Density of states of a two-dimensional *XY* model from the Wang-Landau algorithm

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Using the Wang-Landau algorithm combined with the analytic method, the density of states of a two-dimensional *XY* model on square lattices of sizes 16×16, 24×24, and 32×32 is accurately calculated. Thermodynamic quantities, such as internal energy, free energy, entropy, and specific heat are obtained from the resulted density of states by numerical integration. It is found that both the density of states and the extensive thermodynamic quantities obey the scaling law. From the entropy curve, symptoms of phase transition are observed. A general method of calculation of the density of states of continuous models by simulation combined with analytical method is proposed.

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I. INTRODUCTION

The *XY* model has been widely used for the description of many physical systems and in the studies of phase transitions and other related problems. The two-dimensional *XY* model is especially interested in the studies of the Kosterlitz-Thouless (KT) transition. The model has been extensively studied in the past decades with many different methods, while the density of states (DOS) is yet not determined because of the complexity of the model. Toral and his group computed the DOS of the one-dimensional *XY* model and got some scaling results [1,2]. However, the two-dimensional *XY* model is more interesting and valuable. It is famous for its quasilong range order, vortex pairs, and KT phase transition [3]. It will be helpful for people to understand the nature of the model and to study in more detail the KT phase transition if the DOS of the two-dimensional *XY* model is calculated.

The model can be described by the Hamiltonian

$$H = -J\sum_{\langle ij\rangle} \vec{S}_i \cdot \vec{S}_j, \tag{1}$$

where J is the coupling constant, and $\vec{S}$ is a unit vector (the spin) in a plane. Here i or j is the lattice site on a plane, and the summation is over all nearest neighbor pairs. Different from the Ising model, the *XY* model is a continuous model in which the energy changes continuously. Thus the total number of states of the whole system is infinite, this property gives rise to the difficulties in determining the DOS near the highest and lowest energy level, as we will explain in detail later.

Recently many kinds of simulation algorithms used in the calculation of the DOS have been proposed. In this study we use Wang-Landau algorithm to calculate the DOS of a two-dimensional *XY* model [4,5]. The fast convergence, stability, and the easy to implement method makes it the first choice in a DOS calculation, however, it has some shortcomings in the accuracy of calculation as pointed out by many researchers [6]. In the case of the two-dimensional *XY* model and other continuous models alike, the algorithm usually fails to give good results of DOS close to the boundaries of the spectrum. Fortunately, on the spectrum boundaries, there are usually analytical results of the DOS available or may be obtained in less effort. By combining the analytical results close to spectrum boundaries with simulation, better results of the DOS can be obtained. In the following we show this process using the two-dimensional *XY* model.

II. CALCULATIONAL PROCEDURE

A. Density of states

In order to use the Wang-Landau algorithm to a continuous model, we divide the whole energy range to some subintervals and fine divide each subinterval into many small intervals. Every small interval is regarded as an energy level and represented by its middle energy. The Wang-Landau algorithm can be used to calculate the relative DOS of each subinterval and then the DOS of the whole range can be obtained by smoothly joining the DOS on each subinterval. It should be noted that the DOS calculated this way is the relative DOS of the system, which contains an arbitrary scaling constant. In the case of a discrete model like the Ising model, both the total number of states and the number of the states of the lowest energy level are known and the scaling factor can easily be determined by using either of the known conditions. In the case of a continuous model, one has no knowledge of the DOS at any point so that it is harder to get the scaling factor directly. In fact, the situation is even worse. In the *XY* model, the DOS in the middle range of the spectrum do not change much so that the discretization will not introduce much error to the calculation of DOS. On the other hand, the changes of the DOS close to the spectrum boundary are very large, so accuracy calculation of the DOS close to the spectrum boundary is impossible by simply dividing the small intervals finer and finer. This difficulty is bypassed by the observation that in many cases of the continuous models the analytical expression of DOS close to the spectrum boundaries are known. In this case we can use the known expression for the DOS close to the spectrum boundaries and join them smoothly to the simulated relative DOS in the middle range to get the DOS of the system.

The Hamiltonian of a two-dimensional square lattice *XY* model can be written as

$$H = -\sum_{\langle ij\rangle} \cos(\theta_i - \theta_j). \tag{2}$$

Here we set $(J=1)$ for simplicity, and θ_i is the angle between $\vec{S}_i$ and a reference direction in the plane. The ground state of

the model is the ferromagnetic ordered state where all $\vec{S}_i$ are parallel. Close to the ground state, each spin may deviate from the alignment direction by thermal agitation. The deviation is small at low temperature, so that it can be approximated as

$$H = -2N + \frac{1}{2}\sum_{\langle ij\rangle}(\theta_i - \theta_j)^2 = -2N + \frac{1}{2}\sum_{\vec{k}}|\theta(\vec{k})|^2 f(\vec{k}), \quad (3)$$

where N is the total number of the square lattice sites ($N=L\times L$), and $\vec{k}$ is the wave vector in the plane, $\theta(\vec{k})$ is the Fourier component of θ_i and

$$f(\vec{k}) = \sum_{\vec{a}}[1-\cos(\vec{k}\cdot\vec{a})].$$

Here $\vec{a}$ is the base vector of the square lattice. The partition function of the system is

$$Z(\beta) = \int_{2N}^{-2N} g(E)e^{-\beta E}dE = \int_0^{4N} g(E-2N)e^{-\beta(E-2N)}dE$$

$$\approx e^{2\beta N}\int_0^{\infty} g'(E)e^{-\beta E}dE, \quad (4)$$

where $g'(E)=g(E-2N)$. From Eq. (4) we see that $Z(\beta)e^{-2\beta N}$ is the Laplace transformation of $g'(E)$. Here $\beta=1/T$ is the inverse of temperature (we use a unit system where Boltzmann constant $k_B=1$). From Eq. (4) it is clear that the DOS $g'(E)$ can be obtained if the partition function $Z(\beta)$ is known. In fact the partition function $Z(\beta)$ for the Hamiltonian (3) can be calculated directly,

$$Z(\beta) = \int_{-\infty}^{+\infty}\prod_{\vec{k}\neq 0} d\theta(\vec{k})e^{-\beta H} = e^{2\beta N}\prod_{\vec{k}\neq 0}\sqrt{\frac{\pi}{\beta f(\vec{k})}}. \quad (5)$$

Then the DOS $g'(E)$ is obtained from the inverse Laplace transformation of $Z(\beta)e^{-2\beta N}$,

$$g'(E) = \frac{1}{2\pi i}\int_{\beta'-i\infty}^{\beta'+i\infty} e^{\beta E}Z(\beta)e^{-2\beta N}d\beta$$

$$= \frac{1}{2\pi i}\int_{\beta'-i\infty}^{\beta'+i\infty} e^{\beta E}d(\beta)\prod_{\vec{k}\neq 0}\sqrt{\frac{\pi}{\beta f(\vec{k})}}$$

$$= \frac{\pi^{(N-1)/2}}{2\pi i}\left(\prod_{\vec{k}\neq 0}\frac{1}{\sqrt{f(\vec{k})}}\right)\int_{\beta'-i\infty}^{\beta'+i\infty}\frac{e^{\beta E}}{\beta^{N-1/2}}d\beta = CE^{(N-3)/2}.$$

Finally we have

$$g(E) = C(E+2N)^{(N-3)/2} \quad (6)$$

$$C = \frac{\pi^{(N-1)/2}}{\Gamma\left(\frac{N-1}{2}\right)}\prod_{\vec{k}\neq 0}\frac{1}{\sqrt{f(\vec{k})}}. \quad (7)$$

This expression of DOS is the result from the low temperature approximation of partition function, which is valid only in the vicinity of the ground state.

The DOS of this model is symmetrical, so the DOS close to the higher boundary has a similar expression. As was pointed out before, the Wang-Landau algorithm only calculates the relative values of the density of states. The constant C is of special use in normalization, which is quite valuable in calculating the free energy and the entropy. The Eq. (6) solves the problem of strong variations of DOS close to the boundary, and at the same time, Eq. (7) solves the problem of normalization. Both are hard to obtain in numerical simulations for continuous systems, and we solve them by the analytic derivation. This is a very general method to obtain DOS of a continuous system close to the ground state.

For the model studied, the whole energy range is $4\times L\times L$ on a $L\times L$ lattice, from $-2N$ to $2N$ where $N=L\times L$ is the total sites of the lattice. With the above-mentioned method, we calculate the DOS of the middle energy range $\left[-2N+\frac{N}{256}, 2N-\frac{N}{256}\right]$ directly, and evaluated the DOS close to the spectrum boundaries with the help of the analytic expressions. In real calculation, we extended the range of the middle part slightly so that there are overlap energy ranges of the middle and boundary subintervals. The DOS on subinterval $\left[-2N, -2N+\frac{N}{256}\right]$ is calculated in a way by the use of the analytic expression and simulation relaxation. The subinterval is divided into $4\times N$ small bits, and the DOS for every bit is assigned the value according to the analytical result Eq. (6) as the initial value. Using an initial small f [about $\exp(10^{-4})\sim\exp(10^{-5})$], we then simulate with the Wang-Landau algorithm to relax the analytic DOS for a suitable MCS. This "smooth" simulation is used to modify the DOS close to $-2N+\frac{N}{256}$ a little bit, however, the relative values near $-2N$ are basically unchanged. This is also a check of the consistence of the method since Eq. (6) is strictly valid at the limitation of the ground state. The upper subinterval is treated the same way. The DOS in the middle part is then smoothly connected to the boundary subintervals. To connect the DOS smoothly, we require that the difference of the DOS in the overlap region from calculations in the two subinterval simulations be minimum. The trick of Shulz *et al.* [7] in the accurate calculation of the DOS on the interval boundaries is used in connection. The final result of DOS is shown in Fig. 1. Figure 1(a) is a plot of the part close to the ground state, and we see that the DOS increases dramatically in a small energy range. Figure 1(b) is the overall DOS of the model. The calculation is performed with finite systems of 16×16, 24×24, and 32×32, and periodical boundary condition was used in the simulation. The DOS shows the generic behavior: $g(E,N)\sim e^{N\phi(E/N)}$ where $\phi(E/N)$ is an intensive function. This behavior is consistent with the scaling law in Refs. [1,2,8]. We note here that this also proves the validity of the value of constant C [Eq. (7)]. It should be noted that this scaling relation is strictly satisfied only in the thermodynamic limit where $N\to\infty$. In Fig. 2 we show the small deviations of $\ln g_{16\times 16}/N$ and $\ln g_{24\times 24}/N$ to $\ln g_{32\times 32}/N$ with respect to E/N. From the figure we see that the difference between the case of 24×24 and 32×32 is much smaller than the difference between the case of 16×16 and 32×32. Based on this result we expect that the case of 32×32 is a very good approximation to the infinite system, and the DOS calculated with 32×32 should be good enough in most applications. However, in the case when phase transition occurs, the finite size effect may be important and the 32×32

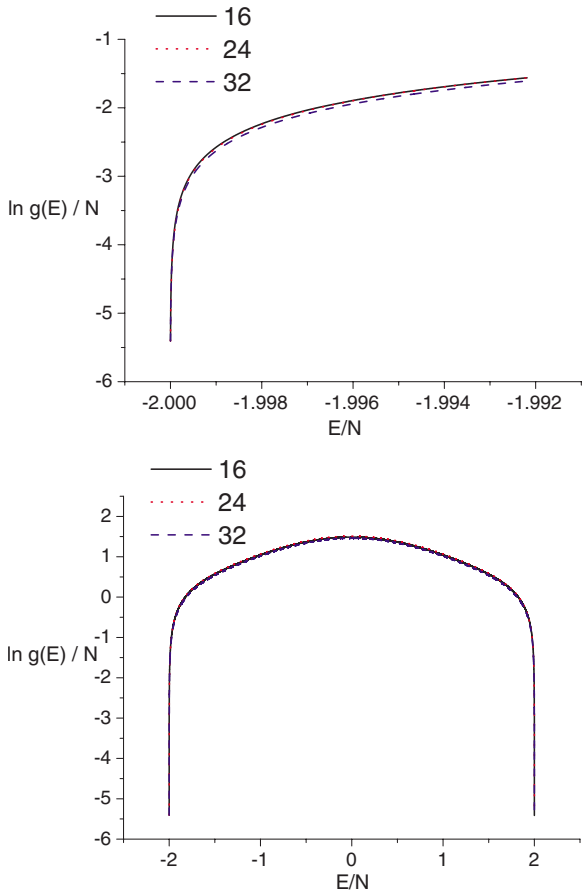

FIG. 1. (Color online) (a) The density of states near the lowest energy of the two-dimensional *XY* model on square lattices of size 16×16, 24×24, 32×32. (b) The density of states in the whole energy range of the two-dimensional *XY* model on square lattices of size 16×16, 24×24, 32×32.

lattice may be too small to obtain accurate results as in the case of KT transition.

B. Thermodynamic quantities

With the accurate result of the DOS obtained, some thermodynamic quantities can be calculated from it by a simple integration. The internal energy, the specific heat, the free energy, and entropy can be immediately calculated according to the equations as follows:

$$U(T) = \frac{\sum_E Eg(E)e^{-\beta E}}{\sum_E g(E)e^{-\beta E}} = \langle E\rangle_T, \tag{8}$$

$$C_V(T) = \frac{\partial U}{\partial T} = \frac{\langle E^2\rangle_T - \langle E\rangle^2{}_T}{T^2}, \tag{9}$$

$$Z = \sum_E g(E)^{-\beta E}, \tag{10}$$

$$F(T) = -T\ln Z, \tag{11}$$

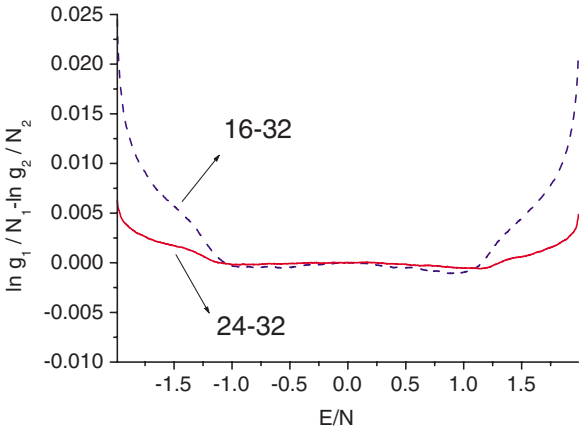

FIG. 2. (Color online) The difference of the two-dimensional *XY* model on square lattices of size 16×16 and 32×32, and 24×24 and 32×32 after scaling. The DOS of energy $E=0$ is adjusted so that they have the same value.

$$S(T) = \frac{U(T) - F(T)}{T}. \tag{12}$$

From the expression we see that the partition function cannot be obtained without the knowledge of the normalization constant C, and neither of the free energy and the entropy. When the temperature $T\to0$ we may use Eq. (6) to get the analytic expressions of thermodynamic quantities at low temperature,

$$Z = \int_{2N}^{-2N} C(E+2N)^{(N-3)/2}e^{-E/T}dE = C\Gamma\left(\frac{N}{2}\right)e^{2N/T}T^{(N-1)/2}, \tag{13}$$

$$F = -T\ln Z = -T\ln\left[C\Gamma\left(\frac{N}{2}\right)\right] - 2N - \frac{N-1}{2}T\ln T, \tag{14}$$

$$S = -\frac{\partial F}{\partial T} = \ln\left[C\Gamma\left(\frac{N}{2}\right)\right] + \frac{N-1}{2}(\ln T + 1), \tag{15}$$

$$C_V = T\frac{\partial S}{\partial T} = \frac{N-1}{2}, \tag{16}$$

$$U = F + TS = -2N + \frac{N-1}{2}T. \tag{17}$$

The low temperature result was obtained in the assumption that the total number of lattice sites is very large, that is, the thermodynamic limit $N\to\infty$ is assumed. By taking the zero temperature limit we get the ground state behavior $F\to-2N$, $S\to-\infty$, $C_V\to\frac{N}{2}$, and $U\to-2N$. The behavior of the entropy does not follow the third law of thermodynamics, which requires that the entropy is zero in the limit. The reason for this discrepancy is the ignorance of the quantum effect of our calculation. In fact, in real physical systems the zero temperature behavior of the system is always quantum. Mathematically the incorrect zero temperature limit of entropy comes from the finite and continuous density of states

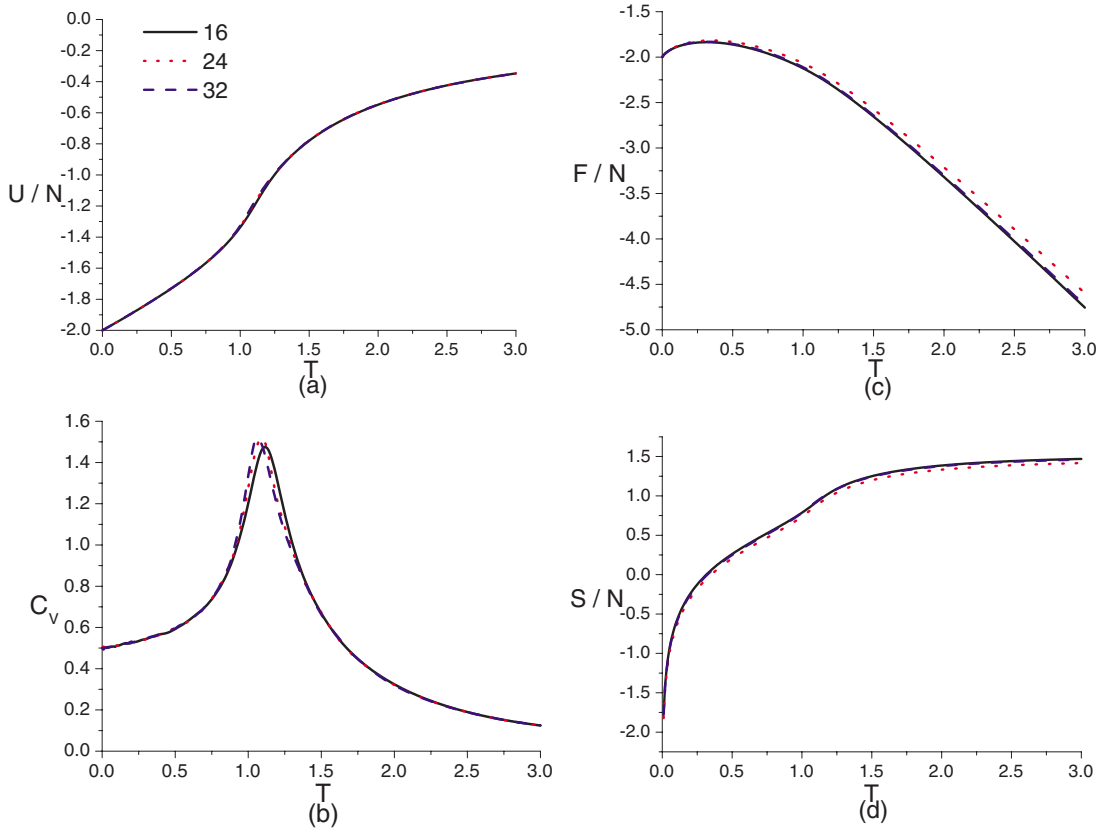

FIG. 3. (Color online) The internal energy (a), specific heat (b), free energy (c), and entropy (d) per lattice site of the two-dimensional *XY* model on square lattices. 16×16 solid line, 24×24 dotted line, and 32×32 dashed line.

close to the ground state. The zero temperature entropy is given by $S(T=0)=\ln g_0$, where g_0 is the degeneracy of the ground state. For the *XY* model, the density of states is continuous so that the number of states at any specific point of energy is zero, thus $g_0=0$ and $S\rightarrow-\infty$.

The results of the thermodynamical quantities in a large temperature range was evaluated by numerical integration and are shown in Fig. 3. The figures plot the quantities per site for different sizes of the system, and it is clear from the figures that the results of different sizes of the lattices basically follow the same curve, which indicates that the size effect is not quite important for system size larger than 16×16, the smallest system we calculated. The scaling law of extensive thermodynamical quantities is consistent with that of the DOS, as the entropy has the same dimension as the logarithm of the DOS.

As we only consider short range interaction, this result is consistent with Refs. [1,2,8]. The peak of the specific heat differs with the size of the system. In the temperature near $T=1$, the entropy shows a sudden rise, which indicates the rise of the number of microscopic configurations. We know in the temperature of KT transition the vortex pairs break up and the restriction is released [3], which also gives a rise to the number of microscopic configurations. So the abnormal behavior of the entropy curve may probably show the KT transition. As KT transition is very weak, it can hardly be observed from the free energy curve. It is known that the effective vortex pair interaction is long ranged so that our current system size is too small to describe the KT transition properly. Thus the accurate transition temperature is yet not determined by this method.

III. CONCLUSIONS

We calculated the DOS of the two-dimensional *XY* model on a square lattice by using the Wang-Landau algorithm combined with analytical expressions on the spectrum boundaries. And from the DOS we calculated the internal energy, the specific heat, the free energy, and the entropy. We find the scaling law of the DOS and the extensive thermodynamic quantities. From the curve of entropy we see some symptoms of phase transition. We find that simulation algorithms will meet difficulties in the calculation of DOS close to the spectrum boundaries with continuous models. We propose a general method to solve such difficulty by using the analytical expressions at the boundaries.

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