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# The parallel Wang-Landau algorithm for joint density of states calculation

**V I Egorov<sup>1</sup>, O G Maksimova<sup>1</sup>, A R Baidganov<sup>1</sup>**

<sup>1</sup> Cherepovets State University, 5 Lunacharskii Av., Cherepovets, 162600, Russian Federation

E-mail: rvladegorov@rambler.ru

**Abstract.** The Wang-Landau algorithm is used for estimating density of states. The joint density of states (JDOS) with two parameters gives more information than conventional one but it requires a huge computational time. Recently, the developing of fast algorithms for the JDOS calculation is an actual problem. In this work, we employ the modified parallel WL algorithm for JDOS, which combines ideas of global updates and two level methods. This algorithm is checked the three-dimensional Ising and Potts models. The method of obtaining phase diagrams from JDOS is demonstrated for Ising model.

## 1. Introduction

The Wang-Landau (WL) algorithm [1] has been successfully applied to study the different types of phenomena, including statistical physics models, protein molecules [2], complex fluids [3], polymers [4] etc. Successful application of this algorithm is attributed to the feature that thermodynamic state functions (free energy, entropy etc.) can be calculated by means of one simulation in a wide range of temperatures. The standard WL algorithm performs a random walk in the configuration space to obtain the density of states (DOS)  $g(E)$ , where  $E$  is the energy of system. From DOS, the free energy, the entropy and the probability distribution of the energy can be calculated at any temperature. The random walk may be separated by some independent processes. Therefore, a code of WL algorithm may be implemented in parallel (replica exchange Wang-Landau algorithm) [5].

Often, we need probability distribution not only of the energy but also of other parameter such as magnetization. In that case, two-dimensional or joint density of states (JDOS) should be estimated by random walk both in the energy and this parameter. For Ising ferromagnetic model, a phase diagram for whole space of the temperature and the external magnetic field can be built by means of JDOS  $g(E, m)$ , where  $E$  is the energy and  $m$  is the order parameter. However, the obtaining JDOS requires a huge computational time which exponentially grows with lattice size. If the values of  $g(E)$  was obtained for time  $\tau$ , the function  $g(E, m)$  requires the  $\tau * N_m$  time, where  $N_m$  is number of possible values of the order parameter  $m$ . For models with continuous energetic spectrum (e.g., Heisenberg model), the number  $N_m \rightarrow \infty$  and JDOS calculation become very complicated.

Recently, some methods for speed up JDOS calculations are developed: the global updates method [6], the two level method [7], the transition matrix algorithm [8] and etc. The purpose of our work is analyzing of these methods and developing of fast algorithm for obtaining JDOS.



## 2. Models and methods

In this paper we apply the Wang Landau algorithm for Ising and 6-state Potts ferromagnetic spin models. The spin has two possible directions in the Ising model and six ones in the Potts model. The Hamiltonian of these models is determined by the formula:

$$E = -J \sum_{\langle i,j \rangle} \vec{S}_i \vec{S}_j - \vec{H} \sum_i \vec{S}_i \quad (1)$$

where  $\vec{S}_i$  is the value of spin placed in the site  $i$  and index  $\langle i,j \rangle$  denotes pairs of nearest-neighbour segments, the parameter  $J$  is a constant of spin interactions,  $\vec{H}$  is an external magnetic field.

The WL algorithm was used for estimate the JDOS dependence  $g(E,m)$  on the energy  $E$  and the order parameter  $m$  in the absence of external field. This simulation allows obtaining phase diagram for Ising model in wide range of temperatures and external fields. The standard parallel WL algorithm for determination JDOS is next:

1. The energy range of the system as a whole is divided in overlapping energy domain. Value of its overlapping should be 60-85%. For the each domain, the empty histogram  $h(E,m)$ , the matrix of logarithms of JDOS with initial value  $\ln(g(E,m)) = 0$  and the initial modification factor  $f = 1$  are set. Then, in the each domain an independent random walk is completed as described in pp. 2-4.
2. A rotation of the randomly chosen spin is completed that the system changes state from  $i$  state to  $j$  one. The new configuration is accepted with probability:

$$P = \min \left( \frac{g(E_i, m_i)}{g(E_j, m_j)}, 1 \right) \quad (2)$$

3. Then, the histogram and the array of logarithms of JDOS are updated by the rule:

$$\begin{aligned} h(E_k, m_k) &\rightarrow h(E_k, m_k) + 1 \\ \ln(g(E_k, m_k)) &\rightarrow \ln(g(E_k, m_k)) + f \end{aligned} \quad (3)$$

where  $k$  is the current system configuration.

4. After fixed number of steps 2-3 (i.e. 1000-10000 Monte-Carlo steps), the flatness of the histogram is checked. The flatness criterion allows usually the deviation 20-80% from the average value for all components of the histogram. If this criterion is satisfied, the histogram is reset and the modification factor  $f$  is updated:  $f \rightarrow f/2$ . The simulation in the domain is continued before the modification factor of this domain become to equal  $f_{final} = 10^{-5} \dots 10^{-8}$ .
5. When modification factors in all windows are equal to  $f_{final}$ , the simulation is over. On account of board errors in windows, a concatenation of JDOS pieces should be making near a center of overlapping regions. The joining point is chosen by a condition of the best derivative correspondence of JDOS.

The calculation of JDOS for large lattices requires too huge computational time. One of ways for speed up of these calculations is *global updates* method [6]. This method is used for stimulation of walker to move in the unexplored domain. In global updates method, all elements of logarithm JDOS are updated by a kernel function, when JDOS have enough a good estimation inside explored domain. This method may be used for saving time, but the kernel function should be chosen very precisely for different systems.

*Two level method* [7] breaks the simulation into two stages of random walk. In the first stage, WL algorithm is used for obtaining of the function  $g(E)$ . In the second stage, the histogram  $h(E,m)$  is accumulated without any updating of DOS. After fixed number of Monte-Carlo steps, the final JDOS is obtaining as:

$$g(E, m) = g(E)h(E, m) \quad (4)$$

Two level method has some disadvantages. Firstly, a supplementary researching of precision with dependence on number of Monte Carlo steps for studying models is required. Secondly, this method is effective only if the change of the function  $g(E, m)$  with  $m$  for the given value of  $E$  is not too large but it is incorrect for ferromagnetic lattice models (Figure 1 and Figure 2).

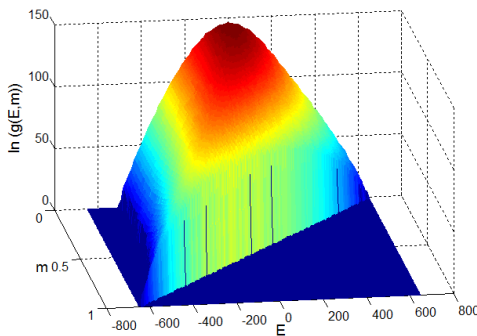
In this work, we use the three-stage method for obtaining JDOS:

1. In the first stage, we implement the conventional WL algorithm for the calculation of the function  $g(E)$  as in two level method.
2. Then, the random walk in the space  $(E, m)$  with global updates is set. Every thousand Monte-Carlo steps, we update  $g(E, m)$  using the Gaussian kernel function:

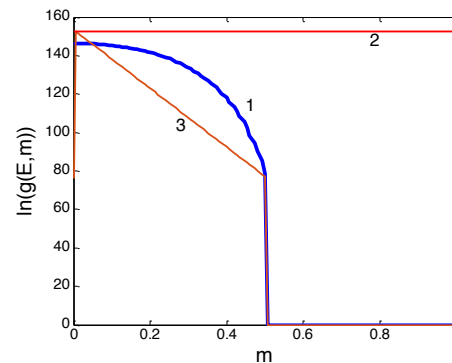
$$\ln(g(E, m)) \rightarrow \ln(g(E, m)) + \kappa \exp\left[\frac{-\lambda}{\ln(g(E, m)) - \omega}\right] \Theta(\ln(g(E, m)) - \omega) \quad (5)$$

with the Heaviside step function  $\Theta$ . We used the values  $\lambda=1$ ,  $\omega=100$ ,  $k=10$ . In this stage, we determine the possible  $(E, m)$  combinations and an approximate profile of JDOS.

3. Using the function  $g(E)$  and data obtained from the random walk with global updates, the initial approximation of JDOS  $g_0(E, m)$  is set. In the point, where  $g(E, m)$  has a maximum for a given value of  $E$ , we propose  $g_0(E, m) = g(E)$ . For board values of  $m$  we take the value  $g_0(E, m)=0$ , for intermediate values, the linear approximation was used (Figure 2). Then, the WL algorithm with the initial approximation  $g_0(E, m)$  of JDOS is completed.



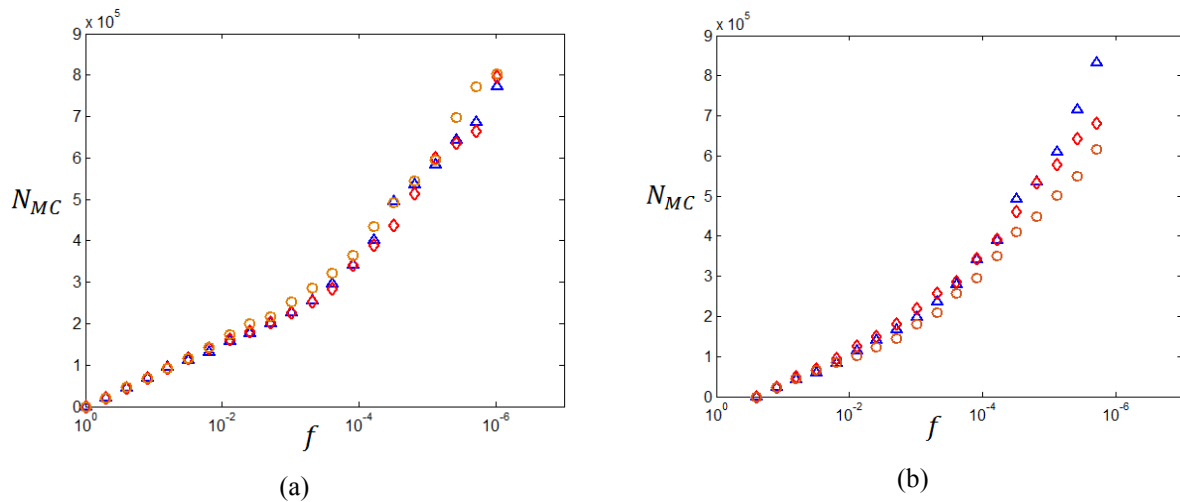
**Figure 1.** Joint density of states for Ising model with 6x6x6



**Figure 2.** Profile of JDOS (1), the initial approximation  $g_0(E, m)$  in the two level (2) and three-stage (3) methods for the value  $E=0$

### 3. Results and discussions.

We studied the efficiency of our method on the example of 6x6x6 Ising ferromagnetic model. The initial approximation of JDOS from two level and three-stage methods is used. The dependencies of number of Monte Carlo steps on the modification factor are represented in figure 2. The total number of Monte Carlo steps for each method is specified in table 1. For the initial modification factor  $f_0=1$ , the simulation with any initial approximation does not accelerate calculations. But for  $f_0=0.125$ , the three-stage method much faster than others.



**Figure 3.** Number of Monte Carlo steps vs. the modification factor in the conventional WL algorithm ( $\Delta$ ), two level method ( $\diamond$ ), our method ( $\circ$ ) at  $f_0=1$  (a), 0.125 (b) for 6x6x6 Ising model.

**Table 1.** Number of Monte Carlo steps for different initial modification factors and simulation methods

Initial modification factor	conventional WL algorithm	two level method	three-stage method
$f_0=1$	$771 \cdot 10^6$ MC steps	$795 \cdot 10^6$ MC steps	$803 \cdot 10^6$ MC steps
$f_0=0.125$	$832 \cdot 10^6$ MC steps	$681 \cdot 10^6$ MC steps	$616 \cdot 10^6$ MC steps

The probability of system configuration with the energy  $E$  and the order parameter  $m$  is determined by the formula:

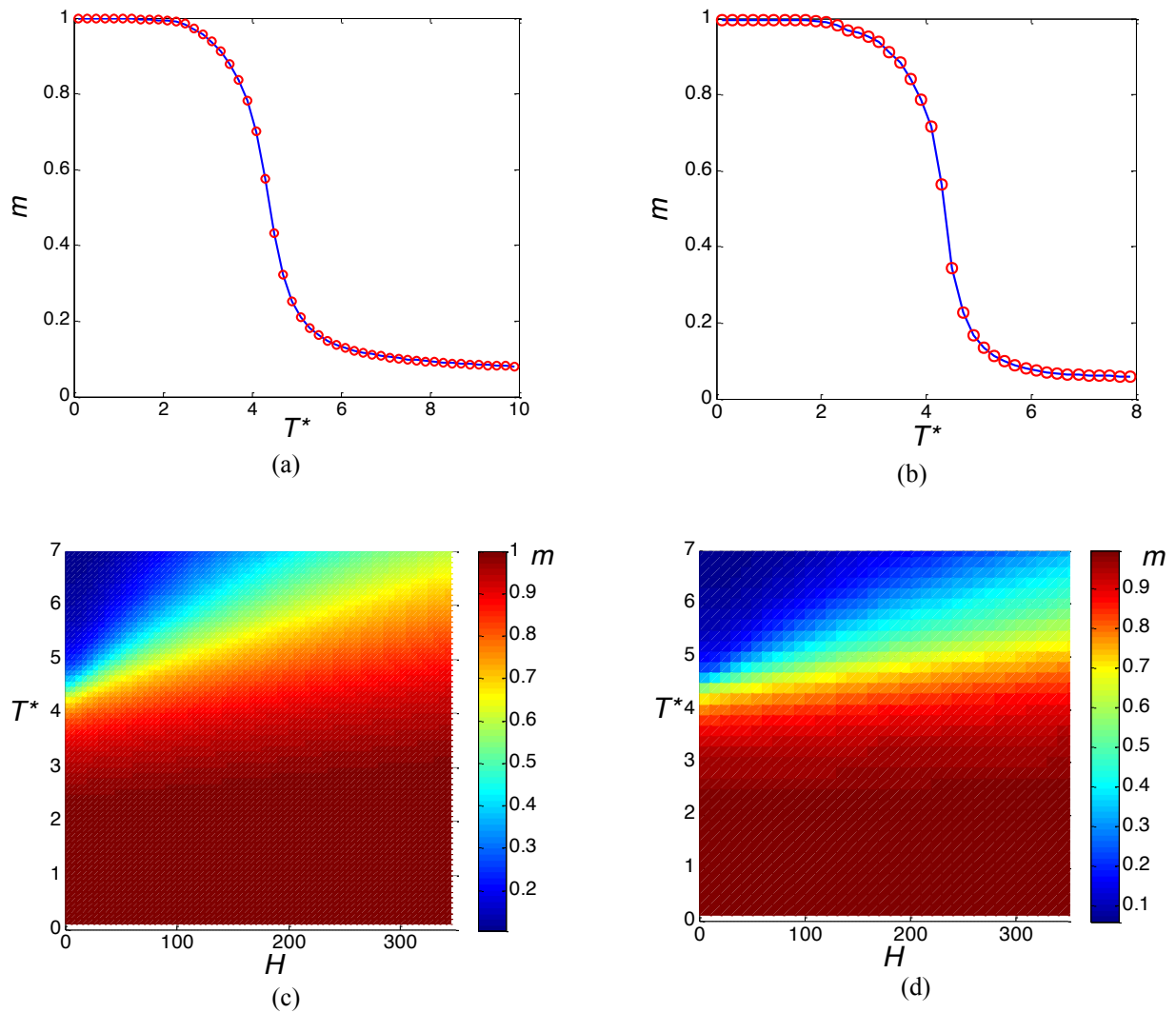
$$P(E, m) = \frac{1}{Z(T)} g(E, m) e^{-E/k_B T} \quad (6)$$

where  $Z(T)$  is the partition function.

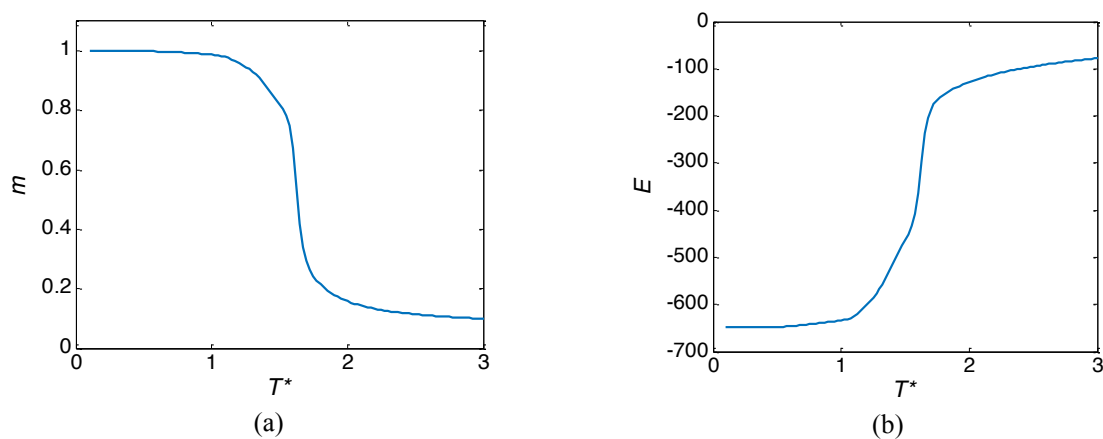
The dependencies of order parameter on temperature calculated on the base of formula (5), by means of standard WL algorithm and three-stage method for the Ising model with the lattice sizes 6x6x6 and 8x8x8 are shown in figure 4a and figure 4b. We can see that results obtained by both methods agree with each other within the error bars.

The dependencies of order parameter on temperature and external magnetic field were obtained (figures 4c, 4d). For this purpose, the density of states  $g(E, M)$ , where  $M$  is a magnetization, was obtained from the function  $g(E, m)$ , using the symmetry considerations:  $g(E, M) = g(E, -M) = g(E, m)/2$ . Then, the system energy was renormalized with considering external field interactions  $E \rightarrow E + M \cdot H$ , and the probability distribution was built on the base of the formula (5). This method may be used for obtaining phase diagrams.

The 6-state Potts model has more possible values of the system energy and the order parameter than the Ising model. Therefore, the calculations of JDOS for the Potts model are more complicated. We obtain the function  $g(E, m)$  on the base of only three-stage method for the 6-state Potts model with the lattice sizes 6x6x6. The random walk was divided in 8 energy domains with 60% of its overlapping. The dependencies of energy and order parameter on temperature are shown in figure 5.



**Figure 4.** (a,b) The order parameter vs. renormalized temperature  $T^* = k_B T/J$ , where  $k_B$  is Boltzmann constant, calculating by standard WL algorithm (solid line) and three-stage method (o) for 6x6x6 (a) and 8x8x8 (b) Ising model in the absence of external magnetic field; (c,d) The order parameter vs. renormalized temperature and external magnetic field for 6x6x6 (c) and 8x8x8 (d) Ising model.



**Figure 5.** The order parameter (a) and energy (b) vs. renormalized temperature for 6x6x6 Potts model

#### 4. Conclusion

The algorithm for fast determination of JDOS is proposed. This algorithm combines ideas of global updates consideration and two level methods. The method is analyzed and validated for the three-dimensional ferromagnetic Ising model. The developed method is applied for 6-state Potts model. We also demonstrated how one may use JDOS for obtaining phase diagrams for Ising model.

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