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MONTE CARLO SIMULATIONS OF THE ISING MODEL ON A SQUARE LATTICE WITH RANDOM GAUSSIAN INTERACTIONS

SYMULACJE MONTE CARLO MODELU ISINGA NA SIECI KWADRATOWEJ Z ODDZIAŁYWANIAMI LOSOWYMI O ROZKŁADZIE GAUSSA

Abstract

The paper shows Monte Carlo simulations of the Ising model on a square lattice with no external magnetic field. In particular, the uncertainty of the spin coupling interactions in the Ising model has been considered. The influence on the phase transition of the Gaussian noise in the spin coupling values has been demonstrated.

Keywords: Ising model, Monte Carlo simulations, Gaussian noise

Streszczenie

W artykule przedstawiono symulacje Monte Carlo modelu Isinga na sieci kwadratowej przy braku zewnętrznego pola magnetycznego. W szczególności rozważono niepewność wartości energii sprzężenia oddziałujących spinów w modelu Isinga. Zademonstrowano wpływ na przejście fazowe obecności szumu gaussowskiego w wartościach stałej sprzężenia oddziałujących spinów.

Słowa kluczowe: model Isinga, symulacje Monte Carlo, szum gaussowski

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1. Introduction

The Ising model, named after Ernst Ising [1] and studied at least 5 years earlier (in early 1920s) by Lenz [2], offers an excellent testing ground for studies of the physics of classical and quantum phase transitions. Despite being subject of numerous, brilliant and extensive research studies over nearly a century, the Ising model still poses some big challenges. For example, the analytical solution for the 2D Ising model with no field was obtained by Onsager [3, 4] in 1944, but up until now, an analytical solution has remained unknown for the case with an external magnetic field. Thus, in many cases, feasible ways to study the model include experiments with quantum simulators with hundreds of spins [5] and numerical methods (Monte Carlo simulations) for finite-size lattices with even more spins included [6–8]. The universality of the Ising model goes far beyond the modelling of purely physical phenomena such as: classical and quantum phase transitions; binary alloys; magnetic properties of condensed-matter materials; strong and long-range correlations; complex systems. Just to give an example, it has been shown by Bornholdt [6], that microscopic models based on the Ising model have a capacity of reproducing complex behavior of real financial and economic markets. Thus, it proves that this model allows for the genuine interdisciplinary research in physics, econophysics and also across other areas of fundamental and applied sciences.

The purpose of this paper is to investigate the two-dimensional (2D) Ising model by means of Monte Carlo simulations. In view of recent progress in engineering two-dimensional Ising interactions in a trapped-ion quantum simulator [5], an important research question arises. Namely, to what extent an uncertainty of the engineered interaction in a real experimental situation may influence the phase transition in the model. In order to provide at least a partial answer to this question, random Gaussian noise is introduced into the Ising interaction coupling constant.

The paper is organized as follows. In the next section, the Ising model is briefly presented. In Section 3, the results are presented for the case of constant interaction coupling energy. This allows for some justification for the applied numerical implementation of the Metropolis algorithm, as such results are fairly standard in the literature. Then, a variant of the model is proposed for which the interaction may vary according to the normal distribution with the mean and standard deviation fixed. Finally, the results are summarized and some conclusions are drawn.

2. The Model

Let us consider 2D Ising model [1, 2, 4], where $N = L^2$ spins $\sigma = \pm 1$ are located in regularly spaced sites of a square lattice $L \times L$. In general, such spins can interact with each other with some coupling energy J (in principle, interactions and thus couplings could depend on interacting spin σ_{ij}, σ_{jk} locations in the lattice). Apart from internal interactions within such an ensemble of spins, one could also take into account interactions of each spin with the external magnetic field. However, for the purpose of the following discussion, let us simplify the model considering the case with no magnetic field and include only equal interactions between nearest neighbors in the square lattice. Hence the Hamiltonian H of the system reads:

$$H = -J \sum_{\{ij,kl\}} \sigma_{ij} \sigma_{kl}$$

where

J – the coupling between interacting nearest-neighbor spins ,

σ_{ij} – the spin $\sigma_{ij} = \pm 1$ located in the site (i, j) of the lattice $(1 \leq 1, j \leq L)$,

$\{ij, kl\}$ – denotes summation only over pairs of the nearest-neighbor sites (i, j) and (k, l) of the lattice.

In the model studied, the usual periodic boundary conditions for the lattice are adopted. This means that any spin has 4 nearest neighbors in the square lattice and for example: $\sigma_{L+1,j} \equiv \sigma_{1,j}$ or $\sigma_{i,L+1} \equiv \sigma_{i,1}$ (the lattice is 'wrapped around').

It is well known that the 2D system exhibits a phase transition between the disordered phase (a paramagnetic state) and the ordered phase (a ferromagnetic state). The order parameter for this transition is simply the total system magnetization M per spin:

$$m = \frac{M}{N} = \frac{1}{N} \sum_{i,j} \sigma_{ij}$$

For a system at a given temperature T, an expectation value $<A>$ of any observable A in the system with spin micro-configurations σ_α on the lattice is evaluated according to probabilities $P(\sigma_\alpha)$, assigned by the canonical ensemble:

$$< A > \; = \sum_{\alpha} P(\sigma_\alpha)\, A(\sigma_\alpha)\,, \quad P(\sigma_\alpha) \; = \; \frac{1}{Z} e^{-E(\sigma_\alpha)/(k_B T)}$$

where:

Z – the partition function,

$E(\sigma_\alpha)$ – the energy of the microstate σ_α,

k_B – Boltzmann's constant.

In the Monte Carlo numerical simulation, such expectation values could be obtained through the Metropolis algorithm (see e.g. [7, 8] for a description of details of the implementation of Metropolis algorithm's).

It also transpires (see e.g. [7, 8]) that the magnetic susceptibility χ (a linear response of the magnetization to the magnetic field) is related to the total magnetization M fluctuations:

$$\chi \; = \frac{1}{N k_B T} \left(\left\langle M^2 \right\rangle - \left\langle M \right\rangle^2 \right)$$

The critical temperature T_C for the order-disorder transition in the 2D Ising model in the limit of an infinite lattice (the so-called thermodynamic limit, with a total spin number $N \rightarrow \infty$), without an external magnetic field, can be found exactly analytically [3, 4]:

$$\frac{k_B T_C}{J} = \frac{2}{\ln\left(1 + \sqrt{2}\right)} \approx 2.2691853$$

An interesting issue is related to the so-called finite-size lattice scaling at the critical temperature [3, 7, 8]. A ratio of any two quantities which have the same finite-size scaling at T_C should be lattice-size independent. Especially useful are the Binder ratios [8] defined in the following way (q is an integer):

$$B_q = \frac{\langle m^{2q} \rangle}{\langle |m| \rangle^{2q}}$$

Therefore, once we have obtained expectation values of the square of the magnetization and the absolute value of the magnetization itself, the first Binder ratio B_1 can be easily found.

3. Results

Monte Carlo simulations of the Ising model using the Metropolis algorithm were performed according to the implementation described by other authors (see [7, 8] for details). Typically, in the present simulations, 50000 Monte Carlo sweeps (MCS) were discarded for equilibration and there were 100 bins used, each with 50000 MCS to obtain expectation values of $\langle m^2 \rangle$, $\langle |m| \rangle$ and χ with estimates of their errors. Figure 1 shows magnetic susceptibility dependence on temperature for lattice sizes L = 16, 32, 64, 128. The data for L = 128 have been obtained with only 20 bins, so Monte Carlo error bars are more pronounced near the critical temperature (its position is denoted by the dashed vertical line) than for smaller lattices studied here (where errors are comparable to data point sizes on the plot). The coupling here is taken to be constant ($J = J_0 = 1.0$).

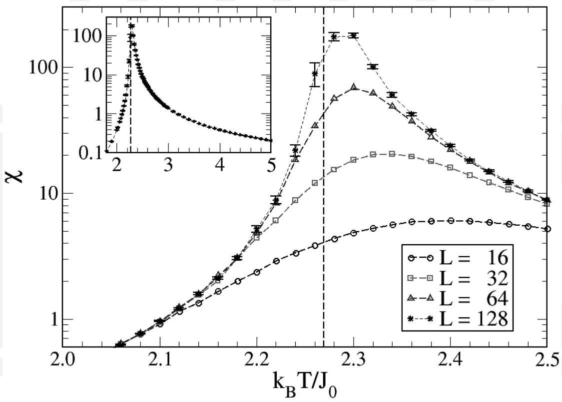

Fig. 1. The magnetic susceptibility χ versus temperature T. Note the logarithmic scale for χ. The dashed vertical line shows the position of the critical temperature T_C. The inset shows the shape of the magnetic susceptibility χ for the lattice of size L = 128 for the given range of temperatures

The corresponding analysis of the Binder ratio is shown in Figure 2. Note, that as expected, the first Binder ratio B_1 is independent of the lattice size at T_C. The inset in Figure 2 shows that in more detail. The horizontal dotted line represents the asymptotic value $\frac{\pi}{2}$

of B_1 for temperatures T much greater than T_C ($T >> T_C$) (for evidence, see [7, 8]). Thus, the results discussed and illustrated in Figures 2 and 3 validate the numerical methods used for the present study to some extent.

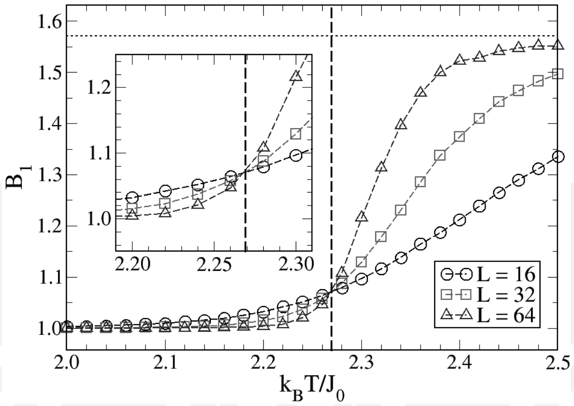

Fig. 2. The Binder ratio B_1 for the studied 2D Ising model ($J = J_0 = 1.0$). The inset shows the Binder ratio scaling in the vicinity of the critical temperature (indicated by the dashed vertical line). The horizontal dotted line indicates the asymptotic value of the Binder ratio

Finally, let us now consider the influence of the Gaussian noise in the value of the interaction coupling. It is assumed that the coupling $J = J_0$ is known with some uncertainty ΔJ_0 ($J = J_0 \pm \Delta J_0$). In the Monte Carlo simulations, the values of coupling energy are now allowed to vary slightly with subsequent MCS (but at any given MCS, they are fixed). The coupling energies are randomly drawn from the Gaussian (normal) distribution with the mean J_0 and the standard deviation ΔJ_0, so that $J = J_0 \pm \Delta J_0 = 1.0 \pm 0.1$ (this corresponds to a relative uncertainty of 10% in the value of the coupling energy). The results for the Binder ratio are shown in Figure 3 – note the shift in the value of the effective critical temperature with respect to the previously discussed case (Fig. 2). The new value of the effective critical temperature T_C' of the phase transition in the noisy system is significantly lower than in the case of noise absence, and in rescaled units, it equals approximately:

$$\frac{k_B T_C'}{J_0} \approx 2.22.$$

In order to understand this phenomenon at least qualitatively, one may regard noise in the coupling energy to be equivalent to the thermal energy in the system with no external field. This additional thermal energy allows for the system to undergo a phase transition at a lower temperature, which otherwise would be too low for the system with no noise (uncertainty) in the spin coupling interaction.

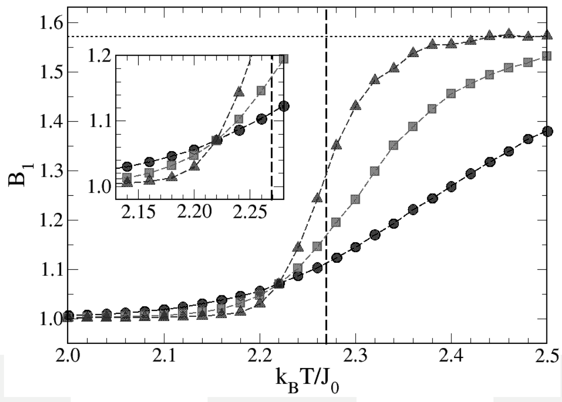

Fig. 3. The Binder ratio B_1 for the studied 2D Ising model with randomly varied coupling J, which is drawn from Gaussian probability distribution with average J_0 and standard deviation $\Delta J_0 = 1.0$

4. Conclusions

In this paper, the 2D Ising model on a square lattice with no external field was considered for various lattice sizes and spin numbers, ranging up to $N = 128^2 = 16\,384$ spins in the complex system. The results of present Monte Carlo simulations are in good agreement with earlier studies and some analytical, exact results. A novel approach has been put forward to consider the influence of the uncertainty of the spin coupling interaction on the effective critical temperatures in the system. This may have an application when comparing experimental results with some phase transition theory predictions. In particular, the results obtained in the present study give some indication regarding possible effects which may arise due to uncertainties of the system parameters in real experimental situations. Another possible application of this noisy 2D Ising model with Gaussian noise adopted would be to represent some many-body corrections or long-range spin correlations which are beyond the description within the standard Ising model, where only the interactions of pairs of spins are taken into account.

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