UNIVERSITÄT LEIPZIG INSTITUT FÜR THEORETISCHE PHYSIK PROF. DR. B. ROSENOW

Statistical Physics, Spring 2011 Problem Set 6

Course Information:

- Class times: lectures Monday and Thursday, 11:00-12:30 in SR 218, tutorials Friday, 9:15-10:45 in SR 221
- ☞ Final exam: July 11, 13:30 in ThHS
- The course website is www.uni-leipzig.de/~stp/Statistical_Physics.html
- In the tutorials you will be expected to present solutions to the class on a volunteer basis. Before each class please decide whether you would like to present any particular problem. If nobody volunteers you may be asked to present. The purpose of this is to gain experience working through problems as a group. Therefore it is informal and need not cause concern. In particular, *please* do not skip a class because you could not complete the problem set. These are the classes you most need to attend!

For questions regarding the problem sets, please email Tony at anthony.wright in the uni-leipzig.de

Problem 18: Conservation of entropy (4 Marks).

Consider a classical ensemble whose dynamics in phase space are given by the Hamiltoinian $H(\vec{X})$. Show that the Gibb's entropy of the ensemble density $\rho(\vec{X}, t)$ is a constant.

Show this also for a quantum mechanical ensemble. For this consider the Gibb's entropy as a function of the density matrix $\hat{\rho}$ whose dynamics follows from the Hamiltonian H.

Problem 19: The one dimensional Ising model with interactions (6 Marks) Here we shall examine a system of *interacting* degrees of freedom: N + 1 Ising spins $S_i = \pm 1$, i = 0, 1, 2, ..., N placed along a single line.

Let the energy of the microstate S be

$$\mathcal{H}(\{S\}) = -J\sum_{i=1}^{N} S_i S_{i-1}.$$

- (a) To count the microstates, it is useful to consider how many states there are with equal energy. The energy of the system can be expressed by the number ν of broken bonds (Neighbouring pairs with anti-parallel spins, see Fig.). Determine the possible energies E_{ν} , and the corresponding number of microstates, and the microcanonical partition function $Z^{(\text{mc})}(E_{\nu})$?
- (b) Using the result of (a), calculate the canonical partition function

$$Z^{(k)}(\beta) = \sum_{\{S\}} e^{-\beta \mathcal{H}(\{S\})} = \sum_{\nu} Z^{(mk)}(E_{\nu}) e^{-\beta E_{\nu}}.$$

(c) For $N \to \infty$, calculate and sketch the following quantities in the canonical ensemble as a function of temperature: The average energy, the heat capacity, and the Gibb's entropy.

Problem 20: Polymers II (6 Marks)

We have previously studied a directed polymer whose starting point was $x_0 = y_0 = 0$, and end point was $x_N = N, y_N = y$. Because all polymer configurations had equal length, we shall assume that the energy of all configurations is equal. Calculate, using the canonical distribution, the internal energy, the entropy, and the free energy of the directed polymer with fixed end-points, and for free end-points. Use appropriate approximations, when necessary.

To investigate the possible configurations of flexible polymers, we can proceed as follows: one can first project the path of the polymer onto the y-axis, and obtain the configurations as in the figure.

In a higher-dimensional configuration, let the polymer configurations now be given as a path of N segments on a three-dimensional cubic lattice. The starting point $\mathbf{r}_0 = 0$ is fixed, and the end-point is flexible, $\mathbf{r}_N = \mathbf{r}$. All configurations have the same energy (this is the so-called Orr-Model for flexible polymers from 1947).



- (a) Calculate $\langle r^2 \rangle$ by dividing r into individual segments, and use that the orientation of each individual segment is independent.
- (b) Try to estimate the number of different configurations $Z(\mathbf{r})$ that relate to the given start and end-points. Avoid if possible, the correct summation over the micro-states, rather use your knowledge of $\langle \mathbf{r}^2 \rangle$. Calculate the entropy and the free energy as a function of \mathbf{r} .
- (c) Calculate, from F(r) the force that must be applied to keep the ends of the polymer within the distance r.

