Letter

Exact expressions for the partition function of the one-dimensional Ising model in the fixed-*M* ensemble

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We obtain exact closed-form expressions for the partition function of the one-dimensional Ising model in the fixed-*M* ensemble, for three commonly used boundary conditions: periodic, antiperiodic, and Dirichlet. These expressions allow for the determination of fluctuation-induced forces in the canonical ensemble, which we term Helmholtz forces. The thermodynamic expressions and the calculations flowing from them should provide insights into the nature and behavior of fluctuation-induced forces in interesting and as-yet unexplored regimes.

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I. INTRODUCTION

Except for the ideal gas, the Ising model is probably the most well-known model in statistical physics. Its solution for the one-dimensional case with a temperature T and external field h—and for the two-dimensional case in zero external field—can be found in most textbooks of statistical mechanics—see, e.g., Refs. [1–4]. Inspection of the literature shows, perhaps surprisingly, that the solution of the Ising model in one or any higher dimension is not available when the magnetization M is fixed. In this Letter we fill that gap and provide closed-form expressions for the cases of the finite Ising chain with fixed total magnetization M under periodic, antiperiodic, and free boundary conditions. The resulting expressions, which involve hypergeometric functions, differ nontrivially from corresponding expressions in the fixed-h ensemble.

The lack of expressions for the one-dimensional Ising model with fixed magnetization M is not due to a lack of interest into the problem. We stress, as noted in Ref. [5], that in customarily considered applications of the equilibrium Ising model to binary alloys or binary liquids, if one insists on full rigor, the case with M fixed must be addressed. Thus, there have been attempts to solve the problem of Ising chain with fixed M [5–7]. In Refs. [5,6] it is attacked via the transfer-matrix method. Reference [5] reports success in deriving a closed-form expression for the partition function for the case $M = 0$ under periodic boundary conditions, when the chain contains an even number of spins. In Ref. [6] the focus is on the asymptotic behavior of the free energy of the Ising chain with $M = 0$ and under periodic boundary conditions and chain length $N \gg 1$ in the temperature regime when the correlation length of the chain ξ is kept finite, i.e., excluding the regime $T \to 0$. In Ref. [7] the finite-size scaling functions for the probability distribution of the magnetization in the one-dimensional Ising model has been investigated. The functions are evaluated in the limit $T \to 0$ and $N \to \infty$ with N/ξ kept finite. Exact results for periodic, antiperiodic, free, and block boundary conditions have been obtained. The approach used there is based on a combinatorial approach to counting the domains of up and down spins. This is similar to the approach we use for our study of a fully finite Ising chain with periodic, antiperiodic, and free boundary conditions.

Knowledge of the partition function leads to the calculation of the Helmholtz free energy, which allows for the determination of a fluctuation-induced force in the fixed-M ensemble. This can be achieved in a manner similar to the derivation of the Casimir force for critical systems in the grand-canonical T-h ensemble,

$$\beta F_{\rm Cas}^{(\zeta)}(T,h,L) \equiv -\frac{\partial}{\partial L} f_{\rm ex}^{(\zeta)}(T,h,L), \tag{1.1}$$

where

$$f_{\rm ex}^{(\zeta)}(T,h,L) \equiv f^{(\zeta)}(T,h,L) - L f_b(T,h) \tag{1.2}$$

is the so-called excess (over the bulk) free energy per area and per k_BT. Here, one envisages a system in film geometry $\infty^{d-1} \times L$, $L \equiv L_\perp$, with boundary conditions ζ imposed along the spatial direction of finite extent L, and with total free energy $\mathcal{F}_{\rm tot}^{(\zeta)}$. Here, $f^{(\zeta)}(T,h,L) \equiv \lim_{A\to\infty} \mathcal{F}_{\rm tot}^{(\zeta)}/A$ is the free energy per area A of the system. Along these lines we define

$$\beta F_{\rm H}^{(\zeta)}(T,M,L) \equiv -\frac{\partial}{\partial L} f_{\rm ex}^{(\zeta)}(T,M,L), \tag{1.3}$$

where

$$f_{\rm ex}^{(\zeta)}(T,M,L) \equiv f^{(\zeta)}(T,M,L) - L f_{\rm H}(T,m), \tag{1.4}$$

with $m = \lim_{L,A\to\infty} M/(LA)$, and $f_{\rm H}$ is the Helmholtz free-energy density of the "bulk" system. We will show that the so-defined *Helmholtz fluctuation-induced force* has a behavior very different from that of the Casimir force. Explicitly, we will demonstrate that for the Ising chain with fixed M

under periodic boundary conditions $F_{\rm H}^{\rm (per)}(T,M,L)$ can, depending on the temperature T, be attractive or repulsive, while $F_{\rm Cas}^{\rm (per)}(T,h,L)$ is only attractive. We note that the issue of the ensemble dependence of fluctuation-induced forces pertinent to the ensemble has yet to be studied. This issue is by no means limited to the Ising chain and can be addressed, in principle, in any model of interest. The analysis reported here can also be viewed as a useful addition to approaches to fluctuation-induced forces in the fixed-M ensemble based on Ginzburg-Landau-Wilson Hamiltonians [8–10] in which one studied the usual Casimir force.

Before turning to the specific calculations related to the Ising chain with fixed magnetization we note that recently one-dimensional and quasi-one-dimensional systems have been the objects of intensified experimental interest—see, e.g., Ref. [11] and references therein. Some of these, such as $TaSe_3$, are quasi-one-dimensional in the sense that they have strong covalent bonds in one direction along the atomic chains and weaker bonds in the perpendicular plane [12]. Others are more properly considered true one-dimensional materials, in that they have covalent bonds only along the atomic chains and much weaker van der Waals interactions in perpendicular directions [13]. One-dimensional van der Waals materials have emerged as an entirely new field, which encompasses interdisciplinary work by physicists, chemists, materials scientists, and engineers [11]. The Ising chain considered here can be seen as the simplest possible example of such a one-dimensional material. Earlier experimental realizations of a one-dimensional Ising model have been considered in Refs. [11,14–17]. The one-dimensional Ising model in a transverse field has proven an important experimental realization of a system with a quantum phase transition [17].

The Ising chain in a T-h ensemble manifests scaling behavior in the vicinity of its zero-temperature ordered state, and it is a test bed for exploring the influence of finite-size scaling on critical properties, including the connection between the behavior of fluctuation-induced forces in the critical regime and scaling predictions [18,19].

Below, we describe the derivation of the exact results for the partition function of an Ising chain with fixed magnetization M under different boundary conditions. In what follows we will assume a lattice constant $a = 1$, so that instead of L we will use N as a measure of the length of the chain.

II. ISING CHAIN WITH FIXED M: THE COMBINATORICS OF DOMAINS

As in the case of all boundary conditions considered here, the partition function to be evaluated is the sum over spin states of the Boltzmann factor

$$\exp\left[K\sum_{i=1}^{N-1} s_i s_{i+1}\right], \tag{2.1}$$

where each spin variable takes on the values ±1. Fixing the total magnetism amounts to the constraint that the difference between the number of up spins, N_+, and the number of down spins, N_-, is equal to M.

The key step in the calculation of the partition function is the determination of the number of ways in which the spins can arrange themselves into alternating spin-up and spin-down domains, subject to the requirement of a fixed value of the total magnetization, M. We start with equations that express the relationships between M, the number of up spins, N_+, and the number of down spins, N_-, along with the total number of spins, N:

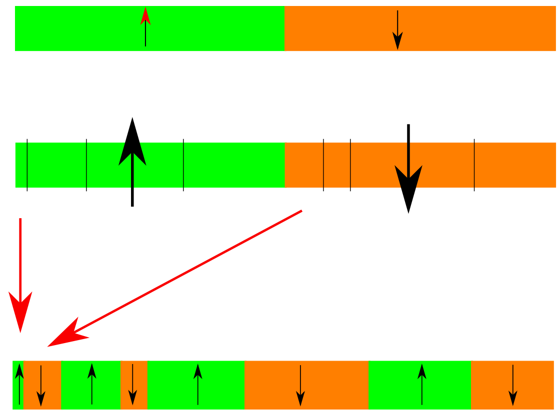

FIG. 1. Top: The domain of up spins (in green) and of down spins (in orange). Middle: The domains are each divided into four smaller domains. Bottom: The smaller domains are now interspersed; see the red arrows.

$$N = N_+ + N_- \quad \text{and} \quad M = N_+ - N_-. \tag{2.2}$$

Inverting these equations we find

$$N_+ = \frac{N+M}{2} \quad \text{and} \quad N_- = \frac{N-M}{2}. \tag{2.3}$$

For insight into the determination of domain statistics, we look at, say, the fourth leading contribution in an expansion of the partition function in powers of $\exp[-K]$. We start with a domain of N_+ up spins. We then partition that domain into four smaller domains. We do this by inserting three "slices" into the domain, effectively three walls between adjacent spins. We then partition a domain of N_- down spins into four smaller domains, which we insert between the domains of up spins. The process is illustrated in Fig. 1.

We now calculate how many ways there are of subdividing each domain into four subdomains. In the case of the spin-up domain, that quantity is

$$(N_+ - 1)(N_+ - 2)(N_+ - 3)/3!, \tag{2.4}$$

which is the number of ways of inserting three partitions between adjacent spins in a linear array of N_+ up spins. A similar expression holds for the number of ways of subdividing the domain of down spins. By making use of relations (2.3) and multiplying the resulting expressions to obtain the number of ways of subdividing both domains, we end up with the factor

$$[(N-2)^2 - M^2][(N-4)^2 - M^2][(N-6)^2 - M^2]/[4^3(3!)^2]. \tag{2.5}$$

We now join the ends of the set of domains up so that they form a ring, consistent with periodic boundary conditions, and we rotate the ring around to find out how many ways we can arrange the subdomains. This yields a factor of N. However, because we take all possible lengths for the set of subdomains we are overcounting by a factor of four, the number of pairs of domains. The overall factor is thus

$$\frac{N}{4}\frac{[(N-2)^2-M^2][(N-4)^2-M^2][(N-6)^2-M^2]}{4^3(3!)^2}. \tag{2.6}$$

To obtain the complete expression, we multiply the above by $\exp(-16K)$, corresponding to the energy cost of the eight walls between the eight domains of the periodically continued array in Fig. 1.

In the general case of $2k$ alternating domains, the first factor of 4 in the denominator of (2.6) is replaced by k, while the two other factors become 4^{k-1} and $(k-1)!^2$. Thus, the general form of the denominator is

$$4^{k-1}k[(k-1)!]^2. \tag{2.7}$$

Then, for the numerator one has

$$N\prod_{p=1}^{k-1}[(N-2p)^2-M^2]. \tag{2.8}$$

Taking into account that the Boltzmann's weight of a configuration with $2k$ domains is $\exp[K(N-4k)]$, for the contribution of this configuration in the statistical sum one obtains

$$Z\ \mathrm{term}(N,M,K,k) = \frac{N\exp[K(N-4k)]\prod_{p=1}^{k-1}[(N-2p)^2-M^2]}{4^{k-1}k[(k-1)!]^2}. \tag{2.9}$$

The form of the right-hand side of (2.9) allows us to sum over k from 0 to ∞ to obtain the partition function $Z^{(\mathrm{per})}(N,M,K)$. The result is a closed-form expression that is exact when N and M are both even or odd integers with $|M|<N$, and that smoothly interpolates between the exact expression for all other values of N and M with $|M|<N$. The case $|M|=N$ is exceptional, but trivial to determine. The result is

$$Z^{(\mathrm{per})}(N,K,M) = Ne^{K(N-4)}\,{}_2F_1\left(\tfrac{1}{2}(-M-N+2),\tfrac{1}{2}(M-N+2);2;e^{-4K}\right), \tag{2.10}$$

where ${}_2F_1(\alpha,\beta;\gamma;z)$ is the generalized hypergeometric function [20].

Similar calculations [21] lead to expressions for the partition functions in the case of antiperiodic and Dirichlet boundary conditions. When the boundary conditions are Dirichlet, we have

$$\begin{aligned} Z^{(D)}(N,K,M) = e^{K(N-1)}\big[&2e^{-2K}\,{}_2F_1\left(\tfrac{1}{2}(-M-N+2),\tfrac{1}{2}(M-N+2);1;e^{-4K}\right)\\ &-\tfrac{1}{2}e^{-4K}(M-N+2)\,{}_2F_1\left(\tfrac{1}{2}(-M-N+2),\tfrac{1}{2}(M-N+4);2;e^{-4K}\right)\\ &+\tfrac{1}{2}e^{-4K}(M+N-2)\,{}_2F_1\left(\tfrac{1}{2}(-M-N+4),\tfrac{1}{2}(M-N+2);2;e^{-4K}\right)\big], \end{aligned} \tag{2.11}$$

and when the boundary conditions are antiperiodic, the partition function is given by

$$\begin{aligned} Z^{(\mathrm{anti})}(N,K,M) = e^{K(N-6)}\big[&2\left(e^{4K}-1\right){}_2F_1\left(\tfrac{1}{2}(-M-N+2),\tfrac{1}{2}(M-N+2);1;e^{-4K}\right)\\ &+N\,{}_2F_1\left(\tfrac{1}{2}(-M-N+2),\tfrac{1}{2}(M-N+2);2;e^{-4K}\right)\big]. \end{aligned} \tag{2.12}$$

As in the case of periodic boundary conditions, the expressions above for the partition function when boundary conditions are Dirichlet and antiperiodic are exact except in the case of perfect alignment of the spins, when $M=\pm N$.

If we write $M=mN$ and focus on the case $N\gg 1$, then the exact expressions above approach different forms. In the case of periodic boundary conditions, the partition function becomes

$$Z_{\lim}^{(\mathrm{per})}(N,K,m) = \frac{2}{N}\frac{e^{NK}x_t}{\sqrt{1-m^2}}I_1(x_t\sqrt{1-m^2}), \tag{2.13}$$

where I_1 is the modified Bessel function of order 1, and $x_t = Ne^{-2K}$ is the scaling combination N/ξ_t, ξ_t being the correlation length [1] in the vicinity of the zero-temperature critical point. This allows us to explore the scaling behavior of thermodynamic quantities close to $T=0$. Limiting forms for the antiperiodic and Dirichlet partition functions can also be obtained.

The explicit formulas (2.10)–(2.12) allow one to obtain expressions involving derivatives with respect to the size N and the total magnetization M of the Ising chain. This is useful in the calculation of fluctuation-induced forces in the one-dimensional Ising system. Because of the nature of the ensemble in which the forces are generated, we refer to them as *Helmholtz* forces. The determination of this kind of force requires that we specify precisely what is held constant in the finite Ising strip (the "film") and the infinite Ising system that borders it (the "bulk"). Three of the possibilities are (1) constant total magnetization M, (2) constant magnetization per site, $m=M/N$, and (3) constant number of up spins, N_+. The last is relevant to lattice gas models. Consideration of the model leads to the following observations.

(1) In the case of periodic and antiperiodic boundary conditions the degeneracy in the position of the borders between the domains with respect to translation results in a contribution to the Helmholtz free energy that is logarithmic in N. The implies lack of a perfect scaling.

(2) When m in the fixed m ensemble is not equal to ± 1, the interfacial energy between the domains with coexisting phases plays a key role in the statistical mechanics of the system.

It is well known that in the grand canonical ensemble, i.e., fixed h, the Gibbs free energy of the finite system approaches the bulk limit *exponentially* in N (i.e., as $e^{-\alpha N}$ with $\alpha>0$) as $N\to\infty$ for periodic boundary conditions. The properties listed above imply that in systems with fixed m the Helmholtz free energy possesses nonscaling contributions that vanish

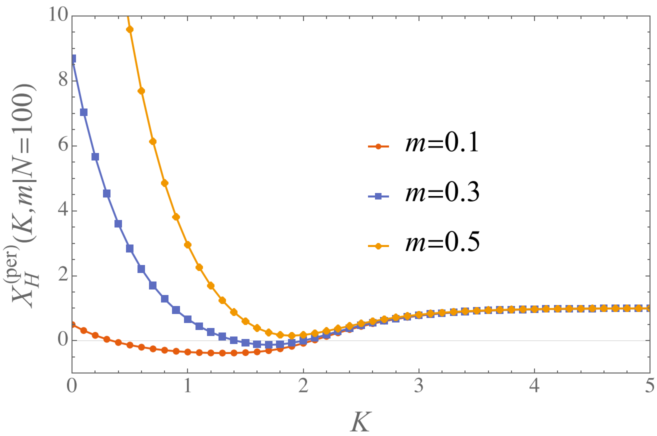

FIG. 2. The behavior of the function $X_{\rm H}^{(\rm per)}(K, m|N)$ [see Eq. (2.15)] with $N = 100$ and for $m = 0.1$, 0.3, and 0.5. We observe that the function is *positive* for large values of K and *negative* for relatively small values of K provided m is also relatively small. For large m the force is always repulsive, irrespective on the value of K. The same is also true for very small values of K, independent on the values of m. The logarithmic behavior of the free energy of the finite Ising chain with periodic boundary conditions noted in item (1) of the comments above lead to the limit $X_{\rm H}^{(\rm per)}(K \to \infty, m|N) = 1$.

significantly more slowly than this exponential approach to the bulk behavior.

Note that m can also be seen as a sort of generalized "charge," or symmetry value, which is conserved both inside and outside the system. Given the free energy derivable from the partition function, one is in a position to determine the fluctuation-induced Helmholtz force on a finite Ising chain in contact with a "bulk," a chain of infinite extent. The results of such a calculation are shown in Figs. 2–4. Along the lines of Eqs. (1.3) and (1.4), in terms of notations used specifically for

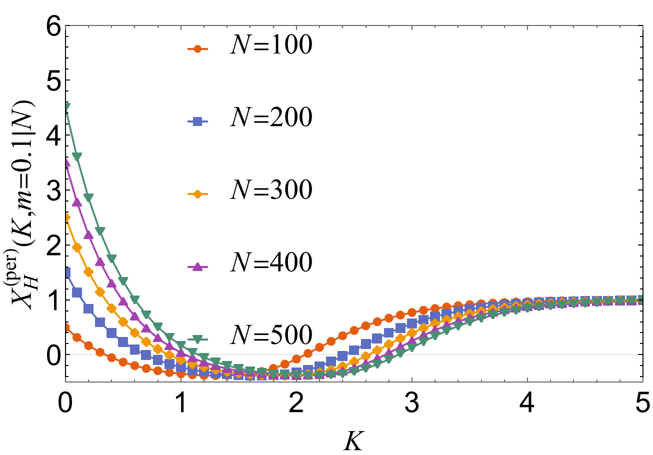

FIG. 3. The behavior of the function $X_{\rm H}^{(\rm per)}(K, m|N)$ [see Eq. (2.15)] with $N = 100$, 200, 300, 400, and 500. We observe that the function is *positive* for large and for small enough values of K, while being *negative* for relatively moderate values of K, *irrespective* of the value of N. The larger N, the stronger the repulsion is for a small enough K; the force in the latter regime is strongly repulsive, irrespective of the value of N.

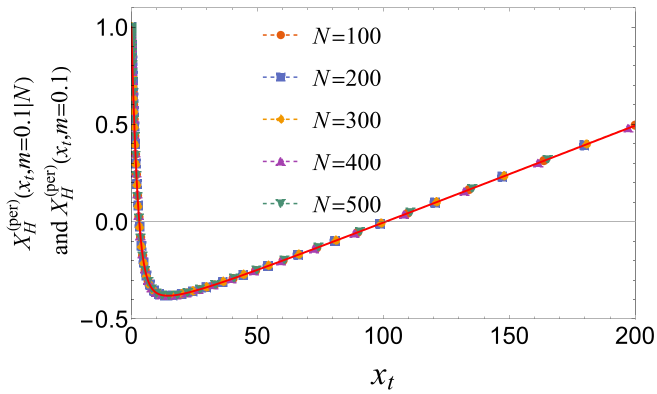

FIG. 4. The behavior of the scaling function $X_{\rm H}^{(\rm per)}(x_t, m)$ for $m = 0.1$. The inspection of the results obtained numerically from Eq. (2.10) with $N = 100$, 200, 300, 400, and 500, and that one from Eq. (2.13) demonstrate perfect scaling and agreement between each other. We observe that the function is *positive* for large values of x_t, *negative* for relatively moderate values of x_t, and again strongly repulsive for small values of x_t.

the Ising chain, the force is minus the derivative with respect to N of the combined Helmholtz free energy

$$\mathcal{F} = -\ln[\mathcal{Z}^{(\rm per)}(N, K, M)] + (\mathcal{N} - N)F_{\rm H}(K, m). \quad (2.14)$$

Here, $F_{\rm H}$ is the Helmholtz free-energy density of a "bulk" neighboring Ising chain. The term proportional to $\mathcal{N}$ can be ignored as a background contribution to the overall free energy. The quantities M, m, and K are kept constant in the process of differentiation, after which M is set equal to mN. This yields the fluctuation-induced Helmholtz force $F_{\rm H}^{(\rm per)}(K, m, N)$. Multiplying the result for $F_{\rm H}^{(\rm per)}(K, m, N)$ by N provides the function $X_{\rm H}^{(\rm per)}(K, m|N)$,

$$X_{\rm H}^{(\rm per)}(K, m|N) = NF_{\rm H}^{(\rm per)}(K, m, N). \quad (2.15)$$

Its behavior is shown in Figs. 2 and 3. Figure 2 shows its behavior as a function of K for $N = 100$, and $m = 0.1$, 0.3, and 0.5, while Fig. 3 shows it for $m = 0.1$ and $N = 100$, 200, 300, 400, and 500. Focusing on the scaling regime (K and N both large compared to 1) we end up with the N-independent scaling function $X^{(\rm per)}(x_t, m)$. Figure 4 shows the behavior of this quantity as a function of x_t for $m = 0.1$.

The plots in Fig. 2 show that the fluctuation-induced force studied has a behavior that is similar to one appearing in some versions of the big bang theory—strong repulsion at high temperatures, transitioning to moderate attraction for intermediate values of the temperature, and then back to repulsion, albeit much weaker than during the initial period of highest temperature [22].

Our Letter demonstrates that one can define *ensemble-dependent* fluctuation-induced forces and study their behaviors. It is worth noting that, as in the studied case of Helmholz's forces, their behaviors can be quite different from the well-known one of the Casimir forces.

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[1] R. J. Baxter, *Exactly Solved Models in Statistical Mechanics* (Academic, London, 1982).
[2] K. Huang, *Statistical Mechanics*, 2nd ed. (Wiley, New York, 1987).
[3] R. K. Pathria and P. D. Beale, *Statistical Mechanics* 3rd ed. (Elsevier, Amsterdam, 2011).
[4] A. J. Berlinsky and A. B. Harris, *Statistical Mechanics* (Springer, Berlin, 2019).
[5] M. Henkel, H. Hinrichsen, S. Lübeck, and M. Pleimling, *Non-Equilibrium Phase Transitions*, Vol. I, Springer Series in Theoretical and Mathematical Physics (Springer, Dordrecht, 2008), see especially Eq. (S.4), p. 305.
[6] Z. J. Wang, F. F. Assaad, and F. P. Toldin, Phys. Rev. E **96**, 042131 (2017).
[7] T. Antal, M. Droz, and Z. Rácz, J. Phys. A: Math. Gen. **37**, 1465 (2004).
[8] C. M. Rohwer, A. Squarcini, O. Vasilyev, S. Dietrich, and M. Gross, Phys. Rev. E **99**, 062103 (2019).
[9] M. Gross, O. Vasilyev, A. Gambassi, and S. Dietrich, Phys. Rev. E **94**, 022103 (2016).
[10] M. Gross, A. Gambassi, and S. Dietrich, Phys. Rev. E **96**, 022135 (2017).
[11] A. A. Balandin, R. K. Lake, and T. T. Salguero, Appl. Phys. Lett. **121**, 040401 (2022).
[12] M. A. Stolyarov, G. Liu, M. A. Bloodgood, E. Aytan, C. Jiang, R. Samnakay, T. T. Salguero, D. L. Nika, S. L. Rumyantsev, M. S. Shur *et al.*, Nanoscale **8**, 15774 (2016).
[13] A. A. Balandin, F. Kargar, T. T. Salguero, and R. K. Lake, Mater. Today **55**, 74 (2022).
[14] C. M. Morris, R. V. Aguilar, A. Ghosh, S. M. Koohpayeh, J. Krizan, R. J. Cava, O. Tchernyshyov, T. M. McQueen, and N. P. Armitage, Phys. Rev. Lett. **112**, 137403 (2014).
[15] C. M. Morris, N. Desai, J. Viirok, D. Huvonen, U. Nagel, T. Room, J. W. Krizan, R. J. Cava, T. M. McQueen, S. M. Koohpayeh *et al.*, Nat. Phys. **17**, 832 (2021).
[16] J. Steinberg, N. P. Armitage, F. H. L. Essler, and S. Sachdev, Phys. Rev. B **99**, 035156 (2019).
[17] Y. Xu, L. S. Wang, Y. Y. Huang, J. M. Ni, C. C. Zhao, Y. F. Dai, B. Y. Pan, X. C. Hong, P. Chauhan, S. M. Koohpayeh, N. P. Armitage, and S. Y. Li, Phys. Rev. X **12**, 021020 (2022).
[18] J. Rudnick, R. Zandi, A. Shackell, and D. Abraham, Phys. Rev. E **82**, 041118 (2010).
[19] D. M. Dantchev and S. Dietrich, arXiv:2203.15050.
[20] M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Functions: With Formulas, Graphs, and Mathematical Tables* (Dover, New York, 1970).
[21] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevE.106.L042103 for more details of the derivation of the exact results for the partition functions under antiperiodic and Dirichlet boundary conditions.
[22] M. Lemoine, J. Martin, and P. Peter, *Inflationary Cosmology*, Lecture Notes in Physics (Springer, Berlin, 2008).