Department of Physics   Prof. R. Bundschuh
The Ohio State University

Fourth Problem Set for Physics 847 (Statistical Physics II)

Winter quarter 2004

Important dates: Feb 10 10:30am-12:18pm midterm exam,
                     Mar 16 9:30am-11:18am final exam

Due date: Tuesday, Feb 3

10. A two-dimensional solid   *10 points*

Consider a two-dimensional lattice in the x-y-plane with sides of length L_x and L_y which contains N atoms (N very large) coupled by nearest-neighbor harmonic forces.

  a) Compute the Debeye frequency for this lattice. Note, that although the atoms are in a two-dimensional lattice they can still oscillate in three space directions. However, in a planar solid, there are three sound velocities: one transversal within the plane of the solid, one transversal out of the plane of the solid, and one logitudinal.

  b) Calculate the heat capacity of this solid. You may use the results from the lecture that are independent of the dimension of the solid without rederiving them.

  c) What is the asymptotic behavior of the heat capacity for very large temperatures?

  d) What is the asymptotic behavior of the heat capacity for very small temperatures? (Hint: $\int\limits_{0}^{\infty} dx\, x^3 \frac{\exp(x)}{(\exp(x)-1)^2} = 6\zeta(3)$.)

11. Rotational degrees of freedom   *10 points*

Hydrogen molecules can exists in two forms: ortho- and para-hydrogen.

  a) The two electrons of H_2 in para-hydrogen form a singlet (antisymmetric) state. The orbital angular momentum can thus only take even values $E_p = \frac{\hbar^2}{2I}L(L+1)$, where $L = 0, 2, 4, \ldots$. Write down the rotational partition function of a single para-hydrogen. You will not be able to actually perform the sum which you get.

  b) In ortho-hydrogen, the electrons are in triply degenerate states, hence $E_o = \frac{\hbar^2}{2I}L(L+1)$, where $L = 1, 3, 5, \ldots$. Write down the rotational partition function of a single ortho-hydrogen. Do not forget the factor of three representing the degeneracy of the electronic states.

  c) For an equilibrium gas of N hydrogen molecules (which contains both para- and ortho-hydrogen), calculate the total partition function coming from the rotational degrees of freedom. (Hint: Sum over contributions from mixtures of N_p para- and $N_o = N - N_p$ ortho-hydrogen particles.)

d) Write down the expression for the rotational contribution to the internal energy $\langle E_{rot} \rangle$, and discuss its low and high temperature limits. (Hint: at high temperatures you can replace the sum by an integral but you should say why.)

12. DNA denaturation *12 points*

DNA is a long molecule consisting of N units called "bases". The natural state of a DNA molecule in a cell is a configuration in which two of these DNA molecules are bound together base by base, i.e., base 1 of the first molecule is bound to base 1 of the second molecule, base 2 of the first molecule is bound to base 2 of the second molecule and so on. In this state the DNA takes on its well-known double helical structure. Chemical differences between the bases prevent the bases at different positions to bind to each other. If temperature rises these bindings can break up. We want to describe this process. To this end, we assign a variable s_i, $i \in \{1, \ldots, N\}$ to each of the N bases of one of the molecules. s_i can take the values 0 and 1. $s_i = 1$ means that the base is bound to its partner base in the other molecule; $s_i = 0$ means that the base is unbound. There are two energetic contributions in this system: A bound pair of bases gains a binding energy ε_0. In addition, there is an energy gain of ε_s whenever two neighboring bases are bound. The latter results from a favorable interaction between neighboring bases of the same molecule which can occur only if both bases are bound to the corresponding bases in the other molecule. The total binding energy of a configuration $(s_1, \ldots, s_N)$ is

$$H(s_1, \ldots, s_N) = -\varepsilon_0 \sum_{i=1}^{N} s_i - \varepsilon_s \sum_{i=1}^{N} s_i s_{i+1}.$$

We assume that the DNA molecule is closed to a ring, i.e., that $s_{N+1} = s_1$ (this is indeed the case for bacterial genomes.)

a) Calculate the partition function of this system in the limit of very long molecules.

b) Calculate the fraction of bound bases. Since the number of bound bases in a given configuration is given by $\sum_{i=1}^{N} s_i$, the fraction of bound bases is $\langle \sum_{i=1}^{N} s_i \rangle / N = \langle s_1 \rangle$ where the equality is due to the translational invariance. Since in reality $\varepsilon_0 \ll \varepsilon_s$, we can set $\varepsilon_0 = 0$ in the result.

c) Calculate the heat capacity of such a pair of DNA molecules at $\varepsilon_0 = 0$.

d) Plot the fraction of bound bases and the heat capacity as functions of dimensionless temperature $k_B T / \varepsilon_s$ at $\varepsilon_0 = 0$.