Problem D1

Consider a particle in a harmonic oscillator with energy levels nhf, where $n = 0, 1, 2, \ldots$, at temperature T.

Question a:

Show that the partition function Z of the particle is

$$Z \simeq \left(\frac{kT}{hf}\right)^{\kappa}$$

for $kT \gg hf$ and give a value for κ.

Consider now a particle, which can sit in two harmonic oscillators. Oscillator A has energy levels nhf, and oscillator B has energy levels $\epsilon_0 + nhf$, where $\epsilon_0 > 0$ and $n = 0, 1, 2, \ldots$. The particle can hop freely between the two oscillators, and the available states for the particle are therefore the harmonic oscillator levels in A and B.

Question b:

Give an expression for the partition function for the particle, when the temperature is T. What is the probability P_A that the particle sits in oscillator A?

Question c:

Give an expression for the average energy $E(T)$ of the particle. Show that $E(T) \approx a + bT$ when kT is large compared to both hf and ϵ_0, and give values for a and b.

Problem D2

Consider a single particle, which can occupy any of the 6 energy levels shown in figure 1. Three of the energy levels are at the energy ϵ_1, two are at the energy ϵ_2, and one is at the energy ϵ_3. Here, $\epsilon_3 > \epsilon_2 > \epsilon_1$. The system is in thermal equilibrium with a reservoir at temperature T.

Question a:

Give an expression for the partition function Z of the system.

Question b:

Compute the mean energy $\bar{E}$ of the system.

Question c:

Compute the limits $T \to 0$ and $T \to \infty$ of $\bar{E}$ and explain both limits physically.

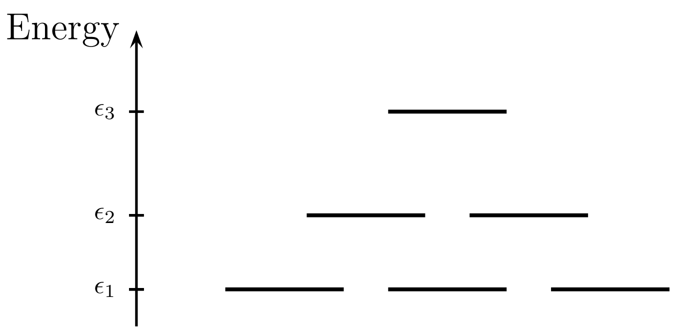

Figure 1: The 6 energy levels of the considered system.

Hand-in D

An alternative definition of the entropy is

$$S = -k \sum_r p_r \ln(p_r), \tag{1}$$

where p_r is the probability of the system to be in microstate r and the sum is over all microstates accessible to the system. We take Eq. (1) to hold for any probability distribution p_r with $\sum_r p_r = 1$ and $p_r \geq 0$.

Question a:

For an isolated system in equilibrium, $p_r = p_0 \equiv 1/\Omega$ for all accessible states r. Show that in this case, Eq. (1) reduces to our basic definition given by Schroeder Eq. (2.45), i.e. $S = S_0 \equiv kln(\Omega)$.

Question b:

Take a system with another probability distribution p_r and entropy S. Show that

$$S_0 - S = k \sum_r p_0 \frac{p_r}{p_0} \ln\left(\frac{p_r}{p_0}\right). \tag{2}$$

Question c:

Show that we can write

$$S_0 - S = kp_0 \sum_r f(p_r/p_0) \tag{3}$$

with $f(x) = xln(x) - x + 1$.

Question d:

Show that $f(x) > 0$ for all $x \geq 0$, except for $x = 1$ where $f(x) = 0$. *Hint*: Look at the sign of $f'(x)$.

Question e:

Prove that $S \leq S_0$ for all probability distributions p_r over microstates, and that the equality sign only holds for $p_r = p_0$.

You have now shown that the entropy is maximum when the probability is constant for all accessible states for an isolated system, i.e. when it is in equilibrium.