Critical exponents of the Ising phase transition

One of the fundamental problems in condensed-matter physics is the phase transition. Most phase transitions can be described by an order parameter, which is zero in one phase and non-zero in the other phase. As a concrete model, Ising model at two-dimension has a ferromagnetic to paramagnetic phase transition. The corresponding order parameter is the magnetization.

$$H = -J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j \ . \tag{1}$$

Following the detailed balance condition and the ergodicity requirement, the single-spin flip algorithm is efficient and accurate in most cases to capture the phase transition of the 2D Ising model.

1. The single-spin flip algorithm is fairly good away from the phase transition point, which becomes inefficient when $T \to T_c$ due to the so-called *critical slowing down* problem. Microscopically, this is due to the formation of large domain with different magnetic moments which makes the flip of any single-spin highly difficult and, thus, is of very low acceptance ratio. One way of reducing the autocorrelation time is to use the cluster update algorithm, one of which is the famous Wolff algorithm. Following the recipe given below to implement the Wolff algorithm and study the phase transition temperature again for the lattices with size of 32×32, 64×64, 128×128, and compare your results to the single spin flipping algorithm. For simplicity, the exchange coupling J and Boltzmann constant are taken as 1. One needs to determine the average magnetization M, the corresponding magnetic susceptibility and the specific heat C_v for all sizes of lattice.

   (a) Choose a seed spin a random from the lattice.

   (b) Look in turn at each of the neighbours of that spin. If they are pointing in the same direction as the seed spin, add them to the cluster with probability $P_{add} = 1 - e^{-2\beta J}$.

   (c) For each spin that was added in the last step, examine each of its neighbors to find the ones with are pointing in the same direction and add each of them to cluster with the same probability. This step is recreated as many times as necessary until there are no spins left in the cluster whose neighbor have not been considered for inclusion in the cluster.

   (d) Flip the cluster.

2. The magnetic phase transition are characterized by critical exponents. In the limit of $T \to T_c$, we have

$$\begin{aligned} M(T) &\sim (T_c - T)^{\beta} \text{ for } T < T_c \ , \\ \chi(T) &\sim |T - T_c|^{-\gamma} \end{aligned} \tag{2}$$

   here β is the critical exponent in stead of the inverse temperature. For the two-dimensional Ising model $\beta = 1/8$ and $\gamma = 7/4$ being as the exact value. The Wolff algorithm has a much better performance around the phase transition and, thus, is suitable to extract the critical exponents. Please carefully measure the $M(T)$ and $\chi(T)$ with fine grid of T. β and γ can be easily extracted from a linear fit to your data if $M(T)$ and $\chi(T)$ are plotted in logarithm as a function of $\log(T - T_c)$ for $T < T_c$.

3. In addition to the way of extracting critical exponents from temperature scaling discussed above, one can also estimate them from finite-size scaling. In infinite-size system, the correlation length ξ diverges near the transition point as $\xi = |T - T_c|^{-\nu}$ (From here one can easily see that ν should be greater or equal 1). In finite-size system, when the correlation length ξ is larger than system size L, the system already becomes effectively long-range ordered. Then $|T - T_c|^{-\nu} \propto L$ for finite-size system, i.e., $T = T_c - \text{const.} \times L^{-1/\nu}$. With this relation, $M(T)$ and $\chi(T)$ can be written as

$$M(T) \sim (T_c - T)^{\beta} \propto L^{-\beta/\nu} \text{ for } T < T_c \ , \tag{3}$$

$$\chi(T) \sim |T - T_c|^{-\gamma} \propto L^{-\gamma/\nu} \ . \tag{4}$$

In addition to fitting $M(T)$ and $\chi(T)$ as functions of T, one now can extract T_{max} where $\chi(T)$ becomes maximal at given L and plot T_{max} as a function of $1/L$. Obviously, one will get a straight line with the slope being $-1/\nu$ and the extrapolation value of T_{max} at $1/L \to 0$ being the true T_c at thermodynamic limit. With the obtained ν, it is straightforward to determine the critical exponents β and γ by fitting $\log(M(T_{max}))$ and $\log(\chi(T_{max}))$ as functions of $\log(L)$. Please follow the above recipe and calculate T_c, ν, β and γ from finite-size scaling. Note, to get reasonable result, one needs results from at least 5 different size clusters.

Please summarize the above required results and compose a project report with an introduction on the Ising model and the two Monte Carlo algorithm in addition to the discussion of your results. The final score is heavily dependent on the quality of your data and the self-consistency of your discussion. Only a few plots without adequate explanation and discussions will not make the job. Personal remarks and suggestions on the improvement of simulations are welcome and appreciated.