New algorithm for the computation of the partition function for the Ising model on a square lattice

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Abstract

A new and efficient algorithm is presented for the calculation of the partition function in the $S = \pm 1$ Ising model. As an example, we use the algorithm to obtain the thermal dependence of the magnetic spin susceptibility of an Ising antiferromagnet for a $8 \times 8$ square lattice with open boundary conditions. The results agree qualitatively with the prediction of the Monte Carlo simulations and with experimental data and they are better than the mean field approach results. For the $8 \times 8$ lattice, the algorithm reduces the computation time by nine orders of magnitude.

Keywords: antiferromagnets; Ising model; magnetic susceptibility; mean field approximation; world records.

1 Introduction

A calculation of the partition function exactly in the thermodynamic limit is equivalent to knowledge of all equilibrium properties of a given system. This task is usually beyond our horizon, except for some selected cases which we call “trivial”. The Ising model seems to be at the border of our possibilities since the beginning of the 20-th century. Even for a finite system of $N$ spins our computational ability is limited by the number of the system configurations, which is $2^N$. Here we describe a new algorithm, designed to improve the speed of the calculation of the partition function for a finite Ising system.
Table 1: The CPU time necessary for investigation of $M$ different configurations of $8 \times 8$ large 2D Ising lattice on SGI 2800 machine.

| $M$   | $10^5$ | $10^6$ | $10^7$ | $10^8$ | $10^9$ | $10^{10}$ |
|-------|--------|--------|--------|--------|--------|-----------|
| $t_{CPU}$ [sec] | 0.86   | 6.90   | 66.4   | 660    | 6648   | 65752     |

In the Ising model [1] only two spin states are possible, say “up” and “down” ($S_i = \pm 1$). The energy $E$ of a given spin configuration may be expressed in terms of the number $n$ of spins pointing “up” (say $S_i = +1$) and the number $k$ of anti-parallel bonds between the nearest neighbors ($S_i S_j = -1$):

$$E(n, k) = -J \sum_{<i,j>} S_i S_j - H \sum_i S_i = 2J(k - L^2 + L) - H(L^2 - 2n),$$

(1)

where $J$ denotes the exchange integral, $H$ is an external magnetic field, and $L$ — the linear size of the lattice.

The partition function can be written as

$$Z = \sum_{n,k} \Omega(n, k) \cdot \exp[-\beta E(n, k)],$$

(2)

where $\Omega(n, k)$ is the number of lattice configurations with given numbers $n$ and $k$, $1/\beta = k_B T$, $k_B$ is a Boltzmann constant and $T$ is temperature. Then, the average value of any quantity $A$ may be calculated as

$$\langle A \rangle = Z^{-1} \sum_{n,k} A(n, k) \cdot \Omega(n, k) \cdot \exp[-\beta E(n, k)].$$

(3)

The magnetic susceptibility per spin $\chi$ may be also expressed in the terms of $n$, $k$ and $L$:

$$\chi = \beta[\langle S_i^2 \rangle - \langle S_i \rangle^2] = \beta[\langle (2n - L^2) \rangle^2 - \langle 2n - L^2 \rangle^2],$$

(4)

where the index $k$ enters through the averaging procedure.

A computation of the partition function (2) requires an evaluation of the histogram $\Omega(n, k)$. Tab. 1 shows the CPU time needed to check the numbers $n$ and $k$ of $M$ configurations of a $8 \times 8$ large lattice on SGI 2800 machine. A rough estimation of the CPU time necessary for full investigation of all of $2^{64} \approx 10^{19}$ possible lattice configurations gives the value larger than four millions years — what makes traditional/direct method practically useless.
2 Calculations

2.1 The algorithm

An effective way of generation $\Omega_{8x8}(n, k)$ is a successive merging of smaller lattices and their histograms, namely $\Omega_{4x4}(n, k)$ and $\Omega_{8x4}(n, k)$. However, the procedure requires storing information on the $\Omega$ dependence not only on $n$ and $k$, but also on $b^r$ — the state of the $r$-sites-long lattice border.

In Fig. 1(a) a $L^2$-long bit-string equivalent to $L \times L$ large array (see Fig. 1(b)) is presented. For $L = 4$ the bit-string corresponds to an integer number from the interval $[-2^{15}, 2^{15}]$. This correspondence allows to investigate all possible lattice configurations in a simple manner. Dark sites in Fig. 1(a) correspond to the dark border of the lattice in Fig. 1(b), and they can be represented by an integer number $0 \leq b^r \leq 127$. The first four bits of $b^r$ (marked as dark sites in Fig. 1(c)) allow to determine the additional number of anti-parallel bonds, created by merging two $4 \times 4$ lattices together to get a $8 \times 4$ lattice (see Fig. 1(f)). On the other hand, the last four digits of $b^r$ (dark sites in Fig. 1(d)) are equivalent to the part of the border $0 \leq b^8 \leq 255$ (the dark sites in Fig. 1(g)) of $8 \times 4$ lattice.

In the next step, two $8 \times 4$ lattices are merged to create the desired $8 \times 8$ large lattice, as presented in Fig. 1(h).
Histograms ($\Omega_{8\times4}$ and $\Omega_{8\times8}$) for the lattices larger than $4 \times 4$ may also be easily computed basing on $\Omega_{4\times4}$:

$$\Omega_{8\times4}(b^8, n_1 + n_2, k_1 + k_2 + k') = \sum_{b_1^7, n_1, k_1, b_2^7, n_2, k_2} \Omega_{4\times4}(b_1^7, n_1, k_1) \cdot \Omega_{4\times4}(b_2^7, n_2, k_2),$$

where $0 \leq k' \leq 4$ is the additional number of anti-parallel bonds in the darker part of Fig. 1(f) and $b^8$ is combined from $b_1^7$ and $b_2^7$.

The histogram $\Omega_{8\times8}(n, k)$ may be constructed in a similar way:

$$\Omega_{8\times8}(n_1 + n_2, k_1 + k_2 + k'') = \sum_{b_1^8, n_1, k_1, b_2^8, n_2, k_2} \Omega_{8\times4}(b_1^8, n_1, k_1) \cdot \Omega_{8\times4}(b_2^8, n_2, k_2),$$

and again $0 \leq k'' \leq 8$ is the number of anti-parallel bonds in the darker part of Fig. 1(h).

This procedure on SGI 2800 machine takes only 22 hours of the machine time instead of a few million years in case of the usage of the traditional/direct method. Successive merging may be repeated recursively to obtain the partition function for larger lattices.

### 2.2 Monte Carlo simulation, mean field approach and experimental data

To evaluate the results obtained for the $8 \times 8$ lattice, we show also the data obtained by the Monte Carlo simulations, the results of the mean field model, and — last but not least — the experimental data. Standard Monte Carlo Metropolis algorithm [2] is applied to determine the magnetic spin susceptibility of a $1000 \times 1000$ Ising lattice. After getting equilibrium, each point of the plot is obtained as the time average over a thousand of time steps.

The mean field model is a direct generalization of the case of a ferromagnet. Namely, we solve numerically a set of two equations for two sublattices $\alpha$ and $\gamma$:

$$\begin{align*}
    m_\alpha &= \tanh (\beta (Jm_\gamma + H)) \\
    m_\gamma &= \tanh (\beta (Jm_\alpha + H))
\end{align*}$$

(5)

where $J < 0$. In this model, the Curie temperature $T_C = -J/k_B$ and the susceptibility $\chi$ is found as $(m_\alpha + m_\gamma)/H$ for a small value of applied magnetic field, e.g. $H = 0.001$.

The experimental data are collected from Ref. [3]. They concern two-dimensional Ising antiferromagnets Rb$_2$CoF$_4$ and K$_2$CoF$_4$ where $S = \pm 1$. The Van Vleck susceptibility is subtracted to obtain a pure spin contribution.
3 Results and discussion

In Fig. 2 the histogram $\Omega_{8\times 8}(n, k)$ obtained by means of the method described in Sec. 2.1 is presented. The numbers are available at our web page [4]. The symbols on $n$-$k$ plane (see Fig. 2(a)) indicate $(n, k)$ pairs with non-zero values of $\Omega_{8\times 8}(n, k)$. In Fig. 2(b) the number of configuration $\Omega_{8\times 8}(n, k)$ is presented. For fixed $n$ different symbols correspond to different $k$.

In Fig. 3 we show the thermal dependence of the antiferromagnetic ($J < 0$) susceptibility, defined in Eq. (4). The Curie temperature is assumed to be at the inflexion point of the curve, which is at the half of the peak height. Below the Curie temperature, the values of $\chi$ obtained with our new algorithm fit well the results obtained with the Monte Carlo results and the experimental data. Above $T_C$, the agreement is only qualitative. We hope that it can be also quantitative if periodic boundary conditions are applied. However, in this case the lattice border is longer, and so is the computation time. Still, even with the present method the qualitative accordance is better than the results of the mean field theory.

It would be of interest to apply the finite size scaling to our results to evaluate the critical properties of the system. Then, the results could be compared with other methods, e.g. the finite size scaling renormalization group [5] or the phenomenological renormalization [6]. For this purpose, however, periodic boundary conditions seem to be more appropriate as a starting point of the calculations.

The function $\Omega(n, k)$, once known, can be easily used for the calculation of all equilibrium thermodynamic properties, for ferro- and antiferromagnets, various values of temperature and magnetic field. The summation over $n$ and $k$ is much faster, than the summation over $2^{64}$ spin configurations. The results can be relevant also for other applications of the Ising model, e.g. for the percolation problem. As for our knowledge, the partition function has never been calculated exactly for the lattice as large as $8 \times 8$. In principle, the algorithm can be applied to larger lattices, with a cost of more time and memory.

The computational mountain remains infinite, but its slope is a little bit reduced.

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Figure 2: The histogram $\Omega_{8 \times 8}(n, k)$. 
Figure 3: The antiferromagnetic susceptibility $\chi$ normalized to its maximal value $\chi_{\text{max}}$, as dependent on temperature $T$ normalized to the Curie temperature $T_c$.

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