Monte Carlo simulations of Heisenberg magnets by the Wang-Landau method

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Abstract. In this work, we investigate the critical behavior of the three dimensional Heisenberg model by parallel Wang-Landau algorithm developed with using of the OpenMP technology.

1. Introduction

Last time there is a wide range of algorithms to explore the critical behavior of complex spin systems. Wang-Landau algorithm is one of the last introduced [1] Monte Carlo method, which allow us to get thermodynamical quantities of the spin system by calculation density of states. This method has few advantages relative to other Monte Carlo methods like Metropolis or cluster algorithms. There are no critical slowing down effect and wide range of applications e.g. exploring of polymer chains [2], protein folding [3], phase transitions [4] in spin glasses.

If the energy interval is too large we can observe divergence of the method, and, to overcome these constraints, we are using the parallel version of the Wang-Landau algorithm [5] with the partitioning of full energy interval to overlaying subintervals. Each subinterval is proceeding by the independent replica of the algorithm. Exchanges between replicas with overlapped intervals are realized for validation the principle of detailed balance. With some modifications of algorithm we can estimate magnetic properties [6] of the Heisenberg model.

2. Description of the method

Process of simulation based on random walking in the energy space of the spin system and changes spin states randomly. During a random walk, we need to track the number of visits of each energy state and build a histogram. If histogram has become sufficient flat - modifier f changes as $f = f^2$ (formula can be different). At begin of simulation need to initialize the density of states $g[E]$ by one and histogram by zero at each iteration of f. Algorithm is converge when $f$ become $f_{min}$, when value of $f_{min}$ is about one, but initial $f$ value is equal to exponent. With a known density of states, many of thermodynamic quantities can be obtained e.g. energy, free energy, heat capacity, and entropy.
Density of states $g(E)$ is number of microstates with the certain energy $E$

$$g(E) = \sum_{S_i} \delta(E - E\{S_i\})$$

where $\delta(E)$ - Dirac delta function.

To obtain thermodynamic quantities we are used formulas below:

$$U(T) = \frac{\sum_E E g(E) \exp \left(-\frac{E}{k_B T}\right)}{\sum_E g(E) \exp \left(-\frac{E}{k_B T}\right)}$$

$$F(T) = -k_B T \ln \left(\sum_E g(E) \exp \left(-\frac{E}{k_B T}\right)\right)$$

$$C(T) = \frac{1}{k_B T^2} \left[\langle E^2(T) \rangle - \langle E(T) \rangle^2\right]$$

$$S(T) = \frac{U(T) - F(T)}{T}$$

In this work we applied the Wang-Landau algorithm to the three-dimensional Heisenberg model which can be described by hamiltonian:

$$H = -J \sum_{i,j} \left\{ S_i^x S_j^x + S_i^y S_j^y + S_i^z S_j^z \right\}$$

where $S_i = (S_i^x, S_i^y, S_i^z)$, $J$ - exchange interaction constant, which characterized exchange interaction between near spins.

Wang-Landau method have ability to estimate averaged value of any observable quantities:

$$\langle A \rangle_T = \frac{1}{Z(T)} \int A(E) \exp \left(-\frac{E}{k_B T}\right) g(E) dE$$

To obtain magnetization and susceptibility with known density of states we can use equations below[2]:

$$\langle M(T,0) \rangle = \frac{1}{Z} \sum_E  M(E) g(E) \exp \left(-\frac{E}{k_B T}\right)$$

$$\bar{M}(E) = \frac{\sum_{S_i} |M_{S_i}| \delta(E - E\{S_i\})}{\sum_{S_i} \delta(E - E\{S_i\})}$$

Susceptibility can be obtained by this formula:

$$\chi(T,H) = \frac{dM}{dH} = \frac{1}{k_B T} \left[\langle M^2(T) \rangle - \langle M(T) \rangle^2\right]$$
3. Parallel Wang-Landau algorithm

If we studying relative large spin systems with complex model e.g. three-dimensional Heisenberg model which spins is continuously oriented [6], - algorithm can show divergence and calculation time tends to infinity. Those restrictions appear when the energy interval is very large. In our work, we used the replica-exchange method described in article [5]. The main idea of parallelization is subdividing full energy interval at overlapping subintervals and random walking with the different replica of the algorithm at each subinterval. We are providing a process of redistributing density of states logarithm between replicas at each f iteration, and, to save principal of detailed balance, realize density of states exchange with histogram incrementation and $G(E)$ update with neighbor replicas. With a less size of energy interval algorithm shows better convergence, especially for big count of subintervals (many of threads). Selecting of replica for exchanging is done with a probability $1/2$. After that, we are trying to exchange $G(E)$ between intervals with probability:

$$P = \min \left[ 1, \frac{g_i(E[X])g_j(E[Y])}{g_i(E[Y])g_j(E[X])} \right]$$

(11)

If exchange is done we need to modify density of states and histogram:

$$g_i(E(X)) = g_i(E(X)) \times f$$
$$g_j(E(X)) = g_j(E(X)) \times f$$
$$g_i(E(Y)) = g_i(E(Y)) \times f$$
$$g_j(E(Y)) = g_j(E(Y)) \times f$$

$$H_i(E(X)) = H_i(E(X)) + 1$$
$$H_j(E(X)) = H_j(E(X)) + 1$$
$$H_i(E(Y)) = H_i(E(Y)) + 1$$
$$H_j(E(Y)) = H_j(E(Y)) + 1$$

At the end of the estimations, density of states is averaging between threads and gluing together by the main thread. Examples of joined and unjoined $G(E)$ shown at figure 1. On the left figure density of states only averaged between replicas with overlapped intervals. On the right - averaged density of states is joined for the full energy interval.

![Figure 1](image1.png)

**Figure 1.** Unjoined (left) density of states logarithm for $N = 8 \times 8 \times 8$ and joined for the same spin system (right)

For the develop parallel version of the Wang-Landau algorithm we are using OpenMP technology for the shared memory systems. Besides "classical" CPU realizations with MPI or OpenMP[5] libraries, GPU version of this algorithm exists too[7].
4. Results of simulations
Wang-Landau algorithm allows us to provide one estimation of spin system density of energy states and get all thermodynamic quantities. For this method density of states is the main quantity, that slightly different for each calculation (rely on the count of the Monte Carlo steps). All of the thermodynamic quantities relying to the density of states, and, for the low dimensional spin system are slightly diverge for a different count of threads (figure 2). The peak of the heat capacity (figure 3) at the one place for all count of threads.

![Figure 2: Entropy and free energy for $N = 8 \times 8 \times 8$ estimated by different count of threads PP = 4,8,16](image2)

![Figure 3: Energy and heat capacity for $N = 8 \times 8 \times 8$ estimated by different count of threads PP = 4,8,16](image3)

For larger spin systems parallel algorithm shows good agreement with the serial version (figure 4). The peak of the susceptibility is near phase transition point for the isotropic three-dimensional Heisenberg model (figure 5).

5. Conclusion
The computer simulation of complex spin systems is an actual area of theoretical physics research and it requires a lot of computational resources and developing parallel versions of existing algorithms is necessary. We apply parallel version of the Wang-Landau algorithm to
Figure 4. Energy (left) and free energy (right) for Heisenberg model with $N = 32 \times 32 \times 32$ and $L = 48 \times 48 \times 48$ for the three-dimensional Heisenberg model at the parallel threads count PP = 1,4.

Figure 5. Entropy (left) with $N = 32 \times 32 \times 32$ and $N = 48 \times 48 \times 48$ and the susceptibility (right) with $N = 32 \times 32 \times 32$ for the three-dimensional Heisenberg model at the parallel threads count PP = 1,4.

the three-dimensional Heisenberg model and shows that it has good, but not ideal agreement with serial version and between multithread parallelization. For the low dimensional systems, thermodynamical quantities have some diverge for the different count of threads. For the larger systems peak of susceptibility is near phase transition point for Heisenberg model.

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