Indian Institute of Science Education and Research, Trivandrum

PHY-221 **Stat-Mech Problem set 4** **19.2.2015**

Note: Deadline: 27 February 2015 (12:30 PM)

---

1. The hydrocarbon 2-butene, $CH3 - CH = CH - CH3$ occurs in two geometrical structures (conformations) called the cis- and trans-conformations. The energy difference ΔE between the two conformations is approximately $\Delta E/k_B = 4180$ K, with the trans conformation lower than the cis conformation. Determine the relative abundance of the two conformations at $T = 300\ K$ and $T = 1000\ K$.

2. Consider a three level single particle system with five microstates with energies 0, ϵ, ϵ, ϵ and 2ϵ. What is the mean energy of the system if it is equilibrium with a heat bath at temperature T ?

   Based on the above problem, can you generalize the definition of the partition function?

3. In the previous problem set, you might have realised that, in the microcanonical ensemble, extending the analysis of 2-spin system to higher spin system is an Herculian task. In the canonical ensemble, the extension can be handled.

   Consider a system of N atoms each of which may exist in three states of energies $-\epsilon, 0, +\epsilon$. This system is fixed at a temperature T. Let us specify the macrostates of the system by N, n, the number of atoms in the zero energy state, n_+ and n_- are the number of atoms in $+\epsilon$ and $-\epsilon$ states

   (a) Calculate the partition function of this system.

   (b) Calculate the entropy and specfic heat of this system.

4. A rigid quantum rotator has energy levels $E_{rot}(l)$ with degeneracy $g(l)$ given by

$$E_{rot}(l) = l(l+1)\frac{\hbar^2}{2I} \qquad g(l) = 2l + 1 \qquad l = 0, 1, 2, ...$$

   where I is the moment of inertia which is a constant.

   (a) Find the canonical partition function of a N non-interacting of these molecules.

   (b) Evaluate the specific heat at high temperatures and at low temperatures.

   Hint: Use the result of Problem 2

5. Suppose that a system of N atoms of type A is placed in diffusive contact with a system of N atoms of type B at the same temperature and volume. Show that after diffusive equilibrium is reached the total entropy has increased by $2\,N\ln 2$ compared to the entropy when the systems were not in contact. This entropy increase is known as the entropy of mixing. If the atoms are identical (i.e. $A = B$), show that there is no increase in entropy when diffusive contact is established. This difference was first highlighted by Gibbs and is sometimes called Gibbs paradox.