Universität of Göttingen
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Methods of Computational Physics
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Sheet 1: Monte-Carlo Simulation in Statistical Physics

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- **2D Ising model**

  Consider Ising spins, $s_i = \pm 1$, on a two-dimensional, square lattice, where $i = 1, \cdots N^2$ denotes the lattice index and N is the linear dimension of the square lattice. The Hamiltonian of the 2D Ising model in units of the thermal energy scale, $k_{\mathrm{B}}T$, is given by

$$\frac{\mathcal{H}(\{s\})}{k_{\mathrm{B}}T} \equiv -J \sum_{\langle ij \rangle} s_i s_j - H \sum_i s_i \tag{1}$$

  where the first sum runs over all nearest neighbor pairs of the two-dimensional lattice. Periodic boundary conditions are applied in all directions. $H = 0$ and $N = 16$ in the following.

  a) Write a simulation program that performs a Monte-Carlo simulation of this 2D Ising model using the single-spin flip, Metropolis algorithm. Describe the algorithm and the program structure.

  b) Verify the program by (i) comparing the energy difference between the ending and starting configuration with the sum of energy changes of accepted single-spin flips and (ii) by comparing the probability distribution, $P(m)$, of the magnetization per spin, $m \equiv \frac{1}{N}\sum_{i=1}^{N} s_i$, obtained by a Monte-Carlo simulation at $J = 0.4$ with the result of the single-histogram extrapolation from the state $J = J_c = \frac{1}{2}\ln(1+\sqrt{2})$. Explain why the histogram extrapolation works particularly well in the vicinity of the critical point.

  c) Calculate the relaxation of the magnetization per spin, $[m]_k$, averaged over different realizations of the Markov process (i.e., simulation runs) at k steps after starting from the configuration with $m = +1$. Plot $[m]_k$ versus the number of Monte-Carlo steps for $J = 0.3$. A single Monte-Carlo step is comprised of N^2 single-spin flip trials.

  d) Calculate the autocorrelation functions of m in equilibrium for $J = 0.3, 0.4$, and J_c, as well as $J = 0.5$. Plot the autocorrelation functions and extract the correlation times. Compile the results in a table.

  e) Use the block analysis to obtain an alternate estimate of the correlation times.

  f) Extend your program to include Wang-Landau sampling of the magnetization. Explain the algorithm and describe the program structure.

  g) Verify your Wang-Landau program by calculating the entire probability distribution at the critical temperature $J = J_c = \frac{1}{2}\ln(1+\sqrt{2})$ and compare the result to that of part b. Verify the result by using the obtained, $P(m)$, in a non-Boltzmann simulation with the "equilibrium" weight $p_{\mathrm{rw}}(\{s\}) \propto \exp(-\mathcal{H}(\{s\})/k_{\mathrm{B}}T)/P(m(\{s\}))$. Plot the "time" series m_k versus the number of Monte-Carlo steps, k.

  h) Redo part g for $J = 1$. How and why does the "time" series differ from the result in part g?