

Partition functions and finite-size scalings of Ising model on helical tori

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The exact closed forms of the partition functions of a two-dimensional Ising model on square lattices with twisted boundary conditions are given. The constructions of helical tori are unambiguously related to the twisted boundary conditions by virtue of the $SL(2, Z)$ transforms. The numerical analyses on the deviations of the specific-heat peaks away from the bulk critical temperature reveal that the finite-size effect of helical tori is independent of the chirality.

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Since Onsager obtained the exact solution of the two-dimensional (2D) Ising model with a cylindrical boundary condition (BC) in 1944 [1], the exact treatments of Ising models on different 2D surfaces have been continuously attempted. Recently, Lu and Wu [2] have provided analytical treatments for the Ising models with BCs of a particular class, including the Möbius strip, the Klein bottle, and the self-dual BC. The exact study of the model subject to BCs is of fundamental importance. First, it represents new challenges for the unsolved lattice-statistical problems [1–10]. Second, it is crucial for the finite-size analysis [11–15]. Furthermore, it provides an optimal test bed for the predictions of the conformal field theory [18]. Numerical simulations, on the other hand, can be complementary to the exact study and have provided very rich content for the theory of finite-size scalings [12]. For example, based on the exact analysis of dimer statistics, by Lu and Wu ([2], 1998), Kaneda and Okabe [13] have achieved, via computer simulations, a more thorough understanding of the finite-size scaling behavior of the Ising models subject to the boundary types of the Möbius strip and the Klein bottle. While interesting numerical studies, concerning the excess number of percolation [14] and the Binder parameter of the Ising model [15], for the twisted BCs further proceed, the gap of lacking the corresponding closed form of the partition functions has to be filled.

Boundary conditions are characterized by sets of primitive vectors, which specify the periodicity in the corresponding directions [16]. Helical BCs are basically considered by pairwise joining the edges of the sheet spanned by any two orthogonal primitive vectors. This then ends up with tori of distinct orientations, labeled by the chirality [17], with respect to the underlying lattice, as depicted in Fig. 1. The conventional periodic BC is referred to as the helical BC with trivial chirality. In contrast to the Klein bottle and the

Möbius strip, the twisted BCs are formed by cutting, rewinding, and rejoining the tori *without antipode*. One of the primitive vectors for the twisted BCs, \vec{a}_2 of $\{\vec{a}_1, \vec{a}_2\}$ for the example shown in Fig. 2, coincides with one of the basic vectors that specify the lattice orientation. However, there exist equivalence relations among the primitive vector pairs on the lattice. This is given by the $SL(2, Z)$ transform, which is the prototype of the modular symmetry discussed in the context of conformal field theory [18]. Moreover, the helical BCs, specified by the primitive vectors $\{\vec{a}'_1, \vec{a}'_2\}$ in the example of Fig. 2, can be further shown to be the subclass of the twisted BCs by the $SL(2, Z)$ transforms.

In this work, we first obtain the general form of the partition functions subject to the twisted BCs by employing the technique of the Grassman path integral [8]. The effective range of the twisting factor α against the conventional aspect ratio A is given. Subsequently, a helical BC acquires an unambiguous prescription of twisted BC via the $SL(2, Z)$ transform. Then, the finite-size shift of the specific-heat peak from the bulk critical temperature is numerically investigated. For the helical BCs, the scaling behavior turns out to

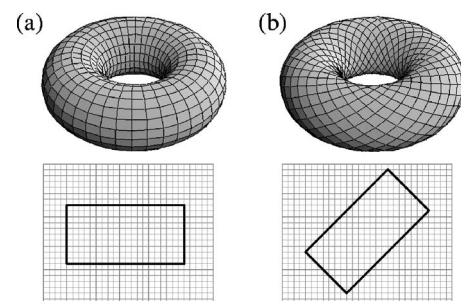


FIG. 1. The formation of helical tori by pairwise joining the edges of the rectangle spanned by any orthogonal set of vectors on the lattice plane: (a) the direction of the primitive vectors coincides with the lattice orientations for the conventional toroidal BC and (b) the helical tori are formed for the noncoincidence.

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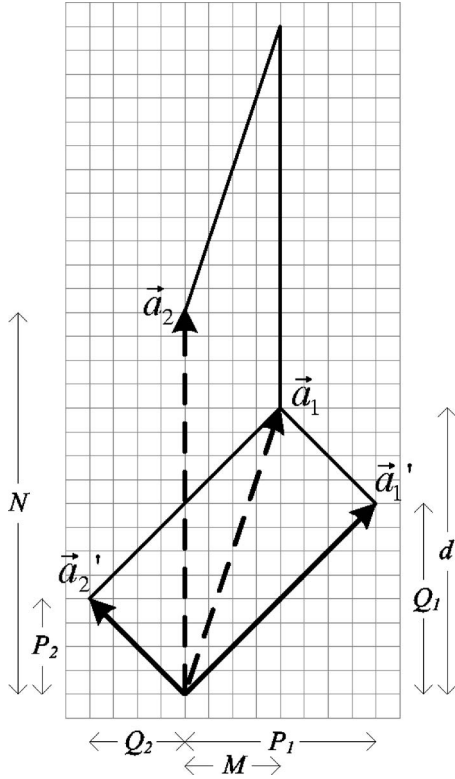


FIG. 2. Equivalence between the BCs in helical and twisted schemes prescribed by $\{\vec{a}_1, \vec{a}_2\}$ and $\{\vec{a}'_1, \vec{a}'_2\}$, respectively, on an $M \times N$ square lattice. For the helical BC, the setting $Q_1/P_1 = Q_2/P_2$ ensures that the two primitive vectors are orthogonal. On the other hand, twisting is generated by a d -unit traverse shift.

be chirality independent. Finally, some notes on the finite-size scaling behaviors are given.

Consider a $M \times N$ square lattice with the coordinates of the lattice sites specified in the form of $\hat{x}m + \hat{y}n$. The partition function of the Ising model is given as $Z_{M,N} = [2 \cosh(\beta J_1) \cosh(\beta J_2)]^{MN} Q_{M,N}$ with the reduced partition function $Q_{M,N} = \prod_{m=1}^M \prod_{n=1}^N \frac{1}{2} \hat{Q}_{m,n}$, where $\hat{Q}_{m,n} = \frac{1}{2} \sum_{\{\sigma_{mn}\}} [(1 + t_1 \sigma_{m,n} \sigma_{m+1,n})(1 + t_2 \sigma_{m,n} \sigma_{m,n+1})]$. Here, we use the notations, $t_i = \tanh(\beta J_i)$ with J_i , for $i=1, 2$, denoting the coupling constants along the x and y directions, and $\beta = 1/k_B T$. The BCs suggest the identifications of the spin variables, whose locations are related by the pair of primitive vectors, say, \vec{a}_1 and \vec{a}_2 . Basically, there are two types of twistings: One is referred to as $Tw_I(M, N, d/M)$ specified by the primitive vectors $\{\vec{a}_1 = M\hat{x} + d\hat{y}, \vec{a}_2 = N\hat{y}\}$ as shown in Fig. 2, and the other is referred to as $Tw_{II}(M, N, d/N)$ specified by $\{\vec{a}_1 = M\hat{x}, \vec{a}_2 = d\hat{x} + N\hat{y}\}$.

According to Plechko ([8(a)]), the reduced partition function takes the form of

$$Q_{M,N} = \sum_{\{\sigma_{mn}\}} \prod_{m=1}^M \prod_{n=1}^N \Psi_{m,n}^{(1)} \Psi_{m,n}^{(2)} \quad (1)$$

with

$$\Psi_{m,n}^{(1)} = \int da_{m,n} da_{m,n}^* e^{a_{m,n} a_{m,n}^*} [A_{m,n} A_{m+1,n}^*],$$

$$\Psi_{m,n}^{(2)} = \int db_{m,n} db_{m,n}^* e^{b_{m,n} b_{m,n}^*} [B_{m,n} B_{m,n+1}^*], \quad (2)$$

where $A_{m,n} = 1 + a_{m,n} \sigma_{m,n}$, $A_{m,n}^* = 1 + t_1 a_{m-1,n}^* \sigma_{m,n}$, $B_{m,n} = 1 + b_{m,n} \sigma_{m,n}$, and $B_{m,n}^* = 1 + t_2 b_{m,n-1}^* \sigma_{m,n}$. In the above equations two pairs of conjugate Grassman variables, $\{a_{m,n}, a_{m,n}^*\}$ and $\{b_{m,n}, b_{m,n}^*\}$ have been introduced. As technically known from Refs. [8–10], the handling of the boundary Boltzmann weights,

$$\Psi_{\Gamma} = \prod_{n=1}^N \Psi_{M,n}^{(1)} \prod_{m=1}^M \Psi_{m,N}^{(2)}, \quad (3)$$

remains central in the treatments. It turns out to be instructive to reexamine the paradigm that solves this problem in the original periodic settings $\sigma_{m+M,n} = \sigma_{m,n}$ and $\sigma_{m,n+N} = \sigma_{m,n}$.

In Ref. [8(a)], the boundary Boltzmann weights Ψ_{Γ} are rearranged such that $\Psi_{\Gamma} = \Psi_{\gamma|\Gamma_1} + \Psi_{\gamma|\Gamma_2} + \Psi_{\gamma|\Gamma_3} - \Psi_{\gamma|\Gamma_4}$ subject to the BCs Γ_i s, imposed on the Grassman variables, with

$$\Psi_{\gamma} = \int \prod_n \bar{A}_{1,n}^* \prod_m \bar{B}_{m,1}^* \prod_n \bar{A}_{M,n} \prod_m \bar{B}_{m,N}, \quad (4)$$

where the arrows indicate the ordering for the multiplications, and we employ the notation \int for all the coming weighted integration over relevant Grassman variables. Subsequently, mirror ordering is applied routinely and furnishes the simple expression of pure Grassmanian integrations,

$$Q_{M,N} = \frac{1}{2} [G|_{\Gamma_1} + G|_{\Gamma_2} + G|_{\Gamma_3} - G|_{\Gamma_4}], \quad (5)$$

$$G = \int \exp \left\{ \sum_{m,n} [a_{m,n} b_{m,n} + t_1 t_2 a_{m-1,n}^* b_{m,n-1}^* + (t_1 a_{m-1,n}^* + t_2 b_{m,n-1}^*) (a_{m,n} + b_{m,n})] \right\}, \quad (6)$$

where the integrations can be diagonalized and carried out straightforwardly [8].

The above reviewing paragraph suggests that the modification is only essential for the twisted BC in the key steps, i.e., from Eq. (3) to Eq. (4). For Tw_I , the $\Psi_{M,n}^{(1)}$ term in Eq. (3) is calibrated in relation to the toroidal term. Then, this leads to

$$\Psi_{\Gamma} = \int \prod_{m=1}^M \overrightarrow{B}_{m,1}^* \prod_{k=1}^{N-d} \overleftarrow{(1 - t_1 a_{M,k+d}^* \sigma_{1,k})} \times \prod_{k=N-d+1}^N \overleftarrow{(1 - t_1 a_{M,k+d-N}^* \sigma_{1,k})} \prod_{n=1}^N \overrightarrow{A}_{M,n} \prod_{m=1}^M \overleftarrow{B}_{m,N}, \quad (7)$$

where the BC $\sigma_{m+M,n+d} = \sigma_{m,n}$ has been explicitly employed. Reordering of the first three products in Eq. (7) is essential such that the form of Eq. (4) can be achieved. By recursive use of the identity for the permutation of the Grassmanian functions [8], we employ, instead,

$$XYZ \equiv \frac{1}{2}(ZYX^- - Z^-Y^-X^- + ZY^-X + ZY^-X^-), \quad (8)$$

where X , Y , and Z stand for the corresponding three objects and the superscript “ $-$ ” denotes flipping the sign of the Grassman variables. Accordingly, the form of Eq. (4) is achieved, which implies Eq. (5). Note that the form of Eq. (6) is preserved under twisting. However, the BCs imposed on the Grassman variables are modified in response to the corresponding sign flipping appearing in the deduction of Eq. (8). For convenience, the compact notation as $\Gamma_i = (\pm, \pm)$ can be employed as follows. The first sign in the parentheses corresponds to $a_{m,n}^* = \pm a_{m,0}^*$, and the second one is for $a_{m,n+d}^* = \pm a_{0,n}^*$. The BCs are given as $\Gamma_1 = (-, -)$, $\Gamma_2 = (+, -)$, $\Gamma_3 = (-, +)$, and $\Gamma_4 = (+, +)$. Henceforth, the exact partition function is straightforward.

For T_{W_1} with the twisting factor $\alpha \equiv d/M$, the reduced partition function is

$$Q_{M,N}^\alpha = \frac{1}{2} \left[I_{M,N}^\alpha \left(\frac{1}{2}, \frac{1}{2} \right) + I_{M,N}^\alpha \left(\frac{1}{2}, 0 \right) + I_{M,N}^\alpha \left(0, \frac{1}{2} \right) - \text{sgn} \left(\frac{T - T_c}{T_c} \right) I_{M,N}^\alpha(0, 0) \right], \quad (9)$$

$$I_{M,N}^\alpha(\Delta, \bar{\Delta}) = \prod_{p=1}^M \prod_{q=1}^N \left\{ \lambda_0 - \lambda_1 \cos \left[2\pi \left(\frac{p + \Delta}{M} - \frac{\alpha(q + \bar{\Delta})}{N} \right) \right] - \lambda_2 \cos \left[2\pi \left(\frac{q + \bar{\Delta}}{N} \right) \right] \right\}^{1/2}, \quad (10)$$

where $\lambda_0 = (1 + t_1^2)(1 + t_2^2)$, $\lambda_1 = 2t_1(1 - t_2^2)$, and $\lambda_2 = 2t_2(1 - t_1^2)$. In addition, the function $\text{sgn}(x)$ denotes the sign of the value x , and T_c is the critical temperature of the bulk system. Meanwhile, for $T_{W_{II}}$, the expression of Eq. (9) remains the same along with the interchange for the roles of p and q and with $\alpha = d/N$ in Eq. (10).

The expression of Eq. (9) implies $Q_{M,N}^\alpha = Q_{M,N}^{-\alpha}$, which reflects the fact that a twisting either clockwise or counter-clockwise is indistinguishable. On employing the transform matrices $\mathcal{M} \in SL(2, Z)$ explicitly, pairs of primitive vectors are related among each other in the manner of

$$\begin{pmatrix} \vec{a}'_1 \\ \vec{a}'_2 \end{pmatrix} = \mathcal{M} \begin{pmatrix} \vec{a}_1 \\ \vec{a}_2 \end{pmatrix}. \quad (11)$$

Consider T_{W_1} , for example. The choice of matrix elements $\mathcal{M}_{11} = 1$, $\mathcal{M}_{12} = J \in Z$, $\mathcal{M}_{21} = 0$, and $\mathcal{M}_{22} = 1$ gives rise to the new pairs of primitive vectors, $\{\vec{a}'_1 = M\hat{x} + (d+N)\hat{y}, \vec{a}'_2 = N\hat{y}\}$, which prescribes the same BC. As evidence, the equality, $Q_{M,N}^\alpha = Q_{M,N}^{\alpha+JA}$ with the conventional aspect ratio $A = N/M$, can be explicitly checked. Thus, the effective range of α is $0 \leq \alpha < A$. Furthermore, T_{W_1} alone suffices for the full prescription of the twisted BCs, because the equivalence $T_{W_1}(M, N, \alpha = A/J) \equiv T_{W_{II}}(JM, N/J, 1/\alpha)$ can be achieved by virtue of $\mathcal{M}_{11} = J \in Z$, $\mathcal{M}_{12} = -1$, $\mathcal{M}_{21} = 1$, and $\mathcal{M}_{22} = 0$. Again, the partition function of Eq. (9) appears to fulfill these relations.

The BC of the helical tori counts on the orthogonal primi-

tive vector pair, $\vec{a}'_1 = \hat{x}P_1 + \hat{y}Q_1$ and $\vec{a}'_2 = -\hat{x}Q_2 + \hat{y}P_2$, where the two radii for the torus are given as $L_i = \sqrt{P_i^2 + Q_i^2}$ for $i = 1, 2$. Let the helical system be denoted by $HI(B, L_1, \chi)$, where the chiral aspect ratio is defined as $B = L_2/L_1$, and the chirality is $\chi = Q_1/P_1 \equiv Q_2/P_2$. Based on Eq. (11) with $\mathcal{M}_{11} = P_1/M$ and $\mathcal{M}_{21} = -Q_2/M$, we can furnish the equivalent structure, $HI(B, L_1, \chi) \equiv Tw_1(A, M, \alpha)$, by using the relations

$$\mathcal{M}_{21} = -B\chi\mathcal{M}_{11}, \quad (12)$$

$$1 = \mathcal{M}_{11}\mathcal{M}_{22} - \mathcal{M}_{21}\mathcal{M}_{12}, \quad (13)$$

$$A = \frac{(\mathcal{M}_{21})^2}{B} + B(\mathcal{M}_{11})^2, \quad (14)$$

$$\alpha = -\frac{\mathcal{M}_{21}\mathcal{M}_{22}}{B} - B\mathcal{M}_{11}\mathcal{M}_{12}. \quad (15)$$

Some notes on the uniqueness of the relations above are given as the following: The $[\mathcal{M}_{12}, \mathcal{M}_{22}]$ pair is unambiguously determined up to \mathcal{M}_{11} and \mathcal{M}_{21} for $0 \leq \alpha < A$. This is because shifting $[\mathcal{M}_{12}, \mathcal{M}_{22}]$ by appending $[J\mathcal{M}_{11}, J\mathcal{M}_{21}]$ for $\forall J \in Z$ leaves Eq. (13) invariant but only deviates the result of Eq. (15) from α to $\alpha + JA$. Meanwhile, the allowable region for $[\mathcal{M}_{12}, \mathcal{M}_{22}]$ appropriate for $0 \leq \alpha < A$ is of exactly one vector section $[\mathcal{M}_{11}, \mathcal{M}_{21}]$. In addition, the ambiguity relating to size dependence can be removed by the coprime properties between \mathcal{M}_{11} and \mathcal{M}_{21} , which ensures the solubility of the integer pair $[\mathcal{M}_{12}, \mathcal{M}_{22}]$ subject to Eq. (13). Consequently, a helical two-tuple (B, χ) corresponds to a unique pair (A, α) for the twisting in the effective range. Moreover, it can be shown that helical tori bearing with different geometry cannot be mapped into each other by $SL(2, Z)$ transforms; thus the distinction of the helical tori via the twisting parameters is unambiguous.

The deviation of the specific-heat peak T_{\max} of a finite system away from the bulk critical temperature T_c , defined as $\theta = (T_{\max} - T_c)/T_c$, is referred to as the critical shift of the system. Based on the parametrization of $T_{W_1}(A, M, \alpha)$ and the exact partition function of Eq. (9) with an isotropic coupling, we study the finite-size scaling of θ for systems with twisted BCs. The numerical results of $\theta(A, \alpha)$ vs $1/L = 1/\sqrt{MN}$ are shown in Fig. 3. These suggest that two parameters, A and α , are required to specify the scaling behaviors, and the leading scaling behavior of $\theta(A, \alpha)$ is $\theta(A, \alpha) \sim c(A, \alpha)/L$ with the constant $c(A, \alpha)$ increasing as α increases for a given A . However, there is an exceptional case $A = 1$ for which, $c(A, \alpha)$ is independent of α .

For helical BCs, the critical shifts $\theta(B, \chi)$ are determined by first employing Eqs. (12)–(15) to find the corresponding twisted BCs and then calculating the equivalent $\theta(A, \alpha)$. Note that the partition function cannot differentiate the rolling up direction in forming the tori, hence there is no distinction between the chiralities χ and $-\chi$, and we take $\chi > 0$. We also note that once $HI(B, \chi) \equiv Tw_1(A, \alpha)$ is established by a $SL(2, Z)$ transform, say $\mathcal{M}^{(a)}$, the equivalence $HI(1/B, 1/\chi) \equiv Tw_1(A, -\alpha)$ is then followed by the $SL(2, Z)$ transform $\mathcal{M}^{(b)}$ with $\mathcal{M}_{11}^{(b)} = -\mathcal{M}_{21}^{(a)}$, $\mathcal{M}_{21}^{(b)} = -\mathcal{M}_{11}^{(a)}$, $\mathcal{M}_{12}^{(b)}$

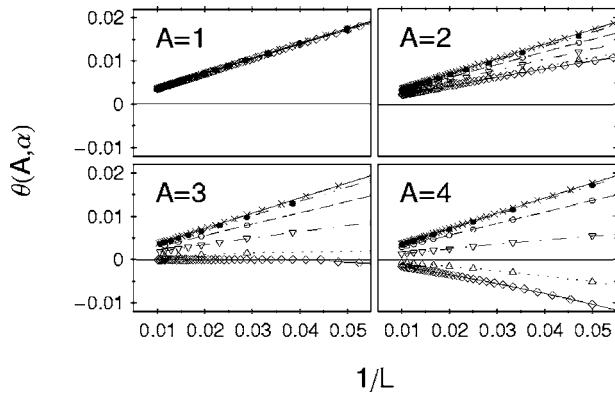


FIG. 3. Plotting $\theta(A, \alpha)$ against $1/L$ for $A=1, 2, 3, 4$ with $\alpha=0$, (\diamond) 0.1A (\triangle), 0.2A (∇), 0.3A (\circ), 0.4A (\bullet), and 0.5A (\times). The scaling behaviors are obviously deviated by α . Nonetheless, for $A=1$ no splitting is found with respect to the twisting factors.

$=\mathcal{M}_{22}^{(a)}$, and $\mathcal{M}_{22}^{(b)}=\mathcal{M}_{12}^{(a)}$. Thus, the equality $\theta(B, \chi)=\theta(1/B, 1/\chi)$ holds, and we may take $B \geq 1$ in calculating $\theta(B, \chi)$ for various χ values. The results of $\theta(B, \chi)$ vs $1/L=1/\sqrt{L_1 L_2}=1/\sqrt{MN}$ are shown in Fig. 4. The finite-size scaling of $\theta(B, \chi)$ for a given B value is chirality independent. The leading scaling behavior takes the form $\theta(B, \chi) \sim c(B)/L$ in which the constant $c(B)$ flips its sign at $B=b_0$ and $1/b_0$ with $b_0 \approx 3$. This sign reversal was anticipated by Ferdinand and Fisher [11] for the conventional periodic BC, where the exact b_0 value was determined as $b_0=3.13927\dots$, a result which now applies for all the helical tori.

In conclusion, we provide the complete description for the finite-size effect of an Ising model subject to the helical BCs, a subclass of the twisted BCs. This is explicitly done by first solving the exact form of the partition function appropriate for all the twisted BCs and then numerically calculating the critical shifts. The finite-size effect is found to be chirality independent. This remarkable fact basically supports the invariance of the scaling behavior of the partition function un-

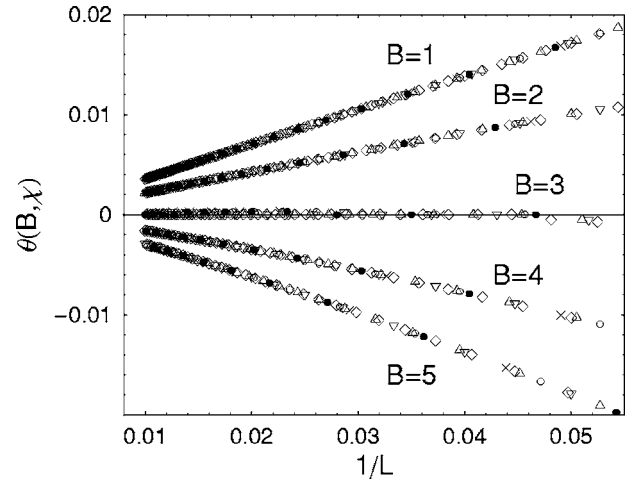


FIG. 4. The plot of $\theta(B, \chi)$ vs $1/L$ for a given chiral aspect ratio B . Results of different chiralities χ collapse into one curve and the curves of both $\theta(B, \chi)$ and $\theta(1/B, 1/\chi)$ vs $1/L$ coincide.

der rotation of the primitive vector pair subject to BCs, conjectured in Ref. [15] which, however, gave the invariant aspect ratio as $A/(1+\alpha^2)$ [19] coinciding with the chiral aspect ratio B only for $\chi=\alpha$. The particular coincidence as the finite-size scaling of critical shift independent of α and χ for $A=1$ and $B=1$ suggests further interesting points exceeding beyond the rotational invariance. For consistency, we stress the fact that $A=1$ does not nontrivially permit any helical structure, as one may observe in Eqs. (12)–(15). As a final remark, Ising systems with helical BCs, a subclass of the twisted BCs, form themselves a reasonable ensemble, and their generalization to the twisted class may also possess interesting issues.

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