CCP5 Summer School: Statistical Mechanics

1. Consider a system of N_A particles of type A and N_B particles of type B that lie on a lattice that contains $N = N_A + N_B$ total sites. Note that each of the A particles are indistinguishable from the other A particles, and the same holds for the B particles.

   Calculate the entropy of difference between a state where all the A and B particles are confined to different parts of the system and another state where both types can roam anywhere in the system. This is the entropy change of mixing. Use the Stirling approximation for $N!$ (i.e. $\ln N! \approx N \ln N - N$, when $N \gg 1$).

2. Consider a system of N free particles in which the energy of each particle can assume two and only two distinct values, 0 and ε ($\varepsilon > 0$). Denote by n_0 and n_1 the occupation numbers of the energy level 0 and ε, respectively. The total energy of the system is U.

   (a) Find the energy for the system in terms of the occupation numbers.

   (b) Find an expression for the entropy of the system in terms of the number of particles N and the total energy U.

   (c) Find the temperature as a function of U, and show that it can be negative. Assume that the system is sufficiently large that the Stirling approximation (i.e. $\ln N! \approx N \ln N - N$) can be used.

   (d) What happens when a system of negative temperature is allowed to exchange heat with a system of positive temperature?

3. Consider a classical system of N noninteracting diatomic molecules enclused in a box of volume V at temperature T. The Hamiltonian for a *single* molecule is taken to be

$$H(\mathbf{p}_1, \mathbf{r}_1, \mathbf{p}_2, \mathbf{r}_2) = \frac{1}{2m}(p_1^2 + p_2^2) + \frac{k}{2}|\mathbf{r}_1 - \mathbf{r}_2|^2$$

   where $\mathbf{p}_1$, $\mathbf{p}_2$, $\mathbf{r}_1$, and $\mathbf{r}_2$ are the momenta and positions of the two atoms in a molecule. Find

   (a) the Helmholtz free energy of the system,

   (b) the pressure of the system,

   (c) the specific heat at constant volume, and

   (d) the mean square molecular diameter $\langle |\mathbf{r}_1 - \mathbf{r}_2|^2 \rangle$.