PHY 831: Statistical Mechanics
Homework 4

Due October 13th, 2020

1. Maximize the Gibbs entropy (with $k_B = 1$) subject to the constraints

$$\begin{aligned}\langle x \rangle &= \sum_i x_i p(x_i) \\ \langle x^2 \rangle &= \sum_i x_i^2 p(x_i),\end{aligned}$$

   to find the probability distribution of x_i. Here, $p(x_i)$ is the probability of x_i. Show that this becomes the normal distribution when x is allowed to be continuous and run from $-\infty$ to ∞, i.e.

$$p(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-(x-\mu)^2/2\sigma^2}$$

   with $\mu = \langle x \rangle$ and $\sigma^2 = \langle x^2 \rangle - \langle x \rangle^2$. Note that for continuous x, $p(x)$ is a probability density, so that the normalization condition is given by $\int_{-\infty}^{\infty} dx p(x) = 1$, for instance.

2. Consider a system in the grand canonical ensemble with two single-particle energy states 0 and ϵ.

   (a) Assuming the particles are Fermions, calculate $\langle N \rangle$ as a function of μ and T. Show the limits as $T \to 0$ and ∞.

   (b) Assuming the particles are Bosons, calculate $\langle N \rangle$ as a function of μ and T. Show the limits as $T \to 0$ and ∞.

3. Consider a system with two single-particle states 1 and 2. This system could also be in the mixed states

$$|\psi_\pm\rangle = \frac{1}{\sqrt{2}} [|1\rangle \pm |2\rangle]$$

   (a) Write down the density matrix for the system in the basis defined by 1 and 2 when the system is in state $|\psi_+\rangle$ and verify $\hat{\rho}^2 = \hat{\rho}$.

   (b) Now consider the density matrix

$$\hat{\rho} = \sum_{\alpha=\pm} p_\alpha |\psi_\alpha\rangle\langle\psi_\alpha|,$$

   $p_+ + p_- = 1$. Find the value of p_+ which minimizes the purity of the ensemble, $\mathrm{Tr}[\hat{\rho}^2]$.

4. In some cases, we might want to talk about systems that have a net macroscopic angular momentum in a particular direction. If the system could exchange angular momentum and energy with the world around it, then it would be natural to describe its properties in terms of an ensemble subject to the constraints $\langle L \rangle = \sum_i p_i L_i$, $\sum_i p_i = 1$, and $\langle E \rangle = \sum_i p_i E_i$, but with every ensemble member having fixed volume V and particle number N.

   (a) Write down the normalized probability p_i for drawing an ensemble member in state i and define the normalization coefficient (or partition function) for this ensemble Z_L.

   (b) Consider a system of N distinguishable quantum rotors that rotate about the same fixed axis, with single particle energies $\epsilon_m = \frac{\hbar^2}{2I} m^2$ and single particle angular momenta $\ell = \hbar m$, where $m = -\infty, ..., -1, 0, 1, ...\infty$. I is the moment of inertia of a single rotor. Calculate Z_L for this system (eventually assuming that the energy levels are closely spaced enough to take sums over m to integrals).

   (c) Calculate the average angular momentum of the system of quantum rotors and show that the Lagrange multiplier associated with the angular momentum constraint multiplied by T can be interpreted as the net angular velocity of the system.

   (d) Calculate the average energy of the system of quantum rotors.

5. Assume there are N random variables labeled by $i = \{1, ..., N\}$ that each obey the arbitrary normalized probability distribution $g(x)$, so that they have averages $\langle x_i^n \rangle = \int dx x^n g(x_i)$. Assume that $\langle x_i \rangle = 0$ and $\langle x_i^2 \rangle = \sigma^2$ for all i. Show that the distribution of the average of these random variables, $\bar{x} = \frac{1}{N} \sum_i x_i$, in the large N limit is given by

$$P(\bar{x}) = \frac{1}{\sqrt{2\pi\sigma^2/N}} e^{-\frac{N\bar{x}^2}{2\sigma^2}},$$

   which is essentially the central limit theorem, which says that the probability distribution of the sum of a large number of random variables tends to a Gaussian (or normal) distribution. Therefore, it is maybe not so surprising that this distribution shows up quite often in statistical mechanics. This also shows the standard deviation of $\bar{x}$ is $\propto 1/\sqrt{N}$, since we have $\int_{-\infty}^{\infty} dx x^2 \exp(-x^2/2\sigma^2) = \sqrt{2\pi}\sigma^{3/2}$, and the distribution of $\bar{x}$ goes to a delta function in the large-N limit [Hints: Use $\delta(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dy e^{ixy}$ and $\int_{-\infty}^{\infty} \exp(iay - by^2) = \sqrt{\pi/b} \exp(-a^2/4b)$.]