Final Exam in SIF4058 Computational Physics

Spring 2002

Use any aid and discuss the problems with whomever. However, you should of course write the programs and do the data analysis yourself. The solutions should be sent to me by email by 21:00 on Wednesday, June 5 at the latest. The solution should be in the form of a report written in any popular format: TeX, LaTeX, Word, PDF, Postscript... Good luck!

Problem 1 The following problem was suggested by Professor Steinar Raaen and constitutes a problem he is actively working on.

Temperature programmed desorption is an important experimental method to study interactions between absorbates and surfaces. The temperature is increased at a constant rate and the rate of desorbing molecules is registered. First order desorbtion can be described by the expression

$$r = -\frac{dN}{dt} = \nu \ N \ \exp(-E/kT) \ , \tag{1}$$

where r is the desorbtion rate, ν is a pre-exponential factor, E is the activation energy for desorbtion, T is the temperature and N is the number of molecules on the surface.

The surface may be represented by a quadratic lattice of size $L \times L$, where each node i is a position where a molcule may be situated. A molecule may be in any of five different configurations $\gamma = 0, ...4$ depending on the number of nearest-neigbor nodes that also contains molecules. By considering all different local configurations of adsorbent on the surface, the desorption rate may be written

$$\frac{-dN}{dt} = \sum_{\gamma} N_\gamma \ \nu \ \exp(-E_\gamma/kT) \ , \tag{2}$$

where ν is the pre-exponential factor of the desorbtion rate (which we will assume equal for all configurations), and N_γ is the number of molecules with local configuration γ, and E_γ is the activation energy for desorbtion of a molecule in a local configuration γ and is given by

$$E_\gamma = E(0) - N_{nn}(\gamma) E_{nn} \ . \tag{3}$$

Here $E(0)$ is the desorbtion energy of an isolated molecule. N_{nn} is the number of nearest neigbor molecules to a molecule with local configuration γ and E_{nn} is the interaction energy with nearest neighbor molecules. The time it takes to desorb one of the N molecules from the surface may be written

$$\tau(N) = 1/\left(\sum_{\gamma} N_{\gamma}\ \nu\ \exp(-E_{\gamma}/kT)\right)\ , \tag{4}$$

where we assume that the diffusion of molecules on the surface is much faster than the desobrion process. Hence, the adsorbed molecules may be assumed to be in thermal equillibrium on the surface at all times.

A Monte Carlo algorithm may then be constructed as follows.

1. Adsorb N molecules initially at random positions on a square lattice with biperiodic boundaries. The initial degree of coverage is $\theta = N/L^2$. Each node is occupied by zero or one molecules.

2. Relax the adsorbate until it has reached thermal equillibrium. This is done in the following way: Choose a molecule at random. This is in position i. Then choose a random neigboring position j. If this position is occupied by another molecule, then the molecule at i cannot move into this position. If this is so, choose another pair i and j. If j is not occupied, the molecule at i may jump into this position with probability $P_{i,j} = \exp[-(E_j - E_i)/kT]$ if $E_j > E_i$ and with probability one if $E_j < E_i$. Here E_i and E_j are defined using Eq. (3) — i.e. count the number of neighbors the molecule in i has and how many it would get if it moved to position j. This procedure is repeated untill thermal equillibrium has been reached.

3. Calculate the desorbtion rate for each molecule k by using $r_k = \nu\ \exp(-E_k/kT)$. The highest desorbtion rate $r_{\max}$ is identified.

4. Choose a random molecule with position n. Let this molecule desorb with probability $P_n = r_n/r_{\max}$. If desorbtion results, increase time τ by $\tau(N) = 1/\sum_i N_\gamma r_\gamma$. The temperature T is also increased by $\rho\tau(N)$ where ρ is the heating rate of the system.

5. Return to 2 and repeat the procedure untill all molecules are desorbed. The desorbtion rate in the time interval Δt is given by $R_d = \Delta N/\Delta t$, where ΔN is the number of molecules that desorb in the time interval Δt.

Typical parameter values are as follows: $\nu = 10^{13}\, s^{-1}$, $E(0) = 1\, eV$, $E_{nn} = 0.1\, eV$, and $\rho = 5\, K/s$.

Write a program that simulates and plots thermal desorbtion rate as a function of temperature.

Problem 2 In February this year, Ulrich Hansmann and Luc T. Wille published a paper entitled *Global Optimization by Energy Landscape Paving* in Physical Review Letters (**88**, 068105 (2002)) describing a very clever new algorithm. They tested the algorithm on the protein folding problem.

This algorithm has, however, never been tested on the Ising spin glass, and it would be of interest to see how it performs in comparison to a standard algorithm such as simulated annealing. Hence, write a code using energy landscape paving and one doing standard simulated annealing and compare these.

Implement the Ising spin glass on a 6×6 lattice with biperiodic boundary conditions. The hamiltonian of the system is

$$H = -\sum_{\langle i,j \rangle} J_{i,j} S_i S_j \ , \tag{5}$$

where $\sum_{\langle i,j \rangle}$ runs over all nearest neighbor nodes and $J_{i,j}$ is ± 1 with 50% probability. The values of the $J_{i,j}$s are fixed at the beginning of the simulation of a given sample. The spins, S_i, take the values ± 1.