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Department of Physics
Monte Carlo methods
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Examination, Monte Carlo methods, 7.5hp, 2010–06–01, at 9.00–15.00, Östra paviljongen.

Allowed aids: Calculator, Beta, Physics Handbook.

Hand in each problem on a separate page.
The calculations and the reasoning should be easy to follow.
Good luck!

1 Basic statistics

a) Consider independent, random variables x_i with average μ and variance σ^2. The average of N such variables is

$$m = \frac{1}{N} \sum_{i=1}^{N} x_i.$$

What is σ_m^2, the variance of m? (1p)

b) Derive this result. (2p)

c) Specialize to the case where the x_i are from a uniform distribution between -1 and 1 and $N = 100$. What is the distribution of m? (2p)

2 Theory behind Markov chains (3p)

A Markov chain may be described as a transition matrix p_{ij}. Describe the three conditions that have to be fulfilled by this matrix and motivate why they are necessary. *Hint: The first has to be true for all* p_{ij}, *the second is for* p_{ii}, *and the last concerns* $\sum_j p_{ij}$.

3 1D Ising model

Show that the 1D Ising model is disordered for all $T > 0$. (4p)

4 Scaling analysis

One way to analyze experimental data (or simulations at big lattices) is to plot $m/|t|^a$ versus $h/|t|^c$. Start from $m \sim \partial f/\partial h$ and

$$f(t, h) = b^{-d} f(tb^{y_t}, hb^{y_h}),$$

and express a and c in terms of d, y_t, and y_h. (4p)

5 Expectation values

For small lattices it is possible to use three different methods to calculate the properties of the Ising model:

(1) Through a complete enumeration of all the possible states.

(2) By generating a set of randomly produced configurations.

(3) Through a Monte Carlo simulation.

a) Describe the formulas that should be used to calculate expectation values in methods (1), (2), and (3). Assume that we have access to A_ν and the energy E_ν for each generated configuration and want to calculate $\langle A \rangle$. (3p)

b) Why could it sometimes be motivated to study a system through a complete enumeration? (1p)

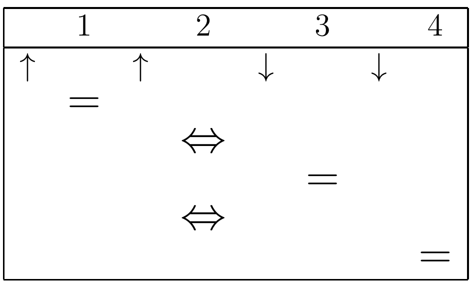
c) Consider a complete enumeration of a $L \times L$ Ising model. What is the maximum size L that would be possible to study in 24 hours on a single 3GHz-processor. Base your answer on some reasonable assumptions. (2p)

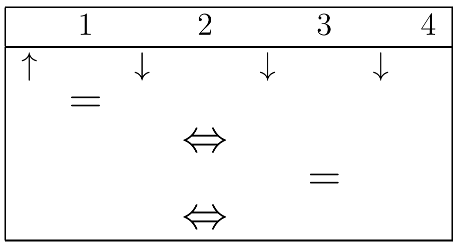
6 Quantum Monte Carlo

The figures below show representations of two terms in the space of spin states and operators for the spin-1/2 Ising model with four spins. The symbol "$\Leftrightarrow$" symbolizes an off-diagonal operator whereas "$=$" is a diagonal operator.

a) Which of these states represents a non-vanishing term? Why? (2p)

b) What is the order of the expansion (denoted by n) of the non-vanishing term? (1p)





7 Master-equation solution of a two state system

A simple system has two states 0 and 1 with energies E_0 and E_1 respectively. Transitions between the two states take place at rates $P(0 \to 1) = R_0 \exp[-\beta(E_1 - E_0)]$ (β is the inverse temperature) and $P(1 \to 0) = R_0$. Let $w_0(t)$ and $w_1(t)$ be the probabilities of the system being in state 0 or 1 as a function of time t with the initial conditions $w_0(0) = 0$ and $w_1(0) = 1$.

a) Express $\mathrm{d}w_0/\mathrm{d}t$ in terms of β, R_0, E_0 and E_1. (3p)

b) Solve this equation and show that the system obeys the Boltzmann distribution in the limit $t \to \infty$. (3p)

8 Conserved-order-parameter Ising model

The conserved-order-parameter Ising model is defined just like the regular Ising model but with the extra condition that the magnetization is fixed M (i.e. a control parameter of the model). The traditional way of simulating the conserved-order-parameter Ising model is by the Kawasaki algorithm defined as follows on a lattice with N spins:

1. Start with any configuration of $(N+M)/2$ up-spins and $(N-M)/2$ down-spins.
2. Chose two sites i and j at random.
3. If ν is the current spin-configuration, let μ be the spin configuration where s_i (the value of the spin at site i) has the value that s_j does in ν and s_j of has the value that s_i has in ν.
4. Let $\Delta E = H(\mu) - H(\nu)$, where H is the Ising Hamiltonian.
5. If $\Delta E < 0$, or with a probability $\exp(-\beta\,\Delta E)$ (β is the inverse temperature), swap the spin-values of sites i and j.
6. Go to step 2.

Obviously the magnetization is constantly M. Our questions are:

a) Define *ergodicity.* (1p)

b) Why does the Kawasaki algorithm sample the configurations of the conserved-order-parameter Ising model ergodically? (1p)

c) Define *detailed balance.* (1p)

d) Why does the Kawasaki algorithm fulfill detailed balance? (2p)

e) Obviously $s_i = s_j$ (in step 2) implies that $\nu = \mu$. The simulation might be faster if one chose i and j randomly only among all *neighboring* pairs of sites with *different* spin values. This algorithm would however not sample the Boltzmann distribution. Why? Illustrate with a concrete example (with explicit configurations) in a system of just a few spins. (4p)