Racah Institute of Physics
The Hebrew University

Computational Physics of Complex Systems
Course no. 77732, by Prof. Ofer Biham

Problem set number 1

This problem set can be submitted as the work of a single student or as the joint project of two students. The solution should be submitted by email as a pdf file. It should include a brief description of the analysis, graphs with the main results and relevant discussion and interpretation. There is no need to include computer codes in the submission.

This is the first in two problem sets that will be given in the course. Some of the problems involve writing codes and simulations and other problems are mostly theoretical. To get credit in this course, submission of both sets is required. The problem sets will have a weight of 20 % in the final grade and the final exam will have a weight of 80 %.

Problem 1

Use the Metropolis algorithm to simulate the *two* dimensional Ising model on a square lattice under equilibrium conditions at several values of the temperature above and below T_c. Try to simulate systems as large as you can for the given computational resources available to you. Calculate the magnetic susceptibility using the fluctuations in the magnetization and plot the results vs. T. Evaluate the magnetic field vs. T in the vicinity of the transition and try to calculate the critical exponent β.

By plotting the magnetic susceptibility vs. T near T_c you can identify the effective value of the critical temperature, $T_c(L)$, as it appears for the given system size, L. This is simply the temperature for which the magnetic susceptibility is maximal. Repeating this for several system sizes you can plot $T_c(L)$ as a function of $1/L$ and extrapolate it in order to find T_c of the infinite system. Knowing $T_c(L)$ will be useful for the calculation of the critical exponent β. This is done by calculating the magnetization per spin $m(T)$ for system size L below $T_c(L)$, and then fitting it to $m \sim (T_c(L) - T)^\beta$ on a log-log scale. The fit on log-log is simply linear regression, using the fact that $T_c(L)$ is known.

Problem 2

Use the Wolff algorithm to simulate the two dimensional Ising model for the same system sizes and the same temperatures as in problem no. 1. Again, try to calculate the magnetic susceptibility from the fluctuations in the magnetization.

Problem 3

- In class we considered the Wolff algorithm for the two dimensional (2D) Ising model with nearest neighbor interactions. Show how to design a Wolff-like algorithm for the the case in which there are also next-nearest neighbor interactions. Show that detailed balance is maintained.
- Show how to design a Wolff-like algorithm for the 2D Ising model in a magnetic field.
- For an XY model in two dimensions - show how to construct a Metropolis algorithm and a Wolff algorithm.
- Show how to construct a heat bath algorithm for the q-state Potts model in two dimensions. Using this approach to simulate the 3-state Potts model, which exhibits a second order transition and the 5-state Potts model, which exhibits a first order transition. You can choose what properties to measure in order to observe the difference between the two transitions.

Problem 4

The following Master Equation describes the reaction $A + A \to A_2$ on the surfaces of small grains:

$$\begin{aligned}
\dot{P}(0) &= -FP(0) + WP(1) + 2 \cdot 1 \cdot KP(2) \\
\dot{P}(1) &= F\left[P(0) - P(1)\right] + W\left[2P(2) - P(1)\right] + 3 \cdot 2 \cdot KP(3) \\
\dot{P}(2) &= F\left[P(1) - P(2)\right] + W\left[3P(3) - 2P(2)\right] \\
&+ K\left[4 \cdot 3 \cdot P(4) - 2 \cdot 1 \cdot P(2)\right]
\end{aligned}$$

$$
\begin{aligned}
&\vdots \\
\dot{P}(N) &= F\,[P(N-1) - P(N)] + W\,[(N+1)P(N+1) - NP(N)] \\
&+ K\,[(N+2)(N+1)P(N)+2) - N(N-1)P(N)]\,. \qquad (1) \\
&\vdots
\end{aligned}
$$

Each grain is exposed to a flux F of atoms of type A. At any given time the number of A atoms adsorbed on the grain may be $N = 0, 1, 2, \ldots$. The probability that there are N adsorbed atoms on the grain at time t is given by $P(N)$ (we do not write the time explicitly here but the probabilities are time dependent) where

$$\sum_{N=0}^{\infty} P(N) = 1. \qquad (2)$$

1. Show that the equations are balanced, namely that the time derivative of the sum of all probabilities vanishes.

2. Sum up the set of equations in this Master Equation in a way that will reproduce the form of a rate equation. What is the difference between the equation you obtained and the original rate equation? What should be the distribution $P(N)$ in order that the reaction rate obtained from the rate equation will coincide with that obtained from the master equation.

3. Use the generating function $G(s,t) = \sum_{N=0}^{\infty} s^N P(N)$ and write down a differential equation for $dG(s,t)/dt$. Solve this equation for steady state and from this solution find an expression for $P(N)$ at steady state. If you need some hints, take a look at N.J.B. Green, T. Toniazzo, M.J. Pilling, D.P. Ruffle, N. Bell and T.W. Hartquist, Astronomy & Astrophysics 375, 1111(2001).

4. Try to explain why in the case that $\langle N \rangle$ is small, the rate equation results for the reaction rates do not coincide with those of the master equation.

Good Luck!!