Course: Statistical Mechanics
Problem Set: 1
Due: 11th Apr 2007

1. Harmonic Oscillator in Microcanonical Ensemble: Let us take N classical one-dimensional harmonic oscillators which have the same mass and the same spring constant. The hamiltonian for the ith oscillator is

$$H_i = \frac{p_i^2}{2m} + \frac{m\omega^2 x_i^2}{2}$$

and the hamiltonian of the full system is given by $H = \sum_i H_i$. Calculate entropy S as function of energy E (the value of H), using microcanonical ensemble.

2. Particles in a Vertical Cylinder: We have semi-infinite vertical cylinder under the action of gravity (assume the acceleration due to gravity, g, to be constant). The cylinder has N independent particles of mass m. The potential energy is mgz with when the particle is at a height z above the lowest point.

a) Calculate the partition function of the system.

b) Calculate internal energy per particle from the partition function.

c) Calculate number density as a function of height z. How far up from the lowest point do you have to go to have density drop by a factor of e? Call this length h. How much would h be if these particles had molecular weight 30 and the temperature was 300K?

d) What is the pressure at the base of the cylinder, when the base area is A? For ideal gas $PV = Nk_BT$ or $V = Nk_BT/P$. What is the Nk_BT/P for the model of particles in the cylinder, with P being the pressure at base? Could you interpret this result?

3. Debye Model in Two Dimensions: Let us make a 2-dimensional version of Debye model! The number of modes between the frequencies ω and $\omega + d\omega$ is given by

$$\Omega(\omega)d\omega = \frac{A\omega d\omega}{\pi c^2}, \text{ for } 0 \leq \omega \leq \omega_D$$

where A is the area and c is the velocity of sound. $\Omega(\omega)$ is zero outside the range $[0, \omega_D]$.

a) Calculate the specific heat of the system at low temperature (i.e. get the leading power law term in the dependence on temperature for low temperature).

b) For an energy eigenstate of the a quantum harmonic oscillator, the average kinetic energy is the same as the average potential energy. Using this one can show that

$$< \vec{x}_n^2 >= \frac{1}{mN} \sum_{\text{modes}} \frac{1}{\omega^2} < E(\omega) >$$

where $< E(\omega) >$ is the thermal average of energy in the mode with frequency ω, and N is the number of particles.

Compute this sum for low temperatures for 3-dimesional Debye model (for the density of modes).

What happens if you compute the same quantitity ($< \vec{x}_n^2 >$) in the 2-dimensional version of Debye model? What does is say about the nature of two dimensional crystals?

4. One Dimensional Ising Model: One Dimensional Ising model with periodic boundary condition has

$$E = -J \sum_{i=1}^{N} S_i S_{i+1} - h \sum_{i=1}^{N} S_i$$

with $S_{N+1} = S_1$.

Calculate the correlation function

$$C(n) =< S_i S_{i+n} > - < S_i >< S_{i+n} >$$

using the transfer matrix method, when N goes to infinity.

5. Simulating Two Dimensional Ising Model: Two dimensional Ising model on a square lattice as interaction parameter J for each bond.

$$E = -J \sum_{i,j NN} S_i S_j - h \sum_{i} S_i$$

(NN means the sites are nearest neighbors on the square lattice). The total magnetization M is given by $\sum_i S_i$.

Set $h = 0$ to begin with so that

$$E = -J \sum_{i,jNN} S_i S_j$$

a) Simulate the system by Metropolis Algorithm for 20×20 lattice with periodic boundary conditions for $\beta J = 0.1, 0.2, 0.3, 0.4, 0.5$.

Explore how long you need to run the system to get to the equilibrium distribution. Calculate $< E >$ and $< M^2 >$ for each of these values of βJ. Estimate errors.

b) For this problem, set $J = 1$. Turn on a small field h. Measure the per spin magnetization $m = M/N$ and calculate the susceptibility $\chi = \partial m / \partial h$ around $h = 0$, for $\beta = 0.1, 0.2, 0.3, 0.4, 0.5$. Compare χ obtained this way to the the linear response expression $\beta < M^2 > /N$. (Pay attention to noise, once more.)