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Exact partition functions of the Ising model on $M \times N$ planar lattices with periodic–aperiodic boundary conditions

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Abstract
The Grassmann path integral approach is used to calculate exact partition functions of the Ising model on $M \times N$ square (sq), plane triangular (pt) and honeycomb (hc) lattices with periodic–periodic (pp), periodic–antiperiodic (pa), antiperiodic–periodic (ap) and antiperiodic–antiperiodic (aa) boundary conditions. The partition functions are used to calculate and plot the specific heat, C/k_B, as a function of temperature, $\theta = k_BT/J$. We find that for the $N \times N$ sq lattice, C/k_B for pa and ap boundary conditions are different from those for aa boundary conditions, but for the $N \times N$ pt and hc lattices, C/k_B for ap, pa and aa boundary conditions have the same values. Our exact partition functions might also be useful for understanding the effects of lattice structures and boundary conditions on critical finite-size corrections of the Ising model.

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1. Introduction

Universality and scaling are two important concepts in the theory of critical phenomena [1, 2] and the Ising model [3] has been widely used in such studies. Recently, exact universal amplitude ratios and finite-size corrections to scaling in a critical Ising model on planar lattices have received much attention [4–12]. This may be due to the fact that the hypothesis of universality naturally leads to the consideration of universal critical amplitudes and amplitude combinations [13], and for the comparison between experiment and theory in relation to scaling and universality, it is often a more rigorous test to use amplitude relations rather than critical exponent values. Moreover, it is also well known that the finite-size scaling functions depend on the boundary conditions [14], and there has been considerable recent interest in studying the lattice model with various boundary conditions [15–21]. The study of exact universal amplitude ratios and finite-size corrections to scaling in the critical Ising model is

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usually based on the analytical solutions of the model on finite lattices. Although the exact solution of the Ising model on the $M \times N$ square (sq) lattice was obtained a long time ago [22], and the exact expression of the partition function of the Ising model on the $M \times N$ plane triangular (pt) lattice was obtained by lattice field theories recently [23], there are still no published results for the exact solutions of the Ising model on $M \times N$ pt and honeycomb (hc) lattices with periodic–aperiodic boundary conditions. The purpose of this paper is to fill this gap. In the present paper we use the Grassmann path integral to calculate the exact partition functions of the Ising model on $M \times N$ sq, pt and hc lattices with periodic–periodic (pp), periodic–antiperiodic (pa), antiperiodic–periodic (ap) and antiperiodic–antiperiodic (aa) boundary conditions. The partition functions are used to calculate and plot the specific heat, C/k_B, as a function of temperature, $\theta = k_B T/J$. We find that for the $N \times N$ sq lattice, C/k_B for pa and ap boundary conditions are different from those for aa boundary conditions, but for the $N \times N$ pt and hc lattices, C/k_B for ap, pa and aa boundary conditions have the same values. Our exact partition functions might also be useful for understanding the effects of lattice structures and boundary conditions on critical finite-size corrections of the Ising model.

The two-dimensional Ising model on the sq lattice at vanishing magnetic field was first solved by Onsager by the use of Lie algebra [3]. The exact solution he obtained was an Ising model on an infinite lattice. The original method was rather complicated, and it was later improved by Kaufman [22] who obtained the exact solution of the Ising model on a finite torus by using the theory of spinor representation. The successful treatments of the two-dimensional Ising model brought the studies of phase transition into the modern era. Onsager's solution, on the one hand, showed that the previous classical theories were unreliable in their quantitative predictions, and on the other, provided a great stimulus to explore the true behaviour near the critical point. After Onsager's original solution, many quite different mathematical approaches were developed, but the approaches were still complicated. Among them, Schultz *et al* gave explicitly the fermionic treatment in the framework of transfer-matrix formalism [24], and Kac and Ward developed the combinatorial method [25, 26]. Both methods reformulated the two-dimensional Ising model as a free-fermionic field theory in terms of anticommuting Grassmann variables, which enclosed the fact that the Ising model on two-dimensional regular lattices may be viewed as free-fermionic theory. The other alternative method in the literature was the Pfaffian representation, which was introduced by Kasteleyn [27] to translate Ising spins into dimers that can be reduced to some Pfaffian [28]. Stephenson has used the Pfaffian representation to solve the Ising model on the pt lattice, but the solution was restricted to the $6L \times 6L$ lattice due to its 6×6 basic nonvanishing matrix elements and was exact only in the limit of $L \to \infty$ [29]. Recently, by using the connections between Pfaffian, dimer and Ising models, Nash and O'Connor have obtained the exact expression of the partition function of the pt lattice Ising model on a finite torus [23]. They first employed the lattice field theories to obtain the exact partition function of the Gaussian model, and then established the exact expression of the partition function of the pt lattice Ising model from the analysis of the appropriate lattice determinants and the parametrization according to the results in [29].

On the other hand, in view of the simplification of the approach, remarkable progress was achieved by Plechko who modified the traditional fermionic interpretation and introduced a nonstandard approach [30]. By the use of this approach, Plechko himself not only rederived Onsager's and Kaufman's results in a relatively simple way [30], but also obtained the partition functions of a class of triangular-type decorated lattices [31], and a triangular lattice net with holes [32]. Quite recently, by using the same approach, Wu *et al* [4] have obtained the $M \times N$ sq lattice Ising model with the periodic–aperiodic boundary condition, and Liaw *et al* [33] have successfully solved the triangular and hexagonal lattices on a cylinder geometry

($M \times \infty$) with periodic and antiperiodic boundary conditions. This approach is based on the integration over the anticommuting Grassmann variables and the mirror-ordered factorization principle in two-dimensional density matrix [30–33], and does not involve the traditional transfer-matrix or combinatorial considerations. The whole scheme of the method can be illustrated schematically as shown below [30]:

$$Z = \underset{(\sigma)}{\mathrm{Sp}}\{Z(\sigma)\} \rightarrow \underset{(\sigma|\chi)}{\mathrm{Sp}}\{Z(\sigma|\chi)\} \rightarrow \underset{(\chi)}{\mathrm{Sp}}\{Z(\chi)\} = Z$$

where 'Sp' stands for the average over spin variables (σ) or Grassmann variables (χ). The original partition function Z is expressed purely by spin variables (σ) at each lattice site. With a set of anticommuting Grassmann variables (χ) being introduced to factorize the local bond Boltzmann weight such that spin variables are decoupled, the partition function passes to a mixed $Z(\sigma|\chi)$ representation. Then, by eliminating the spin variables in the mixed $Z(\sigma|\chi)$ representation, the fermionic interpretation $Z(\chi)$ of the two-dimensional Ising model can be obtained, and after carrying out the Grassmann integral, the analytical solution for the partition function and free energy can be achieved [30–33].

In the present paper, we work in this framework to obtain exact partition functions of $M \times N$ pt and hc lattices with different boundary conditions, including pp, pa, ap and aa boundary conditions. We used these results to calculate and plot specific heat, C/k_B, as a function of temperature, $\theta = k_B T/J$. Our results show that for the sq lattice, C/k_B for pa and ap boundary conditions are different from those for aa boundary conditions, but for the pt and hc lattices, C/k_B for ap, pa and aa boundary conditions have the same values. Besides these analyses, our exact partition functions may also be used for understanding the effects of lattice structures and boundary conditions on critical properties and critical finite-size corrections of the Ising model.

This paper is organized as follows. In section 2, we set up a general form of the partition function for pt and hc lattices. Then, three pairs of conjugate Grassmann variables are introduced for a lattice site to factorize the Boltzmann weights, and the principle of mirror ordering is used to rearrange the Grassmann factors so we can perform the summation over Ising spins to obtain a pure fermionic expression of the partition function. In section 3, using the Fourier transform technique we complete the integrations over the Grassmann variables to obtain the exact solution of the partition function. Then, the solution is subjected to periodic–aperiodic boundary conditions, including pp, pa, ap and aa boundary conditions. We further consider the shift behaviour of the maximum of the specific heats of these systems in section 4. Finally, we discuss some problems for further studies in section 5.

2. The partition function

Consider Ising ferromagnets on $M \times N$ pt and hc lattices as shown in figure 1, in which the former is considered as a sq lattice with a single second-neighbour interaction, and the latter contains an inner spin in each lattice cell. The corresponding Hamiltonians, respectively, read

$$H_t = -\sum_{m=1}^{M}\sum_{n=1}^{N}(J_1\sigma_{mn}\sigma_{m+1n} + J_2\sigma_{mn}\sigma_{mn+1} + J_3\sigma_{m+1n}\sigma_{mn+1}) \tag{1}$$

and

$$H_h = -\sum_{m=1}^{M}\sum_{n=1}^{N}(J_1\sigma_0\sigma_{mn} + J_2\sigma_0\sigma_{mn+1} + J_3\sigma_0\sigma_{m+1n}) \tag{2}$$

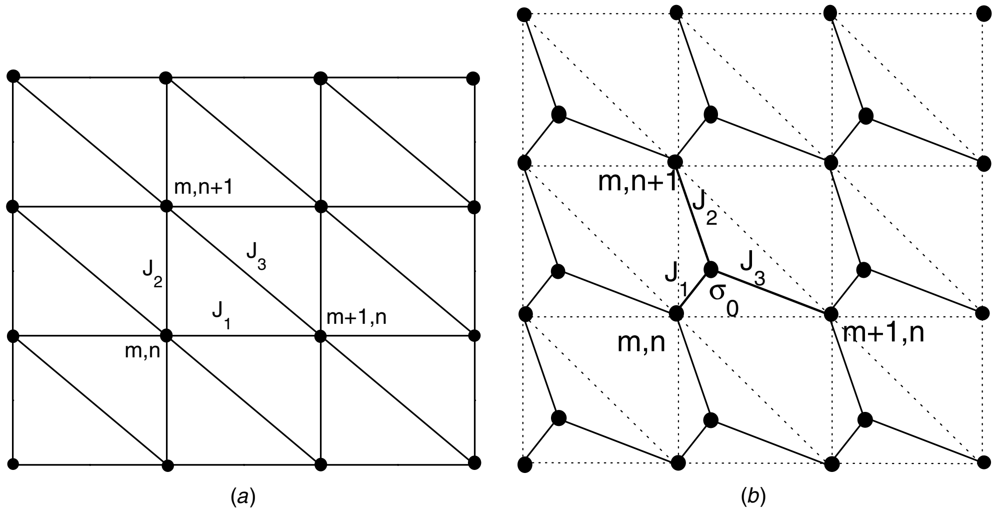

Figure 1. (*a*) The global structure of the triangular lattice used in this paper. A basic cell of the lattice site is given by (m, n), and the coupling constants are J_1, J_2 and J_3. (*b*) The global structure of the honeycomb lattice used in this paper. Each basic cell contains an inner Ising spin σ_0.

where J_i with $i = 1, 2, 3$ are the coupling constants ($J_i > 0$ for ferromagnetic lattices), $\sigma_{mn} = \pm 1$ is the Ising spin located at the site (m, n), and σ_0 denotes the inner Ising spin in the hc lattice. Using the identity of the Boltzmann weight,

$$\exp(\beta J_i \sigma_\mu \sigma_\nu) = \cosh(\beta J_i)[1 + \tanh(\beta J_i)\sigma_\mu \sigma_\nu] \tag{3}$$

$\beta = (k_B T)^{-1}$, and performing the sum over σ_0, the partition functions of the two lattices can be formulated in a single three-spin-polynomial representation,

$$Z = 2^{N_s} \left[\prod_{i=1}^{n_b} \cosh(\beta J_i) \right]^{N_s} \mathop{\mathrm{Sp}}_{(\sigma)} \left\{ \prod_{m=1}^{M} \prod_{n=1}^{N} (\alpha_0 + \alpha_1 \sigma_{mn}\sigma_{m+1n} + \alpha_2 \sigma_{mn}\sigma_{mn+1} + \alpha_3 \sigma_{m+1n}\sigma_{mn+1}) \right\} \tag{4}$$

where N_s is the number of lattice sites ($N_s = MN$ for sq and pt lattices, $N_s = 2MN$ for the hc lattice) and n_b is the number of bonds per lattice cell ($n_b = 2$ for sq lattice, $n_b = 3$ for pt and hc lattices), the symbol 'Sp' stands for the spin average defined by

$$\mathop{\mathrm{Sp}}_{(\sigma_i)}[\cdots] = \frac{1}{2} \sum_{(\sigma_i = \pm 1)} [\cdots] \qquad \mathop{\mathrm{Sp}}_{(\sigma_i)}[1] = 1 \qquad \mathop{\mathrm{Sp}}_{(\sigma_i)}[\sigma_i] = 0 \tag{5}$$

and α_i are defined as

$$\alpha_0^T = 1 + t_1 t_2 t_3 \qquad \alpha_1^T = t_1 + t_2 t_3 \qquad \alpha_2^T = t_2 + t_3 t_1 \qquad \alpha_3^T = t_3 + t_1 t_2 \tag{6}$$

$t_i = \tanh(\beta J_i)$ with $i = 1, 2, 3$, for the pt lattice, and

$$\alpha_0^H = 1 \qquad \alpha_1^H = t_1 t_3 \qquad \alpha_2^H = t_1 t_2 \qquad \alpha_3^H = t_2 t_3 \tag{7}$$

for the hc lattice.

To factorize the partition, we rewrite the partition function as

$$Z_H = 2^{N_s}\left[\prod_{i=1}^{n_b}\cosh(\beta J_i)\right]^{N_s} \underset{(\sigma)}{\mathrm{Sp}}\left\{\prod_{m=1}^{M}\prod_{n=1}^{N} r_0(1+r_1\sigma_{mn}\sigma_{m+1n})(1+r_2\sigma_{mn}\sigma_{mn+1}) \times (1+r_3\sigma_{m+1n}\sigma_{mn+1})\right\} \tag{8}$$

where r_i with $i = 0, 1, 2, 3$ vary from one lattice to the other, and are related to α_i as

$$\alpha_0 = r_0(1+r_1r_2r_3) \qquad \alpha_1 = r_0(r_1+r_2r_3) \qquad \alpha_2 = r_0(r_2+r_1r_3) \qquad \alpha_3 = r_0(r_3+r_1r_2). \tag{9}$$

For the pt lattice, the relation between r_i and t_i is trivial, i.e. $r_0 = 1$ and $r_i = t_i$, but for the hc lattice, the relation is nontrivial and is determined by equations (7) and (9).

It is more convenient to define the generalized reduced partition function as

$$Q = r_0^{MN}\tilde{Q} \tag{10}$$

with

$$\tilde{Q} = \prod_{m=1}^{M}\prod_{n=1}^{N} \underset{(\sigma_{mn})}{\mathrm{Sp}}\,[(1+r_1\sigma_{mn}\sigma_{m+1n})(1+r_2\sigma_{mn}\sigma_{mn+1})(1+r_3\sigma_{mn+1}\sigma_{m+1n})]. \tag{11}$$

To construct the fermionic representation of the generalized partition function, we associate each lattice site (m, n) with three pairs of conjugate Grassmann variables, $\{a_{mn}, a^*_{mn}; b_{mn}, b^*_{mn}; c_{mn}, c^*_{mn}\} \in \chi$. All of these Grassmann variables are anticommuting, and their squares are zero. Their integrals obey the basic rules [34]

$$\int \mathrm{d}\chi = 0, \qquad \int \mathrm{d}\chi\cdot\chi = 1 \tag{12}$$

$$\int \mathrm{d}\chi\cdot\Omega(\chi+\eta) = \int \mathrm{d}\chi\cdot\Omega(\chi) \tag{13}$$

for an arbitrary vector η with anticommuting components, and there is the relation

$$1 + r_i\sigma_\mu\sigma_\nu = \int \mathrm{d}\chi^*\,\mathrm{d}\chi\,\mathrm{e}^{\chi\chi^*}(1+\chi\sigma_\mu)(1+r_i\chi^*\sigma_\nu). \tag{14}$$

Using these Grassmann variables, we can rewrite the reduced partition function as [30]

$$\tilde{Q} = \prod_{m=1}^{M}\prod_{n=1}^{N} \underset{(\sigma_{mn})}{\mathrm{Sp}}\left[\underset{(a_{mn},b_{mn},c_{mn})}{\mathrm{Sp}}(A_{mn}A^*_{m+1n}B_{mn}B^*_{mn+1}C_{mn+1}C^*_{m+1n})\right] \tag{15}$$

where '$\underset{(\chi_i)}{\mathrm{Sp}}$' stands for the averaging with Gaussian weight

$$\underset{(\chi_i)}{\mathrm{Sp}}[\cdots] = \int \mathrm{d}\chi_i^*\,\mathrm{d}\chi_i\,\mathrm{e}^{\chi_i\chi_i^*}[\cdots] \tag{16}$$

with the rules

$$\underset{(\chi_i)}{\mathrm{Sp}}[\chi_i\chi_i^*] = -\underset{(\chi_i)}{\mathrm{Sp}}[\chi_i^*\chi_i] = 1 \tag{17}$$

$$\underset{(\chi_i)}{\mathrm{Sp}}[\chi_i] = \underset{(\chi_i)}{\mathrm{Sp}}[\chi_i^*] = 0 \tag{18}$$

and the Grassmann factors, A, A^*, B, B^*, C and C^*, are defined as

$$A_{mn} = 1 + a_{mn}\sigma_{mn} \qquad A^*_{mn} = 1 + r_1 a^*_{m-1n}\sigma_{mn} \tag{19}$$

$$B_{mn} = 1 + b_{mn}\sigma_{mn} \qquad B^*_{mn} = 1 + r_2 b^*_{mn-1}\sigma_{mn} \tag{20}$$

$$C_{mn} = 1 + c_{mn-1}\sigma_{mn} \qquad C^*_{mn} = 1 + r_3 c^*_{m-1n}\sigma_{mn}. \tag{21}$$

In this way, a Boltzmann weight is decoupled to the product of two factors of separated spins.

For simplicity, we express the reduced partition function as

$$\tilde{Q} = \underset{(a,b,c)}{\mathrm{Sp}} \left\{ \prod_{m=1}^{M} \prod_{n=1}^{N} \Psi^A_{mn} \Psi^B_{mn} \Psi^C_{mn} \right\} \tag{22}$$

where Ψ^A_{mn}, Ψ^B_{mn} and Ψ^C_{mn} are defined by

$$\Psi^A_{mn} = \underset{(\sigma_{mn})}{\mathrm{Sp}} \left(A_{mn} A^*_{m+1n} \right) \tag{23}$$

$$\Psi^B_{mn} = \underset{(\sigma_{mn})}{\mathrm{Sp}} \left(B_{mn} B^*_{mn+1} \right) \tag{24}$$

$$\Psi^C_{mn} = \underset{(\sigma_{mn})}{\mathrm{Sp}} \left(C_{mn+1} C^*_{m+1n} \right). \tag{25}$$

We first treat the boundary weight and consider periodic boundary condition in both directions:

$$\begin{aligned} \Psi^A_{Mn} &= \underset{(\sigma_{Mn})}{\mathrm{Sp}} \left[(1 + a_{Mn}\sigma_{Mn})(1 + r_1 a^*_{Mn}\sigma_{M+1n}) \right] \\ &= \underset{(\sigma_{Mn})}{\mathrm{Sp}} \left[(1 + r_1 a^*_{0n}\sigma_{1n})(1 + a_{Mn}\sigma_{Mn}) \right] \\ &= \underset{(\sigma_{Mn})}{\mathrm{Sp}} \left(A^*_{1n} A_{Mn} \right) \end{aligned} \tag{26}$$

which implies

$$a^*_{0n} = -a^*_{Mn}. \tag{27}$$

Similarly, from

$$\Psi^B_{mN} = \underset{(\sigma_{mN})}{\mathrm{Sp}} \left(B_{mN} B^*_{mN+1} \right) = \underset{(\sigma_{Nn})}{\mathrm{Sp}} \left(B^*_{m1} B_{mN} \right) \tag{28}$$

$$\Psi^C_{Mn} = \underset{(\sigma_{Mn})}{\mathrm{Sp}} \left(C_{Mn+1} C^*_{M+1n} \right) = \underset{(\sigma_{Mn})}{\mathrm{Sp}} \left(C^*_{1n} C_{Mn+1} \right) \tag{29}$$

$$\Psi^C_{mN} = \underset{(\sigma_{mN})}{\mathrm{Sp}} \left(C_{mN+1} C^*_{m+1N} \right) = \underset{(\sigma_{mN})}{\mathrm{Sp}} \left(C_{m1} C^*_{m+1N} \right) \tag{30}$$

we have

$$b^*_{m0} = -b^*_{mN} \tag{31}$$

$$c^*_{0n} = -c^*_{Mn} \tag{32}$$

$$c_{m0} = c_{mN}. \tag{33}$$

Since $c_{m0} = c_{mN}$, Ψ^C_{mN} need not be treated as a boundary weight, and only Ψ^A_{Mn}, Ψ^B_{mN} and Ψ^C_{Mn} should be considered. However, this situation becomes ambiguous when we take a Fourier transform of these Grassmann variables with a single set of exponential factors in equations (56) and (57). Because the Fourier exponential factors are associated with directions in M and N, the sign factor in front of b^*_{mN} takes effect simultaneously on b^*_{mN} and c_{mN}. Therefore, the real situation is that instead of the relation in equation (33), we must take

$$c_{m0} = -c_{mN}. \tag{34}$$

A self-consistent way to assign a minus sign to c_{m0} and obtain the relation in equation (34) is interchanging C_{m1} in equation (30) with another Grassmann factor. An equivalent but more convenient approach is to consider the rearrangement of B^*_{m1} in the boundary weight together with the rearrangement of C_{m1} in the reduced partition function. To see this, we express the reduced partition function as

$$\tilde{Q} = \underset{(a,b,c)}{\mathrm{Sp}} \left\{ \underset{(\sigma)}{\mathrm{Sp}} \left[\left(\prod_{m=1}^{M-1} \prod_{n=1}^{N} \Psi^A_{mn} \Psi^C_{mn} \right) \Psi_B \left(\prod_{m=1}^{M} \prod_{n=1}^{N-1} B_{mn} B^*_{mn+1} \right) \right] \right\} \tag{35}$$

with the boundary weight Ψ_B

$$\begin{aligned} \Psi_B &= \underset{(a,b,c)}{\mathrm{Sp}} \left[\left(\prod_{n=1}^{N} \Psi^A_{Mn} \right) \left(\prod_{m=1}^{M} \Psi^B_{mN} \right) \left(\prod_{n=1}^{N} \Psi^C_{Mn} \right) \right] \\ &= \underset{(a,b,c)}{\mathrm{Sp}} \left[\left(\prod_{m=1}^{M} \overrightarrow{B^*_{m1}}^{\,m} \right) \left(\prod_{n=1}^{N} \overleftarrow{C^*_{1n} A^*_{1n}}^{\,n} \right) A_{M1} \left(\prod_{n=2}^{N} \overrightarrow{C_{Mn} A_{Mn}}^{\,n} \right) C_{M1} \prod_{m=1}^{M} \overleftarrow{B_{mN}}^{\,m} \right] \end{aligned} \tag{36}$$

and

$$\begin{aligned} \prod_{m=1}^{M-1} \prod_{n=1}^{N} \Psi^A_{mn} \Psi^C_{mn} &= \prod_{m=1}^{M-1} \prod_{n=1}^{N} A_{mn} C_{mn+1} C^*_{m+1n} A^*_{m+1n} \\ &= \prod_{m=1}^{M-1} A_{m1} \left(\prod_{n=2}^{N} \overleftarrow{C_{mn} A_{mn}}^{\,n} \right) C_{m1} \left(\prod_{n=1}^{N} \overrightarrow{C^*_{m+1n} A^*_{m+1n}}^{\,n} \right). \end{aligned} \tag{37}$$

Here, arrows have been used to indicate the orders of the products in m and n. When we move B^*_{m1} from the left of $\prod_{n=1}^{N} \overleftarrow{C^*_{1n} A^*_{1n}}^{\,n}$ to the right of $\prod_{n=1}^{N} \overleftarrow{C^*_{1n} A^*_{1n}}^{\,n}$ in equation (36), B^*_{m1} passes $2N$ Grassmann factors, but for moving C_{m1} from the right of $\prod_{n=2}^{N} \overleftarrow{C_{mn} A_{mn}}^{\,n}$ to the left of A_{m1} in equations (36) and (37), C_{m1} passes only $2N - 1$ Grassmann factors. Then by moving B^*_{m1} from left to right, and simultaneously moving C_{m1} from right to left, we can assign to the Grassmann variable in C_{m1} an additional minus sign compared with the Grassmann variable in B^*_{m1}, and hence obtain the relation of equation (34).

Accordingly, we interchange B^* and C^*A^* in equation (36) to obtain the arrangement of $C^*A^*B^*$ according to the identity [30]

$$B^+(CA)^+ = \tfrac{1}{2}[(CA)^+B^+ + (CA)^+B^- + (CA)^-B^+ - (CA)^-B^-] \tag{38}$$

with superscripts + and − being the sign factors in boundary Grassmann factors A^*_{1n}, B^*_{m1} and C^*_{1n}, and simultaneously move C_{m1} from the right of $\prod_{n=2}^{N} \overleftarrow{C_{mn} A_{mn}}^{\,n}$ to the left of A_{m1} in equations (36) and (37). Here we note that the superscripts + and − respectively correspond to periodic and antiperiodic boundary conditions imposed on the spin variables and in turn on the Grassmann variables. Hence, the reduced partition function becomes

$$\tilde{Q} = \tfrac{1}{2} \left(\tilde{Q}_\gamma\big|_{\Gamma_1} + \tilde{Q}_\gamma\big|_{\Gamma_2} + \tilde{Q}_\gamma\big|_{\Gamma_3} - \tilde{Q}_\gamma\big|_{\Gamma_4} \right) \tag{39}$$

with

$$\tilde{Q}_\gamma = \underset{(a,b,c)}{\mathrm{Sp}} \left\{ \underset{(\sigma)}{\mathrm{Sp}} \left[\left(\prod_{m=1}^{M-1} \overrightarrow{\Theta_m \Theta^*_{m+1}}^{\,m} \right) \Psi_\gamma \left(\prod_{m=1}^{M} \prod_{n=1}^{N-1} B_{mn} B^*_{mn+1} \right) \right] \right\} \tag{40}$$

and

$$\Psi_\gamma = \underset{(a,b,c)}{\mathrm{Sp}} \left\{ \underset{(\sigma)}{\mathrm{Sp}} \left[\Theta_1^* \left(\prod_{m=1}^{M} \overrightarrow{B_{m1}^*}^{m} \right) \Theta_M \left(\prod_{m=1}^{M} \overleftarrow{B_{mN}}^{m} \right) \right] \right\} \tag{41}$$

where we have defined

$$\Theta_m = \prod_{n=1}^{N} \overrightarrow{C_{mn} A_{mn}}^{n} \quad \text{and} \quad \Theta_m^* = \prod_{n=1}^{N} \overleftarrow{C_{mn}^* A_{mn}^*}^{n} \tag{42}$$

and the boundary conditions $\Gamma_1, \Gamma_2, \Gamma_3, \Gamma_4$ are defined as

$$\Gamma_1 = (a_{0n}^* = -a_{Mn}^*,\ b_{m0}^* = -b_{mN}^*,\ c_{0n}^* = -c_{Mn}^*) \tag{43}$$

$$\Gamma_2 = (a_{0n}^* = -a_{Mn}^*,\ b_{m0}^* = +b_{mN}^*,\ c_{0n}^* = -c_{Mn}^*) \tag{44}$$

$$\Gamma_3 = (a_{0n}^* = +a_{M,n}^*,\ b_{m0}^* = -b_{mN}^*,\ c_{0n}^* = +c_{M,n}^*) \tag{45}$$

$$\Gamma_4 = (a_{0n}^* = +a_{M,n}^*,\ b_{m0}^* = +b_{mN}^*,\ c_{0n}^* = +c_{M,n}^*). \tag{46}$$

In this way, the configurations of the reduced partition function can be further rearranged and expressed as

$$\begin{aligned} \tilde{Q}_\gamma &= \underset{(a,b,c)}{\mathrm{Sp}}\ \underset{(\sigma)}{\mathrm{Sp}} \left\{ \left(\prod_{m=1}^{M-1} \overrightarrow{\Theta_m \Theta_{m+1}^*}^{m} \right) \Theta_1^* \left(\prod_{m=1}^{M} \overrightarrow{B_{m1}^*}^{m} \right) \Theta_M \left(\prod_{m=1}^{M} \overleftarrow{B_{mN}}^{n} \right) \prod_{m=1}^{M} \prod_{n=1}^{N-1} B_{mn} B_{mn+1}^* \right\} \\ &= \underset{(a,b,c)}{\mathrm{Sp}}\ \underset{(\sigma)}{\mathrm{Sp}} \left\{ \left(\prod_{m=1}^{M} \overrightarrow{\Theta_m^* B_{m1}^* \Theta_m}^{m} \right) \left(\prod_{m=1}^{M} \overleftarrow{B_{mN}}^{n} \right) \left(\prod_{m=1}^{M} \prod_{n=1}^{N-1} B_{mn} B_{mn+1}^* \right) \right\}. \end{aligned} \tag{47}$$

To have a complete mirror-ordered form, we have to rearrange the terms in the last two brackets. To achieve this, first we note that

$$\begin{aligned} \tilde{Q}_\gamma &= \underset{(a,b,c)}{\mathrm{Sp}}\ \underset{(\sigma)}{\mathrm{Sp}} \left\{ \prod_{m=1}^{M} \overrightarrow{\Theta_m^* B_{m1}^* \left(\prod_{n=1}^{N-1} \overrightarrow{C_{mn} A_{mn}}^{n} \right) C_{mN} A_{mN}}^{m} \left(\prod_{m=1}^{M} \overleftarrow{B_{mM}}^{m} \right) \prod_{m=1}^{M} \prod_{n=1}^{N-1} B_{mn} B_{mn+1}^* \right\} \\ &= \underset{(a,b,c)}{\mathrm{Sp}}\ \underset{(\sigma)}{\mathrm{Sp}} \left\{ \prod_{m=1}^{M} \overrightarrow{\Theta_m^* \left(\prod_{n=1}^{N-1} \overrightarrow{B_{mn}^* C_{mn} A_{mn} B_{mn}}^{n} \right) B_{mN}^* C_{mN} A_{mN}}^{m} \left(\prod_{m=1}^{M} \overleftarrow{B_{mN}}^{m} \right) \right\}. \end{aligned} \tag{48}$$

The boundary term of $m = M$, denoted by T, can be formulated as

$$\begin{aligned} T &= \Theta_M^* \left(\prod_{n=1}^{N-1} \overrightarrow{B_{Mn}^* C_{Mn} A_{Mn} B_{Mn}}^{n} \right) B_{MN}^* C_{MN} A_{MN} B_{MN} \\ &= \left(\prod_{n=1}^{N} \overleftarrow{C_{Mn}^* A_{Mn}^*}^{n} \right) \left(\prod_{n=1}^{L_y} \overrightarrow{B_{Mn}^* C_{Mn} A_{Mn} B_{Mn}}^{n} \right) \\ &= \prod_{n=1}^{N} C_{Mn}^* A_{Mn}^* B_{Mn}^* C_{Mn} A_{Mn} B_{Mn} \end{aligned} \tag{49}$$

due to the fact that $\mathop{\mathrm{Sp}}\limits_{(\sigma_{mn})}[C^*_{Mn}A^*_{Mn}B^*_{Mn}C_{Mn}A_{Mn}B_{Mn}]$ for a given n is a commutable object. By continuing such construction from $m = M$ down to $m = 1$, we can obtain the expression

$$\tilde{Q}_\gamma = \mathop{\mathrm{Sp}}\limits_{(a,b,c)} \left\{ \prod_{m=1}^{M} \prod_{n=1}^{N} \mathop{\mathrm{Sp}}\limits_{(\sigma_{mn})} [C^*_{mn}A^*_{mn}B^*_{mn}C_{mn}A_{mn}B_{mn}] \right\}. \tag{50}$$

For this partition function, the factors containing the same spin are grouped together and we can perform the average over the spins. As a result, we have

$$\tilde{Q}_\gamma = \int \prod_{m=1}^{M} \prod_{n=1}^{N} \mathrm{d}a^*_{mn}\,\mathrm{d}a_{mn}\,\mathrm{d}b^*_{mn}\,\mathrm{d}b_{mn}\,\mathrm{d}c^*_{mn}\,\mathrm{d}c_{mn} \exp\left(\sum_{m=1}^{M} \sum_{n=1}^{N} F_{mn} \right) \tag{51}$$

with

$$\begin{aligned} F_{mn} = {} & a_{mn}a^*_{mn} + b_{mn}b^*_{mn} + c_{mn}c^*_{mn} + r_1r_3c^*_{m-1n}a^*_{m-1n} + (r_3c^*_{m-1n} + r_1a^*_{m-1n})r_2b^*_{mn-1} \\ & + (r_3c^*_{m-1n} + r_1a^*_{m-1n} + r_2b^*_{mn-1})c_{mn-1} + (r_3c^*_{m-1n} + r_1a^*_{m-1n} + r_2b^*_{mn-1} \\ & + c_{mn-1})a_{mn} + (r_3c^*_{m-1n} + r_1a^*_{m-1n} + r_2b^*_{mn-1} + c_{mn-1} + a_{mn})b_{mn}. \end{aligned} \tag{52}$$

Since there is no mix on a_{mn} and b_{mn}, the integral in the above expression can be simplified by integrating the a_{mn} and b_{mn} fields by means of the identity

$$\int \mathrm{d}b\,\mathrm{d}a\, \exp(\lambda ab + aL + L'b) = \lambda \exp(\lambda^{-1}LL') \tag{53}$$

where a, b are Grassmann variables, L, L' are linear fermionic forms independent of a, b and λ is a parameter. The result then becomes

$$\tilde{Q}_\gamma = \int \prod_{m=1}^{M} \prod_{n=1}^{N} \mathrm{d}g^*_{mn}\,\mathrm{d}g_{mn}\,\mathrm{d}c^*_{mn}\,\mathrm{d}c_{mn}\ \exp\left(\sum_{m=1}^{M} \sum_{n=1}^{N} G_{mn} \right) \tag{54}$$

with

$$\begin{aligned} G_{mn} = {} & c_{mn}c^*_{mn} + g_{mn}g^*_{mn} + r_1r_3c^*_{m-1n}g_{m-1n} - (r_3c^*_{m-1n} + r_1g_{m-1n})r_2g^*_{mn-1} \\ & + (r_3c^*_{m-1n} + r_1g_{m-1n} - r_2g^*_{mn-1})c_{mn-1} \\ & - (r_3c^*_{m-1n} + r_1g_{m-1n} - r_2g^*_{mn-1} + c_{mn-1})(g_{mn} + g^*_{mn}) \end{aligned} \tag{55}$$

where we have changed the notation for the fields by $(a^*_{mn}, b^*_{mn}) \to (g_{mn}, -g^*_{mn})$. This is the pure fermionic representation of the reduced partition function.

3. Exact solution

Next, to carry out the integration, we have to use the technique of Fourier transform to treat the Grassmann variables which mix together with the variables at different sites. The Fourier transformation is defined as

$$X_{mn} = \frac{1}{\sqrt{MN}} \sum_{p=0}^{M-1} \sum_{q=0}^{N-1} X_{pq}\, \mathrm{e}^{-\mathrm{i}\frac{2\pi}{M}mp}\, \mathrm{e}^{-\mathrm{i}\frac{2\pi}{N}nq} \tag{56}$$

and

$$X^*_{mn} = \frac{1}{\sqrt{MN}} \sum_{p=0}^{M-1} \sum_{q=0}^{N-1} X^*_{pq}\, \mathrm{e}^{\mathrm{i}\frac{2\pi}{M}mp}\, \mathrm{e}^{\mathrm{i}\frac{2\pi}{N}nq} \tag{57}$$

where the variables X_{mn} and X^*_{mn} denote one of the variables $\{c_{mn}, g_{mn}\}$ and $\{c^*_{mn}, g^*_{mn}\}$ respectively.

After performing the Fourier transformation, the partition function becomes

$$\tilde{Q}_\gamma = \prod_{p=0}^{M-1}\prod_{q=0}^{N-1}\int \mathrm{d}V_{pq}\exp(H_{pq}) \tag{58}$$

with the measure $\mathrm{d}V_{pq}$ defined as

$$\mathrm{d}V_{pq} = \mathrm{d}g^*_{pq}\,\mathrm{d}g_{pq}\,\mathrm{d}c^*_{pq}\,\mathrm{d}c_{pq} \tag{59}$$

and the function H_{pq} is given by

$$\begin{aligned}
H_{pq} = {} & \left(1 - r_3\,\mathrm{e}^{-\mathrm{i}\frac{2\pi}{M}p}\,\mathrm{e}^{\mathrm{i}\frac{2\pi}{N}q}\right)c_{pq}c^*_{pq} + \left(r_2 - \mathrm{e}^{\mathrm{i}\frac{2\pi}{N}q}\right)c_{pq}g^*_{pq} + r_3\left(r_1 - \mathrm{e}^{-\mathrm{i}\frac{2\pi}{M}p}\right)c^*_{pq}g_{pq}\\
& - \mathrm{e}^{\mathrm{i}\frac{2\pi}{N}q}\left(1 + r_1\,\mathrm{e}^{-\mathrm{i}\frac{2\pi}{M}p}\right)c_{pq}g_{M-pN-q} - r_3\,\mathrm{e}^{-\mathrm{i}\frac{2\pi}{M}p}\left(1 + r_2\,\mathrm{e}^{\mathrm{i}\frac{2\pi}{N}q}\right)c^*_{pq}g^*_{M-pN-q}\\
& + \left(1 - r_1\,\mathrm{e}^{\mathrm{i}\frac{2\pi}{M}p} - r_2\,\mathrm{e}^{-\mathrm{i}\frac{2\pi}{N}q} - r_1r_2\,\mathrm{e}^{\mathrm{i}\frac{2\pi}{M}p}\,\mathrm{e}^{-\mathrm{i}\frac{2\pi}{N}q}\right)g_{pq}g^*_{pq}\\
& - r_1\,\mathrm{e}^{\mathrm{i}\frac{2\pi}{M}p}g_{pq}g_{M-pN-q} + r_2\,\mathrm{e}^{-\mathrm{i}\frac{2\pi}{L_y}q}g^*_{pq}g^*_{M-pN-q}.
\end{aligned} \tag{60}$$

Because H_{pq} contains not only the variables, X_{pq} and X^*_{pq}, but also the variables, X_{M-pN-q} and X^*_{M-pN-q}, instead of calculating $\tilde{Q}_\gamma$ it is easier to calculate $\tilde{Q}^2_\gamma$ given by

$$\tilde{Q}^2_\gamma = \prod_{p=0}^{M-1}\prod_{q=0}^{N-1}\int \mathrm{d}V_{pq}\,\mathrm{d}V_{M-pN-q}\exp(H_{pq} + H^*_{M-pN-q}). \tag{61}$$

Here H^*_{M-pN-q} can be obtained from H_{pq} by replacing p by $M-p$ and q by $N-q$ for the Grassmann variables and replacing the coefficient in front of the Grassmann variables by its complex conjugate. Completing the integration yields

$$Q_\gamma = \prod_{p=0}^{M-1}\prod_{q=0}^{N-1}\left[A_0 - A_1\cos\frac{2\pi p}{M} - A_2\cos\frac{2\pi q}{N} - A_3\cos\left(\frac{2\pi p}{M} - \frac{2\pi q}{N}\right)\right]^{1/2} \tag{62}$$

with

$$A_0 = \alpha_0^2 + \alpha_1^2 + \alpha_2^2 + \alpha_3^2 \tag{63}$$

$$A_1 = 2(\alpha_0\alpha_1 - \alpha_2\alpha_3) \tag{64}$$

$$A_2 = 2(\alpha_0\alpha_2 - \alpha_1\alpha_3) \tag{65}$$

$$A_3 = 2(\alpha_0\alpha_3 - \alpha_1\alpha_2) \tag{66}$$

where α_0, α_1, α_2 and α_3 are given by equations (6) and (7) for pt and hc lattices respectively.

3.1. Periodic–periodic boundary condition

According to equation (39), the reduced partition function for ferromagnetic lattices with pp boundary condition is

$$Q^{\mathrm{pp}} = \frac{1}{2}\left[\Omega_{\frac{1}{2},\frac{1}{2}} + \Omega_{\frac{1}{2},0} + \Omega_{0,\frac{1}{2}} - \mathrm{sgn}\left(\frac{\theta - \theta_c}{\theta_c}\right)\Omega_{00}\right] \tag{67}$$

where the superscript p refers to periodic boundary condition and

$$\begin{aligned}
\Omega_{\mu\nu} = \prod_{p=0}^{M-1}\prod_{q=0}^{N-1}\Bigg[& A_0 - A_1\cos\frac{2\pi(p+\mu)}{M} - A_2\cos\frac{2\pi(q+\nu)}{N}\\
& - A_3\cos\left(\frac{2\pi(p+\mu)}{M} - \frac{2\pi(q+\nu)}{N}\right)\Bigg]^{1/2}.
\end{aligned} \tag{68}$$

The sign factor in front of the last term is a result of the standard consideration of the Grassmann integral over the zero-mode variable $p = q = 0$ for ferromagnetic couplings [30, 35]. When the integral of equation (61) is carried out, it is always positive, but this is not the case for equation (58). There are unpaired terms from zero-mode in equation (58) under various boundary conditions and they contribute a sign factor to Q_4 for $0 \leqslant t_i \leqslant 1$. The partition function for pp boundary condition then becomes

$$Z^{\mathrm{pp}} = \frac{1}{2} 2^{N_s} \left[\prod_{i=1}^{n_b} \cosh(\beta J_i) \right]^{N_s} \left[\Omega_{\frac{1}{2},\frac{1}{2}} + \Omega_{\frac{1}{2},0} + \Omega_{0,\frac{1}{2}} - \operatorname{sgn}\left(\frac{\theta - \theta_c}{\theta_c} \right) \Omega_{00} \right]. \tag{69}$$

Furthermore, the free energy density per $k_B T$ of the system defined by

$$f^{\mathrm{pp}} = -\frac{1}{N_s} \ln Z^{\mathrm{pp}} \tag{70}$$

then takes the form

$$f^{\mathrm{pp}} = -\frac{(N_s - 1)}{N_s} \ln 2 - \sum_{i=1}^{n_b} \ln[\cosh(\beta J_i)] - \frac{1}{N_s} \ln \left[\Omega_{\frac{1}{2},\frac{1}{2}} + \Omega_{\frac{1}{2},0} + \Omega_{0,\frac{1}{2}} \right.$$
$$\left. - \operatorname{sgn}\left(\frac{\theta - \theta_c}{\theta_c} \right) \Omega_{00} \right]. \tag{71}$$

3.2. Periodic–antiperiodic boundary condition

For pa boundary condition, equation (38) is replaced by

$$B^-(CA)^+ = \tfrac{1}{2}[(CA)^+B^+ + (CA)^+B^- - (CA)^-B^+ + (CA)^-B^-] \tag{72}$$

and the partition function has the form

$$Z^{\mathrm{pa}} = \frac{1}{2} 2^{N_s} \left[\prod_{i=1}^{n_b} \cosh(\beta J_i) \right]^{N_s} \left[\Omega_{\frac{1}{2},\frac{1}{2}} + \Omega_{\frac{1}{2},0} - \Omega_{0,\frac{1}{2}} + \operatorname{sgn}\left(\frac{\theta - \theta_c}{\theta_c} \right) \Omega_{00} \right] \tag{73}$$

where the superscript a refers to antiperiodic boundary condition. The corresponding free energy density per $k_B T$ is

$$f^{\mathrm{pa}} = -\frac{(N_s - 1)}{N_s} \ln 2 - \sum_{i=1}^{n_b} \ln[\cosh(\beta J_i)] - \frac{1}{N_s} \ln \left[\Omega_{\frac{1}{2},\frac{1}{2}} + \Omega_{\frac{1}{2},0} - \Omega_{0,\frac{1}{2}} \right.$$
$$\left. + \operatorname{sgn}\left(\frac{\theta - \theta_c}{\theta_c} \right) \Omega_{00} \right]. \tag{74}$$

3.3. Antiperiodic–periodic boundary condition

Similarly, for ap boundary condition, equation (38) is replaced by

$$B^+(CA)^- = \tfrac{1}{2}[(CA)^+B^+ - (CA)^+B^- + (CA)^-B^+ + (CA)^-B^-] \tag{75}$$

and

$$Z^{\mathrm{ap}} = \frac{1}{2} 2^{N_s} \left[\prod_{i=1}^{n_b} \cosh(\beta J_i) \right]^{N_s} \left[\Omega_{\frac{1}{2},\frac{1}{2}} - \Omega_{\frac{1}{2},0} + \Omega_{0,\frac{1}{2}} + \operatorname{sgn}\left(\frac{\theta - \theta_c}{\theta_c} \right) \Omega_{00} \right]. \tag{76}$$

The corresponding free energy density per $k_B T$ is

$$f^{\mathrm{ap}} = -\frac{(N_s - 1)}{N_s} \ln 2 - \sum_{i=1}^{n_b} \ln[\cosh(\beta J_i)] - \frac{1}{N_s} \ln \left[\Omega_{\frac{1}{2},\frac{1}{2}} - \Omega_{\frac{1}{2},0} + \Omega_{0,\frac{1}{2}} \right.$$
$$\left. + \operatorname{sgn}\left(\frac{\theta - \theta_c}{\theta_c} \right) \Omega_{00} \right]. \tag{77}$$

3.4. Antiperiodic–antiperiodic boundary condition

For aa boundary condition, equation (38) becomes

$$B^-(CA)^- = \tfrac{1}{2}[-(CA)^+B^+ + (CA)^+B^- + (CA)^-B^+ + (CA)^-B^-] \tag{78}$$

and the partition function is

$$Z^{\mathrm{aa}} = \frac{1}{2}2^{N_s}\left[\prod_{i=1}^{n_b}\cosh(\beta J_i)\right]^{N_s}\left[-\Omega_{\frac{1}{2},\frac{1}{2}} + \Omega_{\frac{1}{2},0} + \Omega_{0,\frac{1}{2}} + \mathrm{sgn}\left(\frac{\theta-\theta_c}{\theta_c}\right)\Omega_{00}\right]. \tag{79}$$

The corresponding free energy density per k_BT is

$$f^{\mathrm{aa}} = -\frac{(N_s-1)}{N_s}\ln 2 - \sum_{i=1}^{n_b}\ln[\cosh(\beta J_i)] - \frac{1}{N_s}\ln\left[-\Omega_{\frac{1}{2},\frac{1}{2}} + \Omega_{\frac{1}{2},0} + \Omega_{0,\frac{1}{2}} + \mathrm{sgn}\left(\frac{\theta-\theta_c}{\theta_c}\right)\Omega_{00}\right]. \tag{80}$$

Note that by taking $t_3 = 0$, $n_b = 2$ and $N_s = N_b = MN$, we have $A_3 = 0$,

$$\Omega_{\mu\nu} = \prod_{p=0}^{M-1}\prod_{q=0}^{N-1}\left[A_0 - A_1\cos\tfrac{2\pi(p+\mu)}{M} - A_2\cos\tfrac{2\pi(q+\nu)}{N}\right]^{1/2} \tag{81}$$

and all the results we obtained reduce to those of the sq lattice.

Accordingly, the critical temperature can be determined in the thermodynamic limit from the zero of the free energy contributed by the zero mode,

$$A_0 - A_1 - A_2 - A_3 = 0. \tag{82}$$

It follows that for isotropic coupling, we have

$$\theta_c = \left[\tfrac{1}{2}\ln(1+\sqrt{2})\right]^{-1} = 2.269\,185\ldots \tag{83}$$

for the sq lattice with $\theta = k_BT/J$,

$$\theta_c = \left[\tfrac{1}{2}\ln(\sqrt{3})\right]^{-1} = 3.640\,956\ldots \tag{84}$$

for the pt lattice and

$$\theta_c = \left[\tfrac{1}{2}\ln(2+\sqrt{3})\right]^{-1} = 1.518\,651\ldots \tag{85}$$

for the hc lattice.

4. Specific heat

The specific heat per spin C/k_B for the Ising model on $M \times N$ sq, pt and hc lattices with isotropic couplings are shown, respectively, in figures 2(*a*), 3(*a*), 4(*a*) for $M/N = 1$, and in figures 2(*b*), 3(*b*), 4(*b*) for $M/N = 1/2$. Figures 3(*c*) and 4(*c*) show, respectively, the results for pt and hc lattices under pa and aa boundary conditions and for $M/N = 1, 1/2, 1/4$. In general, for three lattices with the same lattice size, the specific heat under pp boundary condition is always larger than those under other boundary conditions. Note that for sq lattices with $M/N = 1$, C^{pa} and C^{aa} are distinct in figure 2(*a*), but for pt and hc lattices with $M/N = 1$ in figures 3(*a*) and 4(*a*), they coincide and are non-distinguishable due to the last term in the bracket of equation (68), which is associated with the structure symmetries of pt and hc lattices.

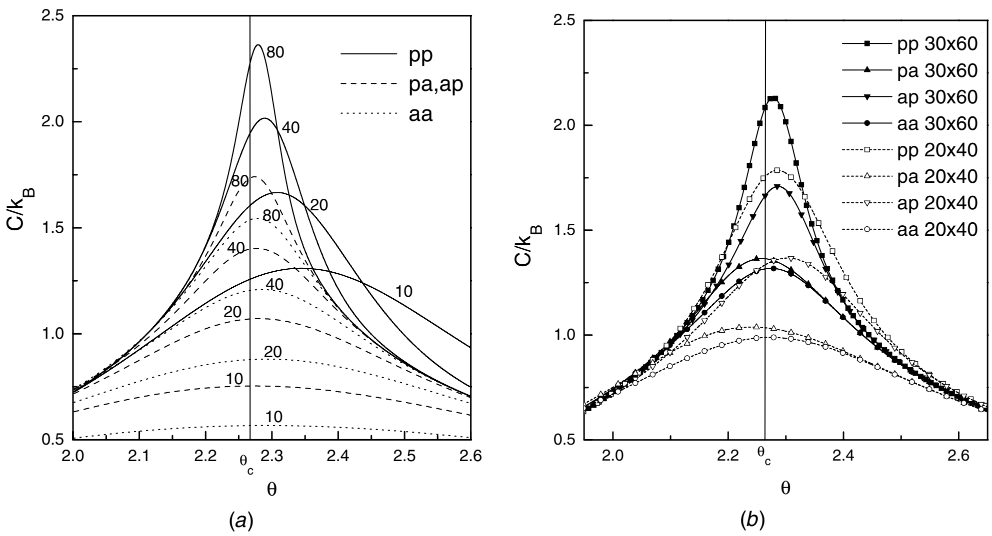

Figure 2. The specific heat per spin for (*a*) $N \times N$ square Ising lattices with isotropic couplings under pp, pa, ap and aa boundary conditions, and (*b*) $M \times N$ square Ising lattices with isotropic couplings and aspect ratio $M/N = 1/2$ under pp, pa, ap and aa boundary conditions. The critical point θ_c is marked by a vertical line.

These behaviours can be violated by taking aspect ratio $\xi = M/N \neq 1$, and the results are shown in figures 3(*b*), (*c*) and 4(*b*), (*c*).

We further study the displacements of the maxima of C^{pp} and C^{pa}. The shift behaviours of the maximum in $C_{NN}(T)$ are shown in figure 5. The slopes of the curves imply the rates of approach of C^{pp} and C^{pa} to their limiting behaviours. For the periodic–periodic boundary condition, these lattices have linear behaviours in $N \to \infty$ and can be described by the formula [36],

$$-\frac{(T_c - T_{\max})}{T_c} \sim \frac{a}{N} \qquad \text{as} \quad N \to \infty. \tag{86}$$

For periodic–antiperiodic boundary condition, the corresponding formula is also provided by the finite-size scaling ansatz. However, for numerical analysis, instead of equation (86), we use

$$-\frac{(T_c - T_{\max})}{T_c} = \frac{a}{N} + \frac{b_1}{N^2} + \frac{b_2}{N^3} + \cdots. \tag{87}$$

As a result, we have $a_s^{\mathrm{pp}} = 0.360$, $b_{1,s}^{\mathrm{pp}} = -0.47$, $a_s^{\mathrm{pa}} = 0.18$, $b_{1,s}^{\mathrm{pa}} = -2.19$, for the sq lattice, $a_t^{\mathrm{pp}} = 0.363$, $b_{1,t}^{\mathrm{pp}} = -0.91$, $a_t^{\mathrm{pa}} = 0.09$, $b_{1,t}^{\mathrm{pa}} = 0.60$ for the pt lattice, $a_h^{\mathrm{pp}} = 0.268$, $b_{1,h}^{\mathrm{pp}} = 0.24$, $a_h^{\mathrm{pa}} = 0.09$, $b_{1,h}^{\mathrm{pa}} = 0.87$ for the hc lattice, and the value of b_2 is of the order of 1. The values of a^{pp} are larger than a^{pa} for three lattices, and this implies that the approach to limiting behaviour for pp boundary condition is faster than the pa boundary condition. Since the logarithmic divergence of the specific heat is independent of the boundary conditions and cannot be used to distinguish C^{pp} and C^{pa} of a large lattice, then the values of a may be used to distinguish the two boundary conditions.

5. Discussion

We have solved the exact partition functions of $M \times N$ pt and hc lattices with different boundary conditions. These results can provide the analytical background for further studies

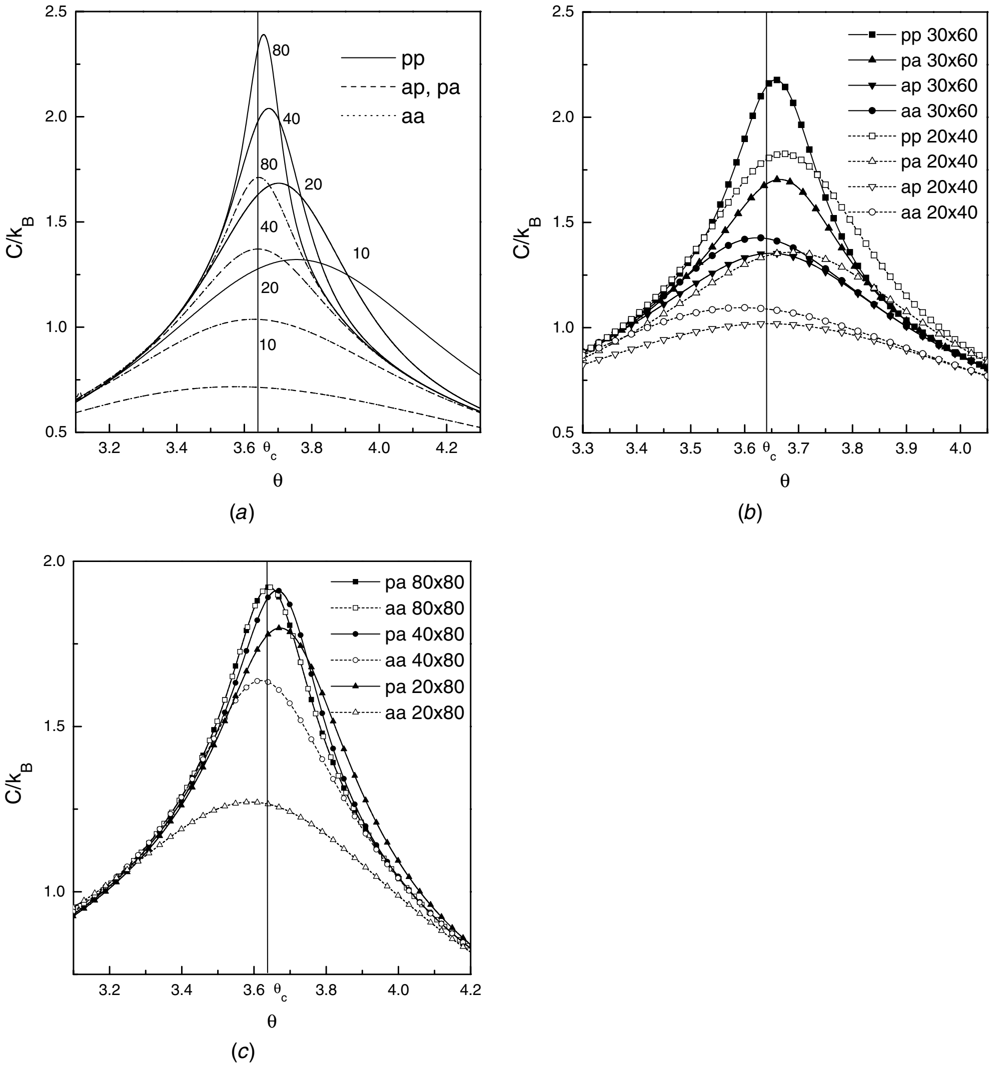

Figure 3. The specific heat per spin for (*a*) $N \times N$ plane triangular Ising lattices with isotropic couplings under pp, pa, ap and aa boundary conditions, (*b*) $M \times N$ plane triangular Ising lattices with isotropic couplings and aspect ratio $M/N = 1/2$ under pp, pa, ap and aa boundary conditions, and (*c*) $M \times N$ plane triangular Ising lattices with isotropic couplings and aspect ratio $M/N = 1, 1/2, 1/4$ under pa and aa boundary conditions. The critical point θ_c is marked by a vertical line.

on the effects of lattice structures and boundary conditions on the critical properties and critical finite-size corrections of the Ising model.

Firstly, universal finite-size scaling functions for critical systems have received much attention in recent years [15–17, 20, 21, 37, 38], and it is well known that the finite-size scaling functions depend on the boundary conditions [14]. Hu *et al* and Okabe and Kikuchi have discussed the difference in the finite-size scaling functions for the lattice models under periodic boundary and free boundary conditions in connection with the universal finite-size scaling function for the percolation problem [15] and the Ising model [17] respectively.

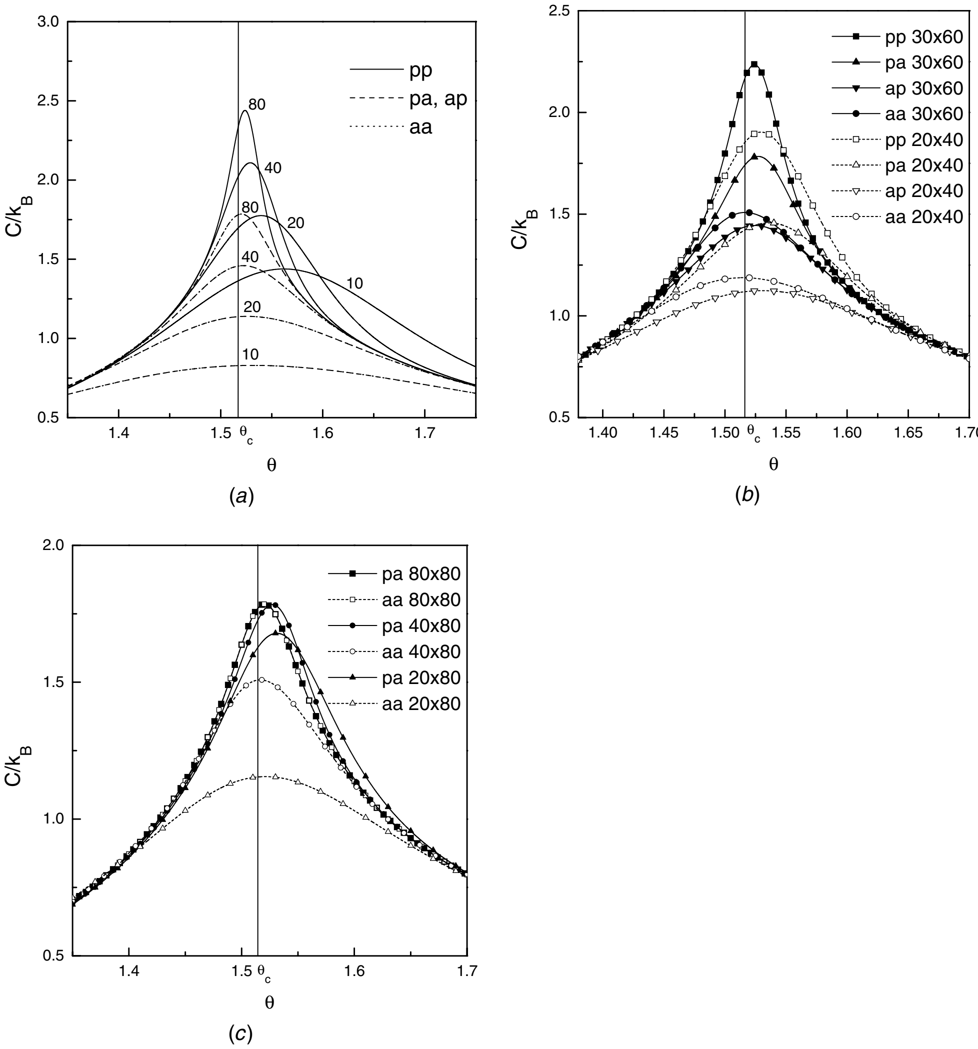

Figure 4. The specific heat per spin for (*a*) $N \times N$ honeycomb Ising lattices with isotropic couplings under pp, pa, ap and aa boundary conditions, (*b*) $M \times N$ honeycomb Ising lattices with isotropic couplings and aspect ratio $M/N = 1/2$ under pp, pa, ap and aa boundary conditions, and (*c*) $M \times N$ honeycomb Ising lattices with isotropic couplings and aspect ratio $M/N = 1, 1/2, 1/4$ under pa and aa boundary conditions. The critical point θ_c is marked by a vertical line.

Other boundary conditions, such as the Ising model on an $M \times N$ simple-quartic lattice embedded on a Möbius strip and Klein bottle have also been studied [18]. Kaneda and Okabe found that there is an interesting aspect ratio dependence of the value of the Binder parameter at criticality for various boundary conditions [19]. It is then interesting to have a rigorous test of finite-size scaling function and critical finite-size corrections for different planar Ising models under various boundaries.

In addition, by using the Monte Carlo method, Hu *et al* [15, 16], and Tomita *et al* [21] have found that the universal finite-size scaling functions of the scaled quantities for sq, pt and hc lattices depend on the aspect ratios and have very good universal finite-size scaling

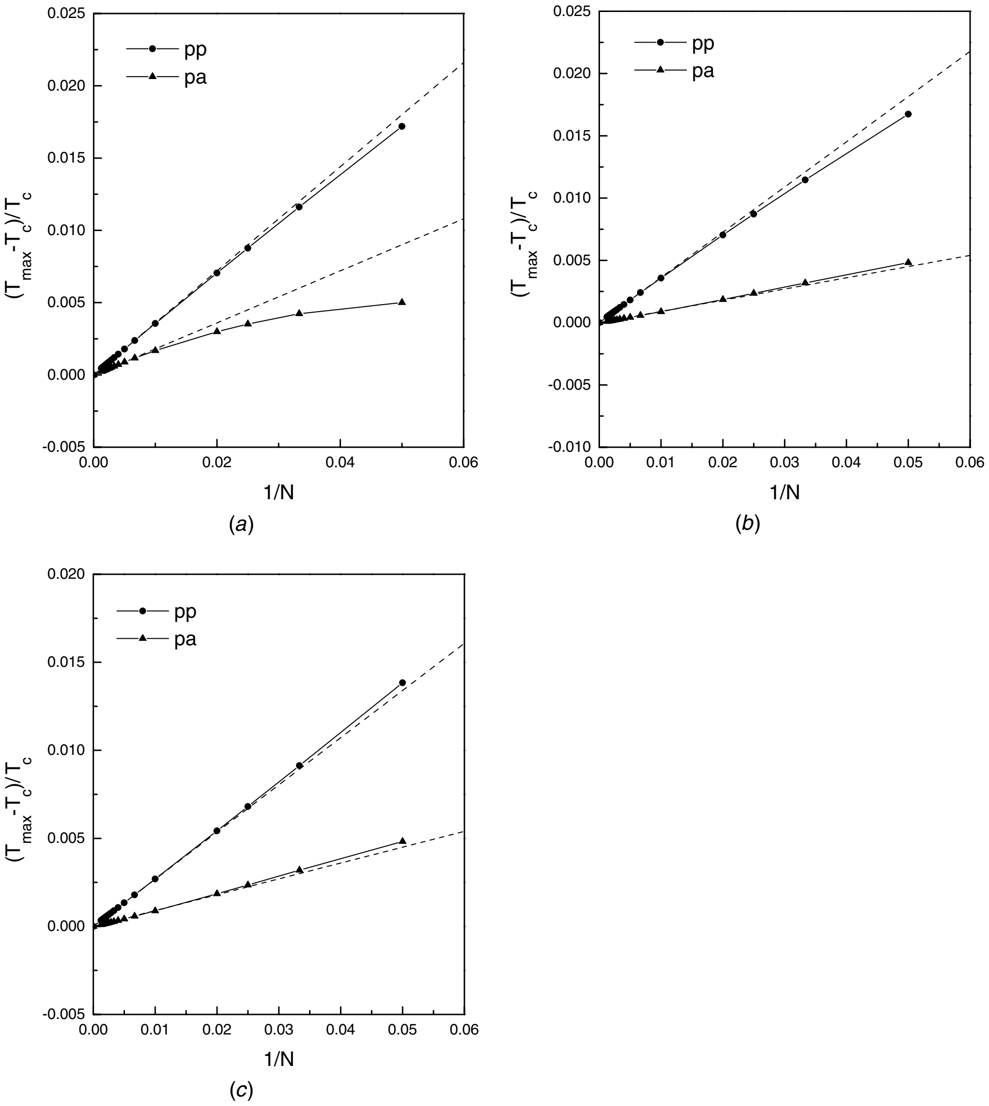

Figure 5. (*a*) Variation of $(T_{\max} - T_c)$ with finite N for $N \times N$ square Ising lattices with isotropic couplings under pp and pa boundary conditions. The broken lines are given by $(T_{\max} - T_c)/T_c = a/N$ and indicate the limiting behaviour as $N \to \infty$. (*b*) Variation of $(T_{\max} - T_c)$ with finite N for $N \times N$ plane–triangular Ising lattices with isotropic couplings under pp and pa boundary conditions. (*c*) Variation of $(T_{\max} - T_c)$ with finite N for $N \times N$ honeycomb Ising lattices with isotropic couplings under pp and pa boundary conditions.

behaviours when the aspect ratios of these lattices have the proportions $1 : \sqrt{3}/2 : \sqrt{3}$. This further implies lattice-structure-dependence of the universal finite-size scaling function and it would be a rigorous test from the analytical perspective. For the aforementioned topics, we have found finite-size scaling behaviours for sq, pt and hc lattices under period–aperiodic boundary conditions. By selecting a very small number of nonuniversal metric factors, we have further found very good universal finite-size scaling behaviours for these lattices, and the results will be presented in another paper.

Finally, the discussion of specific heat in this paper also inspires another problem. Quite recently, Izmailian and Hu have found an exact amplitude ratio and finite-size corrections for the $M \times N$ sq lattice Ising mode on a torus [8], and new sets of the universal amplitude ratios of subdominant correction to scaling amplitudes [9]. The results of section 4 suggest that $a^{\mathrm{pp}}/a^{\mathrm{pa}}$ for sq, pt and hc lattices are roughly 2, 4 and 3. The question is 'are there exact relations between a^{pp} and a^{pa} for these lattices?' It is interesting to study this question and to have a heuristic argument on this simple relation.

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