Efficient algorithm for computing correlation functions of the two-dimensional random-bond Ising model

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Extending the recent work of the bond-propagation algorithm [Y. L. Loh and E. W. Carlson, Phys. Rev. Lett. **97**, 227205 (2006)], we present an efficient algorithm for calculating the correlation functions between any two (or more) spins of Ising models in two dimensions. With this algorithm, the spontaneous magnetization, correlation length, and susceptibility can be calculated. The results for the usual Ising model with different size lattices are compared with the exact results. We also present the correlation functions for the $\pm J$ random-bond Ising model.

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I. INTRODUCTION

It is well known that Ising model is the basic model in study on phase transition. Although it is simple, the exact solutions can be obtained in rare cases. Recently an efficient algorithm is presented for computing the partition function in two dimension (2D) which is exact to machine precision and works for any planar network of Ising spins with arbitrary bond strengths.[1,2] The algorithm executes in $O(N^{3/2})$ time for most planar networks of interest, much faster than other numerical method. This method works by successively integrating in and then integrating out spin degrees of freedom in a way that only introduces local changes to the network, in order to progressively move degrees of freedom to an open edge of the network, where they are eliminated. It is called the bond-propagation (BP) algorithm. There are two basic transformations required: a series reduction and the so-called Y-Δ transformation (along with its corresponding inverse). Using these ingredients, a 2D bond network can be efficiently reduced to a single net bond. Then one can get the partition function and heat capacity, etc. In fact BP algorithm is an extension of a bond-propagation algorithm originally developed for resistor networks.[3]

In Ref. 2, a method to evaluate the correlation function between two corner spins of a finite lattice is also presented. However we find that extending BP algorithm the correlation functions between any two spins (even many spins) can be evaluated. In our algorithm the concerned spins are propagating, so it can be called site-propagation (SP) algorithm. With this algorithm the spontaneous magnetization, correlation length, susceptibility can be calculated. As the BP algorithm, it also can be applied to random-bond Ising models (RBIM) and geometric frustration as in the case of triangular Ising antiferromagnets but without external field.

For the pure 2D Ising model, beside the famous work of Onsager on the partition function[4] and Yang's work on spontaneous magnetization,[5] Wu and McCoy had done formidable work to study the correlation functions.[6–8] As a test of SP algorithm, we calculate the spontaneous magnetization, the critical correlation function, and correlation length on lattices with size up to 1024×1024. The results agree with the famous Yang's work on the spontaneous magnetization and Wu *et al.*'s work on the correlation functions. Our results are obtained on a common workstation and in several weeks, so one can see the high efficiency of this algorithm easily.

Of course there is nothing new for the pure 2D Ising model. However, the Ising models with randomness are still of much interest. The models with weak randomness has been studied for more than 20 years, they are still controversial.[9–15] The RBIM with strong randomness, the Ising spin glass, have been intensively studied, especially on Nishimori point, by renormalization group, numerical transfer matrix and Monte Carlo simulation.[16–22] As an example we show some typical correlation functions for the $\pm J$ RBIM at the end of paper. SP algorithm can provide another powerful tool to study this kind of models.

We arrange this paper as follows. In Sec. II, we give the SP algorithm. In Sec. III, we calculate the correlation function for the pure two-dimensional Ising model with SP algorithm. The spontaneous magnetization, correlation length, and the critical correlation are calculated and compared with the exact results. In Sec. IV, SP algorithm is applied to RBIM simply. Section V is a summary.

II. SITE-PROPAGATION ALGORITHM

Our goal is to calculate the two point correlation on a 2D lattice

$$\langle\sigma_{\mathbf{r}}\sigma_{\mathbf{r}'}\rangle = \frac{1}{Z}\sum_{\{\sigma_i\}}\sigma_{\mathbf{r}}\sigma_{\mathbf{r}'}e^{-\beta H}, \tag{1}$$

where Z is the partition function. We call $\sigma_{\mathbf{r}}$ and $\sigma_{\mathbf{r}'}$ the concerned spins in the following. The Ising Hamiltonian is given by

$$-\beta H = \sum_{\langle i,j\rangle} J_{ij}\sigma_i\sigma_j. \tag{2}$$

where the nearest-neighbor dimensionless couplings $J_{ij}=\beta\tilde{J}_{ij}$ are arbitrary real numbers. The denominator in Eq. (1), the partition function, can be calculated with the bond-propagation (BP) algorithm.[1,2] The numerator in Eq. (1) can be calculated with the site-propagation algorithm, which is shown schematically in Fig. 1. Besides the BP "series" reduction and BP Y-Δ transformation defined in Refs. 1 and 2,

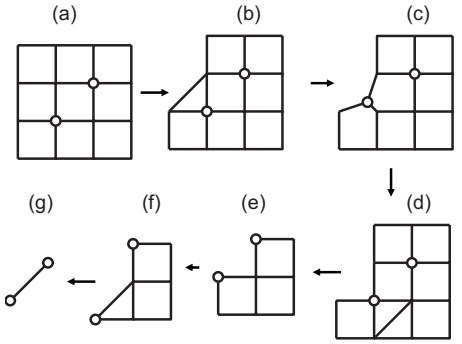

FIG. 1. The algorithm for calculating the numerator in Eq. (1). The two open circles represent the concerned spins. Using BP series reduction, BP Y-Δ and its inverse, one can transform the lattice from (a) to (b). From (b) to (c), the SP Δ-Y transformation is used. From (e) to (f), the SP series reduction is used. Finally the two concerned spins are shifted to the right down corner.

a site-propagation "series" reduction and a SP Y-Δ transformation are necessary in the algorithm.

We define the SP series reduction and SP Δ-Y transformation. These building blocks are transformations of the J's that preserve the value of the numerator in Eq. (1). SP "series" reduction corresponds to integrating out a spin with two neighbors, generating an effective coupling J_{12} to make the

$$\sum_{\sigma} \sigma e^{\sigma(J_1\sigma_1+J_2\sigma_2)} = \sigma_1 e^{\delta G+J_{12}\sigma_1\sigma_2}, \tag{3}$$

[see Fig. 2(a)]. It is convenient to use variables $j_i=e^{-J_i}$, $j_{ij}=e^{-J_{ij}}$, and $\delta g=e^{\delta G}$. Then we get the solution $\delta g=\sqrt{z_0 z_1}$, $j_{12}=z_1/\delta g$, where $z_0=\frac{1}{j_1 j_2}-j_1 j_2$ and $z_1=j_2/j_1-j_1/j_2$. Because the solutions in SP series reduction and Δ-Y transformation are usually complex even if the initial couplings are real, we need use complex algorithm. We do not use another solution $\delta g=\sqrt{z_0}\sqrt{z_1}$, $j_{12}=\sqrt{z_1}/\sqrt{z_0}$, because it contain more computations of square root than the former solution. Although the former solution is different from the latter one in some cases, it can be shown that the former solution satisfy also Eq. (3). For example, given $z_0=a_0 e^{i\phi_0}$, $z_1=a_1 e^{i\phi_1}$ with $\phi_0+\phi_1>2\pi$, $2\pi>\phi_1-\phi_0>0$. The former solution leads to $\delta g=\sqrt{a_0 a_1}e^{i(\phi_0/2+\phi_1/2-\pi)}$ and $j_{12}=\sqrt{a_1/a_0}e^{i(\phi_1/2-\phi_0/2+\pi)}$ and the latter one leads to $\delta g=\sqrt{a_0 a_1}e^{i(\phi_0/2+\phi_1/2)}$ and $j_{12}=\sqrt{a_1/a_0}e^{i(\phi_1/2-\phi_0/2)}$. However both of them satisfy Eq. (3).

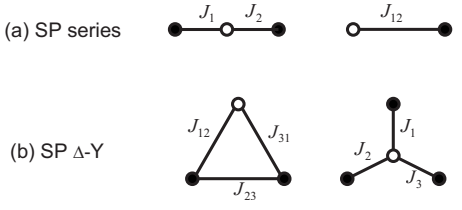

FIG. 2. Building blocks of site propagation. (a) SP series. In a SP series reduction, the middle spin (which is the concerned spin) is integrated out. The concerned spin is shifted to be the right spin. (b) SP Δ-Y and Y-Δ. In a SP Δ-Y transformation, a new spin (the center spin in Y) is introduced. After SP Δ-Y the concerned spin (the top spin in Δ) is shifted to be the center spin of Y. See Eq. (4) for formulas relating the coupling constants in these transformations. After SP Y-Δ the concerned spin (the center spin of Y) is shifted to be the top spin in Δ. See Eq. (6) for formulas.

The SP Δ-Y transformation corresponds to introducing a new spin σ to make

$$\sigma_1 e^{J_{12}\sigma_1\sigma_2+J_{23}\sigma_2\sigma_3+J_{31}\sigma_3\sigma_1} = e^{\delta G}\sum_{\sigma} \sigma e^{J_1\sigma_1\sigma+J_2\sigma_2\sigma+J_3\sigma_3\sigma}. \tag{4}$$

The concerned spin σ_1 is shifted to the center spin σ in the "Y" [see Fig. 2(b)]. The couplings of the resulting "Y" and the correlation shift are

$$j_1=\sqrt{\frac{t_1-1}{t_1+1}}, \quad j_2=\sqrt{\frac{z_2+z_3 j_1^2}{z_0+z_1 j_1^2}},$$

$$j_3=\sqrt{\frac{z_3+z_2 j_1^2}{z_0+z_1 j_1^2}}, \quad \delta g=\frac{z_0}{\frac{1}{j_1 j_2 j_3}-j_1 j_2 j_3}, \tag{5}$$

where $t_1=\sqrt{c_2 c_3/(c_0 c_1)}$, with $c_0=z_0+z_1+z_2+z_3$ and $c_1=z_0+z_1-z_2-z_3$, and c_2, c_3 are obtained by cyclic permutation, and $z_0=\frac{1}{j_{12}j_{23}j_{31}}$, $z_1=\frac{j_{12}j_{31}}{j_{23}}$ and $z_2=\frac{j_{12}j_{23}}{j_{31}}$, $z_3=\frac{j_{23}j_{31}}{j_{12}}$. Naive permutation from j_1 to j_2, j_3 will cause errors in phase factor and such solution cannot satisfy Eq. (4). Of course, one can get j_2 at first, then express j_1, j_3 in terms of j_2 like Eq. (5). It can be easily shown that the transformation is the same as BP Δ-Y transformation if the concerned spin remains at the top rather than be shifted to the center of Y.

The inverse of SP Δ-Y transformation is SP Y-Δ transformation defined by the following equation:

$$e^{\delta G}\sigma_1 e^{J_{12}\sigma_1\sigma_2+J_{23}\sigma_2\sigma_3+J_{31}\sigma_3\sigma_1} = \sum_{\sigma} \sigma e^{J_1\sigma_1\sigma+J_2\sigma_2\sigma+J_3\sigma_3\sigma}. \tag{6}$$

where the concerned spin σ is shifted to be top spin σ_1 [see Fig. 2(b)]. One solution is given by

$$\delta g=(z_0 z_1 z_2 z_3)^{1/4}, \quad j_{12}=\frac{\delta g}{\sqrt{z_0 z_3}},$$

$$j_{23}=\frac{1}{j_{12}}\sqrt{\frac{z_2}{z_0}}, \quad j_{31}=\frac{\delta g j_{12} j_{23}}{z_2}, \tag{7}$$

where $z_0=\frac{1}{j_1 j_2 j_3}-j_1 j_2 j_3$, $z_1=\frac{j_2 j_3}{j_1}-\frac{j_1}{j_2 j_3}$, $z_2=\frac{j2}{j_1 j_3}-\frac{j_1 j_3}{j_2}$, and $z_3=\frac{j_3}{j_1 j_2}-\frac{j_1 j_2}{j_3}$. It should be noted that σ_1 is the concerned spin, and not symmetric with σ_2, σ_3, so z_2, z_3 (or j_2, j_3) are not obtained from z_1 (or j_1) by cyclic permutation. It can be easily shown that the transformation is the same as BP Y-Δ transformation if the concerned spin is at the top of Y and stays still at the top of Δ after the transformation. For example, from Figs. 1(c) and 1(d), such a transformation is used.

If the two concerned spins are nearest neighbors, it can be shown that the SP series reduction and Δ-Y transformation (along with its inverse), in which one of the spins is shifted, also exist, and the transformation formulas are the same as those discussed above. In addition, in the propagation process the trajectories of the two concerned spins must not

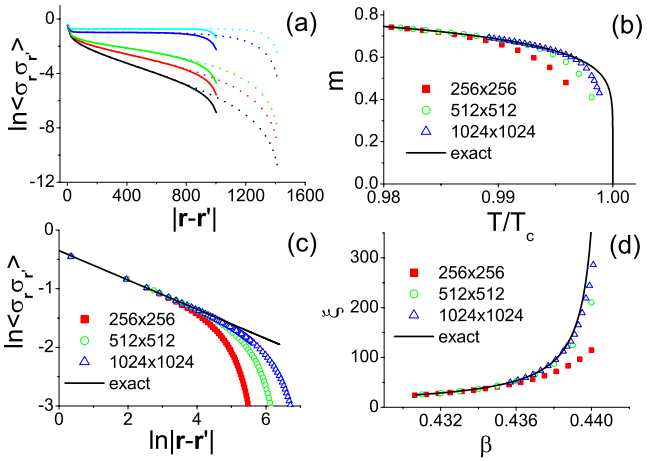

FIG. 3. (Color online) (a) Typical correlation functions calculated with SP algorithm. (b) The spontaneous magnetization on a square lattice with uniform coupling. The black solid curve is the exact result of Yang (Ref. 5) (c). The correlation function at critical point. The results on 256×256 lattice are at $\beta=044125$, 512×512 lattice at $\beta=0.4410$, and 1024×1024 lattice at $\beta=0.4408$. (d) The correlation length for $T>T_c$ on a square lattice with uniform coupling.

intersect because two concerned spins cannot occupy a same site. Although in the intermediate steps the couplings are usually complex, the final result should be real. Due to the round-off error there are small imaginary parts.

As the bond-propagation algorithm,[1] the site-propagation algorithm requires open boundary conditions in at least one direction in order to have a free edge at which propagating bonds can annihilate. Therefore, the algorithm can work with open boundary conditions in both directions, or cylindrical boundary conditions (open in one direction but periodic in the other), but not a torus. Cylinders with skew-periodic or helical boundary conditions may be used as well. The site-propagation algorithm can also be straightforwardly adapted to infinite strips.

III. COMPARISON WITH THE EXACT RESULTS ON PURE ISING MODEL

To test the site-propagation algorithm, we apply it to the uniform ferromagnetic Ising model with $\tilde{J}_{ij}=1$ on a square lattice with open boundary. We show some typical correlation functions on 1024×1024 square lattice in Fig. 3(a). From these correlation functions we obtain spontaneous magnetization as shown in Fig. 3(b), the critical correlation functions in Fig. 3(c), and correlation length for $T>T_c$ in Fig. 3(d).

In Fig. 3(a), from bottom to top the five groups of curves are at temperatures $\beta=0.4401$, 0.4405, 0.04408, 0.4425, 0.4455, respectively. The thick solid curves are correlation along the horizontal (or vertical) direction in the middle of the lattice, where the positions of concerned spins are given by $\mathbf{r}=(512-l,512)$, $\mathbf{r}'=(512+l,512)$ and $|\mathbf{r}-\mathbf{r}'|=2l$, where $l=1,2,\ldots$. The thin dotted curves are correlation along diagonal direction, where the positions of concerned spins are given by $\mathbf{r}=(513-l,512+l)$, $\mathbf{r}'=(512+l,513-l)$, and $|\mathbf{r}-\mathbf{r}'|=2\sqrt{2}l$. They coincide well for distances much less than the lattice size. If the system is infinite, the increases of slopes of the curves should become less as the distances become large. However, as one see in Fig. 3(a), the slopes of curves become larger as the distances approach the lattice size. This is caused by the open boundary. For the correlation function along diagonal direction there is larger range of distance immune from the boundary effect than those along horizontal direction. Therefore the results of spontaneous magnetization, critical correlation and correlation length in Fig. 3(a), 3(b), and 3(d), are obtained from the correlation functions along diagonal direction.

As one can see in Fig. 3(a), there are plateaus for $\beta=0.4425$, 0.4455. From these plateaus we can draw spontaneous magnetization. As we know $\lim_{|\mathbf{r}-\mathbf{r}'|\to\infty}\langle\sigma_{\mathbf{r}}\sigma_{\mathbf{r}'}\rangle=m^2$, where m is the spontaneous magnetization. See the curves for $\beta=0.4425$, 0.4455, after the correlation decays to a plateau, it decays further as the two concerned spins approach the edges because of boundary effect. We choose the correlation as m^2 at the point where the slope is minimum. Then we get the results in Fig. 3(b), which agree well with Yang's exact solution[5] in certain ranges of temperature.

At the critical point $\beta=\beta_c$, the exact correlation function has been calculated in Ref. 8 and it behaves like $\langle\sigma_{\mathbf{r}}\sigma_{\mathbf{r}'}\rangle=0.70338/|\mathbf{r}-\mathbf{r}'|^{1/4}$, which is shown in Fig. 3(c) with the black solid line. Due to the boundary effect, the numerical results deviate the exact result as the distance approaches the lattice size. Since the lattices are finite, the effective critical temperatures are different for different size lattices and different from that for infinite system $\beta_c^{\infty}=0.440\,686\,8$. For 256×256 lattice, we compare the correlation functions for $\beta=0.440625$, 0.441 25, 0.441 875 and find the correlation function for $\beta=0.441\,25$ fit the exact result best. For 512×512 lattice we choose the result for $\beta=0.441$ from the results for $\beta=0.440$, 0.441, 0.442. For 1024×1024 lattice we choose the result for $\beta=0.4408$ from the results for $\beta=0.4407$, 0.4408, 0.4409.

For $\beta<\beta_c$ (or $T>T_c$) the exact correlation function is $\sim e^{|\mathbf{r}-\mathbf{r}'|/\xi}/r^{1/2}$ for $|\mathbf{r}-\mathbf{r}'|/\xi\gg1$, where $\xi\approx|4(\beta-\beta_c)|^{-1}$,[6,7] which is drawn in black solid line in Fig. 3(d). We fit the numerical results then get the correlation length shown in Fig. 3(d). If the critical temperature shift due to the finite size effect is taken into account, the coincidence with the exact results will be better.

IV. CORRELATION FUNCTIONS OF RBIM

Now we present some typical correlation functions for RBIM. Using SP algorithm, one can get the correlation function directly, including the sign. As an example, we show the results on 256×256 square lattice with nearest-neighbor $\pm J$ in Fig. 4. The nearest-neighbor interactions J_{ij} are taken as random variables with a distribution $P_J(J_{ij})$. We consider the simple distribution $P_J(J_{ij})=p\delta(J_{ij}+J)+(1-p)\delta(J_{ij}-J)$, corresponding to a fraction p of antiferromagnetic bonds.

In Fig. 4(a), we calculate the correlation function for a sample (with a particular realization of bonds) with $p=0.05$ and $\mathbf{r}=(128,129)$, $\mathbf{r}'=(128+m,129)$, $m=1,2,3,\cdots,128$ at

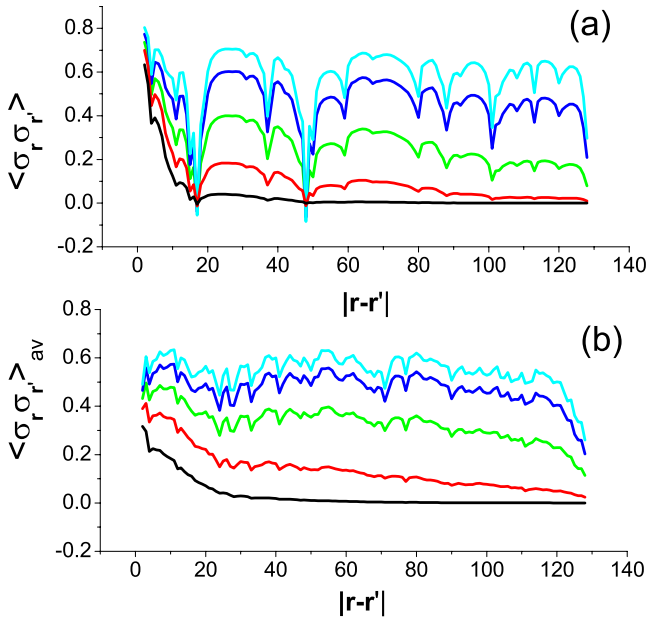

FIG. 4. (Color online) (a)The correlation function for nearest-neighbor $\pm J$ RBIM on a 256×256 square lattice with open boundary. (b) The averaged correlation function over 11 samples. For both (a) and (b), from bottom to top, the temperatures are $\beta=0.51$, 0.53, 0.54, 0.55, 0.56, respectively

five temperatures $\beta=0.51$, 0.53, 0.54, 0.55, 0.56. The maximum of specific heat of this sample is at $\beta=0.536\pm0.005$, which can be regarded the critical temperature. Note that at $\mathbf{r}'=128+17$ and $128+48$ the correlation is negative. The reason is simple. It is found that the bond between sites $(128+16,129)$ and $(128+17,129)$ is antiferromagnetic. So is the negative correlation at $\mathbf{r}'=128+48$. The other drastic drops in correlation functions are due to the antiferromagnetic bonds near the corresponding spin.

We also show averaged correlation functions over 11 samples (with 11 different realizations of bonds) in Fig. 4(b). The parameters for the 11 samples are the same as the sample in Fig. 4(a). The correlation for each sample is calculated with $p=0.05$ and $\mathbf{r}=(128,129)$, $\mathbf{r}'=(128+m,129)$, $m=1,2,3,\ldots,128$ at five temperatures $\beta=0.51$, 0.53, 0.54, 0.55, 0.56. Obviously the averaged correlation function becomes less oscillatory. However the drastic drops become dense although the amplitudes of drop become small. This is because the antiferromagnetic bonds distribute randomly. For different samples, the drops in correlation locate at different sites. Obviously the more the samples are averaged over, the more drops are present, and the smaller the amplitudes of drop become.

There exist some numerical methods to study RBIM. One of an efficient method to study RBIM is the fermion network method fermion-network method of Merz and Chalker.[20] However with this method, odd powers of correlation functions, including the first power, appear to be much harder to evaluate, leaving the sign of the correlation function undetermined. Correlation functions can also be studied with Monte Carlo simulations[23,24] or transfer-matrix calculations in a spin basis.[21,25] However, for Monte Carlo simulations there are the statistical sampling errors. If implemented using the transfer matrix, transfer-matrix dimension grows exponentially with system width that occurs if this matrix is written in a spin basis. For example, the system with width 64 is very large for the transfer-matrix method.[21]

Using SP algorithm, one can get the correlation functions, which can provide more information than its even powers. In addition the lattice size can be as large as $\sim10^3\times10^3$. Therefore this algorithm provide another efficient way to study RBIM.

V. CONCLUSION

In conclusion we have developed a highly efficient algorithm to calculate the correlation functions for the two-dimensional Ising model with arbitrary bond strengths on planar graphs. With this method, only $O(L^2)$ memory is required to store the bond strengths, and $O(L^3)$ time is taken.

We have shown how to calculate the spontaneous magnetization and correlation length with SP algorithm. The susceptibility can also be calculated according to $\beta^{-1}\chi=\Sigma_{\mathbf{r}'}[\langle\sigma_{\mathbf{r}}\sigma_{\mathbf{r}'}\rangle-\langle\sigma\rangle^2]$. Such a calculation will cost huge amount of time if it is carried on a common workstation for large size lattices, say 1024×1024. However it should not be too difficult through large scale parallel computing. In addition, although only two point correlation function is discussed in this paper, the algorithm for many points correlation functions can be developed similarly.

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