Racah Inst. of Physics, The Hebrew University
Computational Physics of Complex Systems: 77732
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Problem set number 2

1. The Potts model is a generalization of the Ising model to the case that each spin can take one of q states, namely $s_i = 1, \ldots, q$. Each bond, between neighboring spins i and j contributes energy $-J$ if they are in the same state and zero otherwise, namely $H = -J \sum_{\langle ij \rangle} \delta_{s_i,s_j}$ where δ_{s_i,s_j} is the Kronecker δ symbol. Design a Metropolis type algorithm and a heat-bath type algorithm for the Potts model in two dimensions. Which of the two you expect to be more efficient and why?

2. The two dimensional (2D) Ising model is described by the Hamiltonian

$$H = -J \sum_{\langle ij \rangle} s_i s_j. \tag{1}$$

where s_i can take the values ± 1. Consider the case in which the dynamics is modified such that the flipping of any site i involves an intermediate state in which the interaction of site i with its neighbors is turned off and the energy of site i is $E_p \geq z \cdot J$ where $z = 4$ is the coordination number of the lattice. The move of flipping the spin s_i thus involves two Metropolis steps: one from the original to the intermediate state and the other from the intermediate to the new state, such that after a complete move the system will never remain in the intermediate state. It is also assume that the second part of the flipping move is instantaneous, namely the system spends zero time in the intermediate state. (a) Write down the master equation for this system. (b) Does it satisfy detailed balance? (c) Does the addition of these intermediate state change the probabilities p_α, $\alpha = 2^N$ of the ordinary states of the system? Does it change the partition function? (d) Will the simulation of this model using, say, the Metropolis algorithm be faster or slower than the simulation of the ordinary 2D Ising model of the same size? By what factor, approximately?

3. You are given a random number generator that produces numbers in the range $[0, 1)$. Show how to obtain random numbers distributed according to the Lorentzian distribution

$$f(x) = \frac{1}{\pi} \frac{\Gamma}{\Gamma^2 + x^2}. \tag{2}$$

This distribution has the property that all its moments diverge. For a given upper cutoff x_{max} such that $|x| < x_{max}$, find a way to obtain random numbers that are bounded by this cutoff, and within this range are distributed according to the Lorentzian distribution.

4. You are given a random number generator that produces numbers in the range $[0, 1)$. Show how to obtain random numbers distributed according to the power-law distribution

$$f(x) = Kx^{-(\alpha+1)} \tag{3}$$

within the range $x > x_{\min}$, where K is a normalization constant that is determined by α and $x_{\min}$.

5. The following Master Equation describes the process of hydrogen recombination on dust grains in dilute (atomic) hydrogen clouds within the interstellar medium:

$$\begin{aligned}
\dot{P}_{\mathrm{H}}(0) &= -F_{\mathrm{H}} P_{\mathrm{H}}(0) + W_{\mathrm{H}} P_{\mathrm{H}}(1) + 2 \cdot 1 \cdot A_{\mathrm{H}} P_{\mathrm{H}}(2) \\
\dot{P}_{\mathrm{H}}(1) &= F_{\mathrm{H}} \left[P_{\mathrm{H}}(0) - P_{\mathrm{H}}(1)\right] + W_{\mathrm{H}} \left[2P_{\mathrm{H}}(2) - P_{\mathrm{H}}(1)\right] + 3 \cdot 2 \cdot A_{\mathrm{H}} P_{\mathrm{H}}(3) \\
\dot{P}_{\mathrm{H}}(2) &= F_{\mathrm{H}} \left[P_{\mathrm{H}}(1) - P_{\mathrm{H}}(2)\right] + W_{\mathrm{H}} \left[3P_{\mathrm{H}}(3) - 2P_{\mathrm{H}}(2)\right]
\end{aligned}$$

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\begin{aligned}
&+ \quad A_{\rm H}\left[4\cdot 3\cdot P_{\rm H}(4) - 2\cdot 1\cdot P_{\rm H}(2)\right] \\
&\;\vdots \\
\dot{P}_{\rm H}(N_{\rm H}) \quad &= \quad F_{\rm H}\left[P_{\rm H}(N_{\rm H}-1) - P_{\rm H}(N_{\rm H})\right] + W_{\rm H}\left[(N_{\rm H}+1)P_{\rm H}(N_{\rm H}+1) - N_{\rm H}P_{\rm H}(N_{\rm H})\right] \\
&+ \quad A_{\rm H}\left[(N_{\rm H}+2)(N_{\rm H}+1)P_{\rm H}(N_{\rm H}+2) - N_{\rm H}(N_{\rm H}-1)P_{\rm H}(N_{\rm H})\right]. \qquad (4) \\
&\;\vdots
\end{aligned}
$$

Each grain is exposed to a flux $F_{\rm H}$ of H atoms. At any given time the number of H atoms adsorbed on the grain may be $N_{\rm H} = 0, 1, 2, \ldots$. The probability that there are $N_{\rm H}$ hydrogen atoms on the grain is given by $P_{\rm H}(N_{\rm H})$, where

$$\sum_{N_{\rm H}=0}^{\infty} P_{\rm H}(N_{\rm H}) = 1. \qquad (5)$$

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?

3. Show that the Master Equation above does not satisfy detailed balance.