Physics 727: Assignment 4

(to be submitted by Thursday, April 4, 2024)

1. Consider a system whose density of states is given by

$$g(\varepsilon) = \delta(\varepsilon + W/2) + 2\delta(\varepsilon + W/4) + \frac{\varepsilon}{W^2}\left(1 - \frac{\varepsilon}{W}\right)\theta(\varepsilon(W - \varepsilon)).$$

   (a) Explain what roles the delta (δ) and Heaviside (θ) functions are playing here. Plot $g(\varepsilon)$ versus ε/W.

   (b) Compute the partition function,

$$Z = \int_{-\infty}^{\infty} d\varepsilon\, g(\varepsilon) e^{-\beta\varepsilon}.$$

   (c) Prove that, in general,

$$S = k_B\left(1 - \beta\frac{d}{d\beta}\right)\ln Z \text{ and } C_V = -\beta\frac{dS}{d\beta}.$$

   Then determine the particular expressions for S and C_V that obtain for this system. (The derivatives are a bit tedious. *Mathematica* may be appropriate here.)

   (d) At what value of $T = W/k_B\beta$ (roughly) does an increase in temperature $T \to T+dT$ lead to the largest gain in internal energy. (*Hint:* Make a plot of S and C_V, each versus βW; the entropy is monotonically decreasing in βW, and that function's inflection point gives rise to a peak in the specific heat.)

   (e) Without actually computing the internal energy $U = -(d/d\beta)\ln Z$, show that $\lim_{\beta\to\infty} U = -W/2$ and $\lim_{\beta\to 0} U = -11W/38$. Just make an argument based on which levels are filled or unfilled in the low ($k_BT \ll W$) and high ($k_BT \gg W$) temperature limits.

2. A free particle in D spatial dimensions has a hamiltonian

$$H(p,x) = H(p) = \frac{1}{2m}(p_1^2 + p_2^2 + \cdots + p_D^2).$$

   According to the equipartition theorem, the internal energy for such a system in the canonical ensemble is $U = D \times (k_BT/2) = Dk_BT/2$, and the corresponding heat capacity if $C_V = Dk_B/2$. Given a partition function (in arbitrary dimension D) of the form

$$Z \sim \int d^D p\, e^{-\beta H(p)} \sim \int_0^{\infty} d\epsilon\, g(\epsilon)\, e^{-\beta\epsilon},$$

   what can you say about the functional form of the density of states, $g(\epsilon)$? [*Hint:* Recall that from previous examples that $g(\epsilon) \sim \sqrt{\epsilon}$ in three spatial dimensions and $g(\epsilon) \sim 1/\sqrt{\epsilon}$ in one.]

3. Consider a one-dimensional classical system with Hamiltonian $H(p,x) = p^2/2m + F_0|x|$. This Hamiltonian describes a particle of mass m subject to a force $F(x) = -F_0\,\mathrm{sgn}(x)$ that pulls the particle with constant force F_0 back toward the origin. Imagine that an ensemble of such systems is prepared at temperature T.

   (a) Compute the partition function. You should be able to show that $Z = (T/T_0)^{3/2}$, where

$$T_0 = \frac{1}{k_B}\left(\frac{h^2F_0^2}{8\pi m}\right)^{1/3}.$$

   (b) Compute the free energy (in terms of k_B, T, and T_0).

   (c) Compute the internal energy

   (d) Compute the entropy.

(e) Compute the heat capacity. You should find that $C_V = 3k_B/2$. In a real-world example, why might you expect this value to drop to $C_V = k_B$ at ultra-cold temperatures? *Hint:* physical realism almost certainly demands that the actual potential deviates from the model potential sufficiently close to the point of nonanalyticity at $x = 0$.

4. A one-dimensional system has a hamiltonian $H = p^2/2m + V(x)$ in which an otherwise free particle of mass m is confined by a trapping potential $V(x) = (K/2)x^2\left[1 + (x/x_0)^2\right]^{-1/3}$.

   (a) Sketch $V(x)$, emphasizing its small-, intermediate-, and large-x behaviour.

   (b) Show that the potential has an expansion

$$V(x) = \frac{K}{2}x^2 - \frac{K}{6x_0^2}x^4 + \frac{K}{9x_0^4}x^6 + \cdots$$

   (c) Compute the partition function, using a cumulant expansion to handle the nonquadratic terms in the integral. You should be able to show that

$$Z = \frac{1}{\beta\hbar}\sqrt{\frac{m}{K}}\exp\left(\frac{1}{2\beta K x_0^2} - \frac{5}{3\beta^2 K^2 x_0^4} + \cdots\right).$$

   (d) Show that the heat capacity has an expansion

$$C_V = k_B\left(1 + \frac{k_B T}{K x_0^2} - \frac{10(k_B T)^2}{(K x_0^2)^2} + \cdots\right)$$

   in terms of the dimensionless parameter $k_B T/K x_0^2$.

5. Start from the partition function of a tilted harmonic well,

$$Z = \int_{-\infty}^{\infty} dx\, \exp\left[-\beta\left(\frac{1}{2}Kx^2 - fx\right)\right] = \sqrt{\frac{2\pi}{\beta K}}\, e^{\beta f^2/2K}.$$

   (a) Find explicit expressions for the first six moments

$$\begin{aligned}
\langle x \rangle &= \frac{1}{\beta Z}\frac{\partial Z}{\partial f} \\
\langle x^2 \rangle &= \frac{1}{\beta^2 Z}\frac{\partial^2 Z}{\partial f^2} \\
&\vdots \\
\langle x^6 \rangle &= \frac{1}{\beta^6 Z}\frac{\partial^6 Z}{\partial f^6}
\end{aligned}$$

   (b) Identify the mean and variance of the distribution.

   (c) Use the relationship

$$\langle e^{\lambda x} \rangle = \exp \sum_{n=0}^{\infty} \frac{\lambda^n \langle x^n \rangle_c}{n!}$$

   to define and compute the cumulants $\langle x^n \rangle_c$.

   (d) You should be able to prove that $\langle x \rangle_c = f/K$, $\langle x^2 \rangle_c = 1/2\beta K$, and that all other cumulants vanish identically.