceding subsystems (separated and enclosed by a totally restrictive wall). What is the entropy of this composite system? Express the entropy as a function of U_1 and U_2.

Answer:

$$S_{total} = k_B \ln\left[\left(\frac{U_1}{\hbar\omega} + 1\right)\left(\frac{U_2}{2\hbar\omega} + 1\right)\right].$$

3. **[PRACTICE PROBLEM] Properties of a Gaussian function**

Consider a probability distribution function for a quantity x given by a Gaussian function

$$f(x) = f(0)e^{-x^2/(2\sigma^2)}.$$

(a) What should be the value of $f(0)$ so that the distribution function is normalised to unity, $\int_{-\infty}^{+\infty} dx f(x) = 1$? Use the value of a Gaussian integral

$$\int_0^\infty dx e^{-a^2x^2} = \frac{\sqrt{\pi}}{2a},\ a > 0.$$

(b) What is the average value of the quantity x, $\langle x\rangle = \int_{-\infty}^{+\infty} dx\, x\, f(x)$?

(c) What is the average value of x^2, $\langle x^2 \rangle = \int_{-\infty}^{+\infty} dx\, x^2\, f(x)$. Use the following integral

$$\int_0^\infty dx\, x^2\, e^{-a^2 x^2} = \frac{\sqrt{\pi}}{4a^3}.$$

(d) Define the rms (root mean square) width of the distribution function $f(x)$ as $w_{\rm rms} = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$. Find $w_{\rm rms}$ for the above $f(x)$. What is the meaning of σ in the above Gaussian $f(x)$?

(e) Plot the function $f(x)$ on a computer for the values $f(0)$ and σ of your choice or sketch $f(x)$ by hand, but indicate the main properties on the graph. Indicate on the graph the length scale corresponding to σ.

(f) Find the half-width at half-maximum of $f(x)$ (define it as $w_{1/2}$) and compare it with $w_{\rm rms}$; which one is greater?

4. **[FOR ASSESSMENT] Stirling Approximation and sharpness of the multiplicity function for a binary system**

(a) Using the Stirling approximation for large $N \gg 1$,

$$N! \simeq \sqrt{2\pi N}\, N^N e^{-N},$$

show that for $|s| \ll N$, the multiplicity function $g(N, s)$ of a binary system with "spin excess" $2s$ can be approximated by a Gaussian distribution

$$g(N, s) \simeq g(N, 0) e^{-2s^2/N},$$

where

$$g(N, 0) \simeq 2^N \sqrt{2/\pi N}$$

(b) Show that the root-mean-square (rms) width σ of this distribution is given by $\sigma = \sqrt{N}/2$, and therefore the fractional width, defined as $s_w = 2\sigma/N$, is equal to $s_w = 1/\sqrt{N}$. Sketch a graph of the function $g(N, s)$ as a function of s (or plot it using Matlab) and indicate on the graph the distance corresponding to 2σ.

5. **[PRACTICE PROBLEM] Flipping 10 coins**

Suppose you flip 10 fair coins

(a) How many possible outcomes (microstates) are there?

(b) What is the probability of getting the sequence HTTHHHTHTH (in exactly that order)?

(c) What is the probability of getting 6 heads and 4 tails (in any order)? Write your answer in percentages.

6. **[PRACTICE PROBLEM] Entropy and temperature**

Consider a system of N particles in a container of volume V with the multiplicty function $g(N, U, V) = f(N) V^N U^{3N/2}$, where U is the energy of the gas and $f(N)$ is a certain function of N (its precise form is not important here).

Show that $U = \frac{3}{2} N k_B T$. This form of $g(N, U, V)$ actually applies to an ideal gas.

7. **[FOR ASSESSMENT] Probability of a royal-flush**

Calculate the number of possible five-card poker hands, dealt from a deck of 52 cards. (The order of cards in a hand does not matter). A royal flush consists of the five highest-ranking cards (ace, king, quoin, jack, 10) of any one of the four suits. What is the probability of being dealt a royal flush (on the first deal)?

Hint: as this is a statistical mechanics course, and this module deals with microcanoncial ensembles, treat this system like a microcanonical ensemble and solve using relevant methods.

8. **[FOR ASSESSMENT] Paramagnetism**

Atoms of many substances have a permanent magnetic dipole moment $\mathbf{m}$. If such a substance is placed in a magnetic field $\mathbf{B}$, the dipoles (or the elementary magnets) try to align in the direction of the field $\mathbf{B}$, so that the potential energy $-\mathbf{m}\cdot\mathbf{B}$ of each dipole becomes minimal. In this case all magnetic moments of the atoms add up to the maximum net magnetic moment $\mathbf{M} = N\mathbf{m}$ of the substance, where N is the total number of dipoles. On the other hand, at a given temperature the statistical motion of the dipoles counteracts the alignment. Namely, there are many more micro-states if the magnetic moments have an arbitrary orientation compared to the case when all of them point in the same direction. In the limit of very high temperature, therefore, all dipoles are statistically distributed, and the magnetic moments cancel each other, so that the net magnetic moment vanishes. In the case of a finite temperature, the mean total moment is somewhere between these extreme cases.

As a model of a paramagnetic substance, consider a binary magnetic system consisting of N sites each occupied by an elementary magnet that can, independently of other magnets, point either up ($\uparrow$) or down ($\downarrow$), corresponding to magnetic moments $\pm m$ (for definiteness, we have assumed that the direction of the magnetic field $\mathbf{B}$ is up). For a configuration with a spin excess of $2s = N_\uparrow - N_\downarrow$, the energy of the system is given by $U = -2smB$, where $B = |\mathbf{B}|$ is the magnetic field strength.

(a) Find the multiplicity $g(N, s)$ of the configuration (macro-state) with a given spin excess $2s$. Hence find the entropy S of the system. Assume that N, as well as $N_\uparrow$ and $N_\downarrow$, are separately much larger than unity. Write down S as a function of N and s.

(b) Hence find the equilibrium temperature of the system T, and express it in terms of U and N.

(c) Invert the result for T to find the thermal equilibrium value of energy U as a function of T. Once this done, the resulting U can be regarded as the thermal average value of energy $\langle U\rangle$ [the thermal average spin excess would then be given by $2\langle s\rangle = -\langle U\rangle/(mB)$]. Express the result for $\langle U\rangle$ in terms of the hyperbolic tanh-function.

(d) What is the limiting behaviour of $\langle U\rangle$ at very high temperatures, $k_B T \gg mB$? To inspect the approach of $\langle U\rangle$ to the limiting value, expand the tanh-function in Taylor series with respect to $mB/k_B T \ll 1$ and keep the first term only. Does your result agree with Curie's law, according to which the net fractional magnetisation, $\frac{M/m}{N} = \frac{2\langle s\rangle}{N}$, decreases as $1/T$ at high temperatures?

(e) What's the limiting behaviour of $\langle U\rangle$ in the opposite limit of $T \to 0$?

9. **[PRACTICE PROBLEM] Paramagnetism (continued)**

For the system considered in the previous problem:

(a) Plot on a computer the function $\langle U\rangle$ for the entire range of temperatures from 0 to ∞. Does your curve agree with the behaviour in the limiting low- and high-temperature regimes found in Problem 8?

(b) Find the heat capacity of the system, $C_B = (\partial\langle U\rangle/\partial T)_{N,B}$. Plot on a computer the heat capacity as a function of T. What is the limiting behaviour of C_B as $T \to 0$ and as $T \to \infty$?

(c) Repeat the derivation for the entropy, the equilibrium temperature, and the thermal average energy $\langle U\rangle$, using the multiplicity function $g(N, s) \simeq g(N, 0)\exp(-2s^2/N)$, which is an approximation valid for $|s| \ll N$ and $N \gg 1$ (see Lecture notes). Do you reproduce the high-temperature result for $\langle U\rangle$, from the previous problem? Explain why the low-temperature behaviour of $\langle U\rangle$ is not recovered.