Statistical Mechanics Fall 2014 — Problem Set 1

due: Wednesday, November 19, 2014

1.1 1-d gas with interactions (50 points)

Not many statistical mechanics models of interacting particles can be solved *exactly*. Such solutions are valuable as they allow to check the validity and reliability of different approximations.

One exactly solvable model, which will be studied in this problem, is a one-dimensional gas with short range interactions. Consider N (indistinguishable) particles of mass m confined to a line of length L, in which they are free to move. The positions of the particles $\{x_i\}$ will be labelled according to their *order*, i.e.,

$$0 \leq x_1 \leq x_2 \leq \ldots \leq x_N \leq L. \quad (1)$$

(a) First, consider a gas of hard impenetrable rods, each of length a. In the microcanonical ensemble, calculates the entropy of the gas as a function of the energy E, the number of particles N and the length L. Obtain the equation of state of the gas and compare the result to that of an ideal gas.

(b) Now consider a general interaction potential. We will assume that the particles screen the interactions, and therefore they only interact with their *nearest* neighbors. In this case he Hamiltonian can be written as

$$\mathcal{H} = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \sum_{i=2}^{N} V(x_i - x_{i-1}), \quad (2)$$

where $V(x)$ is the interaction potential. Write down the expression for the canonical partition function $Z(T, N, L)$. Change variables to $\delta_1 = x_, \delta_2 = x_2 - x_1, \ldots, \delta_N = x_N - x_{N-1}$. Be careful with the allowed ranges of integration.

(c) The trick that allows a general calculation of the expression from (b) is to move to the constant-pressure ensemble. The partition function of the constant-pressure ensemble is obtained from the Laplace transformation

$$\mathcal{Z}(T, N, f) = \int_0^\infty dL \exp(-\beta f L) Z(T, N, L), \quad (3)$$

where f is the force (the pressure in one dimension). Find the standard formula for f in the canonical ensemble via a saddle point approximation of equation (3).

(d) Change variables from L to $\delta_{N+1} = L - \sum_{i=1}^{N} \delta_i$, and find the expression for $\mathcal{Z}(T, N, f)$ as a product of one-dimensional integrals over each δ_i.

(e) At a fixed force f, find expressions for the mean length $L(T, N, f)$, and the density $n = N/L(T, N, f)$ (involving ratios of integrals that should be easy to interpret). Verify that you recover the known equation of state in the case of an ideal gas (i.e., when $V(x) = 0$ for all x).

(f) Calculate the Gibbs free energy and the entropy (as a function of T, N, f) for the interaction energy given by

$$V(x_i - x_{i-1}) = \begin{cases} \epsilon & |x_i - x_{i-1}| \leq a \\ 0 & |x_i - x_{i-1}| > a \end{cases} . \tag{4}$$

Verify that you recover the entropy calculated in (a) in the case of hard rods, i.e., when $\epsilon \to \infty$.

1.2 Virial expansion of hard-core particle gas (50 points)

Consider a particle gas with hard core interparticle interaction

$$u(r) = \begin{cases} \infty & r < \sigma \\ 0 & r > \sigma, \end{cases} \tag{5}$$

where r is the inter-particle distance.

(a) Compute the second and third virial coefficients for a hard-core gas in $d = 1$ dimensions.

(b) Do the same in $d = 2$ dimensions.

(c) Compute the isothermal compressibility κ_T and the constant-pressure heat capacity c_p for the hard-core gas in $d = 1, 2, 3$ dimensions using the virial expansion to third order. The virial coefficients in $d = 3$ dimensions do not need to be calculated, they are given by $B_2^{(3d)}(T) = 2\pi\sigma^3/3$ and $B_3^{(3d)}(T) = 5\pi^2\sigma^6/18$. Discuss the effect of dimensionality on your results.

(d) In question 1.1a you found the equation of state of a 1-dimensional gas of hard rods. From this expression obtain the general virial coefficient $B_\ell(T)$ of this gas. Compare with the results of (a).

1.3 Monte Carlo simulation (10 bonus points) (due: 3/12/2014)

In this question you will use MC simulation to study the magnetization in a two-dimensional Ising model with Metropolis dynamics. Note that although the Metropolis dynamics is probably not a realistic model of the dynamics of real magnets (as was stressed in class), it is nonetheless instructive from a theoretical perspective to explore this dynamics.

Consider a two dimensional Ising model on an $L \times L$ square lattice with periodic boundary conditions. The Hamiltonian of the model is given by

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} s_i s_j, \tag{6}$$

where $s_i = \pm 1$ and $\sum_{\langle i,j \rangle}$ denotes a sum over all nearest neighbour pairs. This model undergoes a phase transition at $T_c = 2J/\log(1+\sqrt{2}) \simeq 2.27J$. In this question, set $T = 3J$ to assure that the system is in the disordered phase.

Implement the metropolis algorithm in your favorite programming language. Work with the largest system for which you can collect enough statistics. In C, Fortran, Java and similar languages you should be able to reach systems of size $L = 200$, while in Matlab you will probably be limited to $L \approx 10$. Therefore, it is preferable that you do not run the simulation in Matlab if possible. You may download from the course website a code example written in C++, which you may alter to model the Ising dynamics. This code can be easily compiled on the computers found in the computer lab, as explained in the instructions in the website.

(a) Verify that you are in the disordered phase by measuring that $\langle M \rangle = \langle \sum_i s_i \rangle = 0$ at $T = 3J$. Attach a plot of $M(t)$.

(b) Measure the correlation function for the magnetization

$$C(\Delta t) = \langle (M(t) - \langle M \rangle)(M(t + \Delta t) - \langle M \rangle) \rangle, \tag{7}$$

for several values of Δt. The correlation function is expected to have an exponential decay, i.e. $C(\Delta t) \sim e^{-\Delta t/\tau_{\text{corr}}}$. Estimate τ_{corr} from $C(\Delta t)$ and attach a plot of $C(\Delta t)$.

(c) Measure the fluctuations in the magnetization by averaging

$$\sigma_M^2 = \left\langle (M - \langle M \rangle)^2 \right\rangle \tag{8}$$

at time steps larger than τ_{corr}. Measure the fluctuations for several system sizes (smaller than the maximal one you can simulate) and plot a graph which demonstrate that σ_M scales with L as you would expect from the central limit theorem.

Note: Please attach your code to your answer. Make sure to save your code, as it will be useful for future homework assignments.