Approaches to numerical solution of 2D Ising model

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Abstract. Parallel algorithm of partition function calculation of two-dimensional Ising model for systems with a finite number of spins was developed. Within a method of complete enumeration by using MPI technology with subsequent optimization of a parallel code time of calculations was reduced considerably. Partition function was calculated for systems of 16, 25, 36 Ising spins. Based on the obtained results, main thermodynamic and magnetic values dependences (such as heat capacity, magnetic susceptibility, mean square magnetization) for ferromagnetic and antiferromagnetic interactions was investigated. The analysis of a different configurations contribution showed, that states with the minimum energy have essential influence on dependences of thermodynamic values. Comparison with the results obtained by the Wang Landau algorithm was performed.

1. Introduction

Studying of systems consisting a large number of interacting particles is one of the most fundamental and actual problems of the modern physics [1]. The task is interesting both from the practical and theoretical points of view. Special attention should paid to behavior of such systems near a stability boundary. First of all, there is a problem of definition of these borders, i.e. limiting values of energies for various systems, then studying a peculiar nature of thermodynamic behavior of the modelled substance in case when loss of stability of the system caused by emergence of particular type of the ordering called by phase transition. For the study of phase transitions and the knowledge of their nature is convenient to use classical lattice models such as the Ising model [2, 3]. In this regard, a comparison of the results of the analytical theory and numerical simulations, developed by the authors in [4–8], would be very useful and productive in terms of the development of our understanding of the processes of ordering and randomization.

2. Partition function

Difficulties in calculation of partition function, for a lattice consisting of a finite number of Ising spins generally consists in calculation of degeneracy multiplicity of spin excess Mᵢ (a difference between number of spins down and number of spins up) by energy Eᵢ (sum of energies of all pair interactions) see equation (1).
\[
Z = \sum_{s_i=\pm 1} \ldots \sum_{s_N=\pm 1} \exp(J \sum_{i,j} S_i S_j + \mu H \sum_{j=1}^N S_j)
\]

It’s important to notice that sums of degeneracy multiplicities of energy within each fixed value of spin excess \( M \), represent binomial coefficients. The developed algorithm based on representation of a spin lattice in the form of bit vectors:

![Figure 1. Representation of a lattice of Ising spins in the form of bit vectors.](image)

- The number of rows and columns (and total number of spins) is set. The array containing integer variable \( \{a_i\} \) is initialize. Every integer variable \( \{a_i\} \) in binary notation represents corresponding lattice column (e.g. \( a_i = 14 \) that means “1110” in binary notation that means \( S_1 = 1, S_5 = 1, S_9 = 1, S_{13} = -1 \) on figure 1).
- By means of serial change of values of each integer variable \( \{a_i\} \) all possible configurations of the system will passed.
- Spin excess (the sum of all one’s) is calculated using the Kernighan’s algorithm [9].
- Exchange pair interactions energy \( E_n \) between spins at lattice sites are calculated by logical XOR (\(^\wedge\)) between all columns and rows including periodic boundary conditions.
- The final value of \( E_n \) is equal to number of all pairs opposite spins. Energy of the system configuration in general:

\[
E_{tot} = -2(N - E_n).
\] (2)

3. Parallel execution

The standard of Massage Passing Interface (MPI) expands possibilities of calculations and does possible parallel algorithmization that allows to solve problems, which could not be solved for acceptable time for single-threaded mode. Parallel algorithm enumerates all possible configurations and calculates energy and spin excess in multithread mode.

Calculation of small systems, such as \( 4 \times 4 \), and \( 5 \times 5 \), shows restriction to increase of efficiency with increase number of involved processes. This result is caused by the Amdahl’s law according to which, the increase of effectiveness of calculations depends on algorithm of a task and is bounded above for any task [10].

The advanced methods of load distribution on the threads had to be used, as some threads received different number of subtasks. The number of \( p \) iterations, approximately identical in duration, which is required to be distributed between \( L \) processes, can be presented through integer numbers of \( a \) and \( b \) in the following form:

\[
p = aL + b, \quad 0 \leq b < L.
\] (3)
Width of an interval of iterations for each process \( p_k, k = 0, ..., L - 1 \) can be calculated as

\[
p_k = \begin{cases} 
  a + 1, & k < b; \\
  a, & k \geq b.
\end{cases}
\]  

(4)

The first \( b \) intervals are wider than the others by one. Left border of each interval \( n_k^l \) is calculated based on the same ratios:

\[
n_k^l = ak + \begin{cases} 
  k, & k < b; \\
  b, & k \geq b.
\end{cases}
\]  

(5)

Thus, interval of iterations \([p_k^l; p_k^l + p_k]\) on each process is distributed. The described approach allows combine conveniences of block distribution and the acceptable balance.

**Table 1.** Run time of the balanced parallel software

| Size 4 × 4 | Size 5 × 5 | Size 6 × 6 |
|-----------|-----------|-----------|
| N,proc    | T,sec     | N,proc    | T,sec     | N,proc    | T,sec     |
| 2         | 0,018     | 2         | 13,17     | 8         | 5741,55   |
| 4         | 0,0078    | 4         | 4,35      | 16        | 2622,05   |
| 8         | 0,0057    | 8         | 1,80      | 32        | 1244,01   |
| 16        | 0,0065    | 16        | 0,82      | 64        | 595,48    |
| 20        | 0,0072    | 32        | 0,42      | 128       | 445,76    |
| 24        | 0,0086    | 48        | 0,46      | 192       | 320,63    |
| 32        | 0,0087    | 64        | 0,41      | 256       | 213,02    |

4. **Wang-Landau algorithm**

To describe a system in the state of thermodynamic equilibrium is necessary to know the partition function that contains all the information about the statistical properties of the system. The problem is that the number of members of the functional series, which is a partition function, increases exponentially with the increasing number of particles; that is, if a system and its parameters are researched by a brute-force method, such an approach would exponentially increase the computation time with the increasing number of particles. Therefore, statistical physics currently uses the Monte Carlo methods. The WL method is an efficient algorithm to calculate the energy density of states (DOS), \( g(E) \), with high accuracy, and was successfully applied to many problems [11-13].

![Figure 2.](image)

Figure 2. (a) Density of states \( g(E) \) for a 6 × 6. (b) Joint density of states \( g(M, E) \) for a 6 × 6.
Wang-Landau method is based on the representation of the partition function $Z$ in the form of an expansion in the number of levels of density of states $g(E)$ with a given energy $E$ [11]:

$$Z = \sum_E g(E) \exp\left(-\frac{E}{kT}\right)$$  \hspace{2cm} (6)

If $g(E)$ is known, we can calculate the mean energy, heat capacity and other thermodynamic quantities at any temperature from the relation:

$$\langle E \rangle = \frac{1}{Z} \sum_E E g(E) \exp\left(-\frac{E}{kT}\right).$$  \hspace{2cm} (7)

In the figure 2, as an example, are represented the density of states for a 6x6 system of spins.

5. Discussion of results

By means of described algorithm, heat capacity, mean square magnetization, magnetic susceptibility for ferromagnetic and antiferromagnetic interactions were calculated. Heat capacity can be calculated as

$$C(h=0) = \frac{SU}{\delta T}.$$  \hspace{2cm} (8)

Heat capacity reaches the maximum in points $T_1 = 2.434$, $T_2 = 2.408$, $T_3 = 2.391$ for systems $4 \times 4$, $5 \times 5$, $6 \times 6$ respectively. When the size of system increasing, the peak becomes sharper, more expressed and displaced to a point $T_C = 2.269$ — to the phase transition temperature calculated by Onsager [14].

![Figure 3. Dependence of a heat capacity for systems with finite number of Ising spins.](image)

Mean square magnetization is calculated by formula (9). The sign of a constant of exchange interaction $J$ of partition function is equal positive for ferromagnetic model, and negative for antiferromagnetic system.

$$\langle M^2 \rangle(h=0) = \frac{1}{N Z_N} \frac{\delta^2 Z_N}{\delta h^2}.$$  \hspace{2cm} (9)
Figure 4. Dependences of mean square magnetization for a ferromagnetic exchange interaction $J > 0$ (a) and antiferromagnetic exchange interaction $J < 0$ (b).

Also, when number of particle increases, angle of the magnetization curve increases relatively to $x$-axis.

An abrupt tendency of magnetization to zero with infinite slope is observed at the limit of infinite number of particles in Curie point $T_C = 2.269$, characterizing the second-order phase transition [14]. Magnetic susceptibility $\chi$ is calculated as

$$\chi(T > 0) = \frac{\delta M}{\delta h}.$$  \hspace{2cm} (10)

Increase of number of particles leads to higher peak of magnetic susceptibility, which becomes sharper at decreasing temperature.

Figure 5. Dependences of magnetic susceptibility at $T = 5$ (a) and at $T = 2.269$ (b).

6. Conclusion

Realized parallel algorithm allows us to calculate coefficients of partition function within two-dimensional Ising model with a finite number of spins, using the minimum amount of resources. Existence of logical parallelism in the considered task gives wide opportunities for application of various approaches to use of parallel programming tools. By means of received results, the curves of main thermodynamic averages were investigated, contribution made in them was estimated too. States with minimum values of energy have the greatest impact, especially at increase number of particles in system. Such states rather easily can be calculated analytically, however complete enumeration of all configurations is the essential necessity for the most correct solution to the problem.

Acknowledgments

This work was supported by RFBR according to the research project No 16-32-00202 mol_a and the Ministry of Education and Science of the Russian Federation in frame of the scholarship of the President of the Russian Federation for young scientists and postgraduate students performing advanced research and development in priority areas of modernization of the Russian Economics for 2015-2017 years (SP-118.2015.5, order #184, 10/03/2015).
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