Frustrated Ising model with competing interactions on a square lattice

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(Received 27 April 2023; revised 1 November 2023; accepted 25 January 2024; published 26 February 2024)

The Ising model with nearest-neighbor and next-nearest-neighbor interactions of the coupling constants J_1 and J_2, respectively, is investigated on a square lattice. For $J_1 = 2$ and $J_2 = 1$, the model becomes frustrated because ground states are infinitely degenerate. We obtain the density of states by using the Wang-Landau Monte Carlo method and calculate the specific heat. We find two separate peaks in the specific heat: a sharp peak related to the critical behavior and a round peak related to the specific heat of a disordered system such as spin glass. As the system size increases, the sharp-peak temperature decreases towards zero, and the maximum height of the sharp peak increases logarithmically, supporting that the spatial correlation length diverges exponentially at zero temperature. The partition-function zeros calculated by the density of states also suggest the zero-temperature phase transition.

DOI: 10.1103/PhysRevB.109.064422

I. INTRODUCTION

In the absence of an external magnetic field, the Ising model with nearest-neighbor (NN) interactions on a square lattice was exactly solved by Onsager [1]. The understanding of phase transitions and critical phenomena has been mainly developed since the Onsager's exact solution. However, this problem becomes unresolved when the next-nearest-neighbor (NNN) interactions are added. The lack of an exact solution has given rise to the challenge of various methods [2–20].

The Hamiltonian of the Ising model with both NN and NNN interactions is

$$\mathcal{H} = J_1 \sum_{\langle i,j\rangle} \sigma_i\sigma_j + J_2 \sum_{\langle i,k\rangle} \sigma_i\sigma_k, \tag{1}$$

where J_1 (J_2) are the coupling constants of NN (NNN) interactions, the sum is over all NN (NNN) pairs, and $\sigma_i = \pm 1$. The coupling ratio is defined as $R \equiv J_2/J_1$. The sign of J_2 produces a very different aspect. For $J_2 < 0$ this model is similar to the typical Ising model, only with NN interaction, and has the well-known ferromagnetic (FM) ground states for $J_1 < 0$ and antiferromagnetic (AF) ground states for $J_1 > 0$ at zero temperature.

Interestingly, two phase transitions exist for $J_2 > 0$. One is transition between paramagnetic (P) and FM phases ($J_1 < 0$) or between P and AF [Fig. 1(a)] phases ($J_1 > 0$) for $|R| < 1/2$. The other is transition between P and superantiferromagnetic (SAF) [Fig. 1(b)] phases for $|R| > 1/2$, where the nonuniversal critical behavior appears, i.e., critical exponents vary continuously depending on R values. Although lots of studies have been conducted on the phase transition for $|R| > 1/2$, the debate on the order of transition remains controversial. Some studies [21–29] have argued for a second-order transition, while others [30–40] have supported the occurrence of a first-order transition in the range $1/2 < |R| < R_c$, where $0.53 \leqslant R_c \leqslant 1.144$. Because this model shows the same critical phenomena regardless of the sign of J_1, only the case $R > 0$ ($J_1 > 0$ and $J_2 > 0$) is covered in this work.

The ratio $R = 1/2$ has been of special interest because the ground states are highly degenerate, i.e., the energies of AF and SAF ground states are the same. The number of ground states for $R = 1/2$ is infinite [Fig. 2] [35,41], in some sense similar to disordered systems [42] such as spin glass [43]. For $R = 1/2$, some studies have claimed the critical temperature T_c is suppressed to zero in the thermodynamic limit [5,8,23,28,29,31,35,40,44,45]. There have also been simulation studies claiming a finite critical temperature, $T_c > 0$ [46,47]. Studies of partition-function zeros [41] and effective field theory [48] have proposed a first-order phase transition. It has been suggested that the system behaves as the one-dimensional Ising model [30,31,44] whose specific heat is a finite peak and the well-known Schottky anomaly [49–53]. Landau [23] and Kim [28] argued that the correlation length diverges exponentially at zero temperature. As such, quite a lot has been revealed for $R = 1/2$, but the results are still not accurate enough to adequately describe the critical behavior of this system.

In this paper we obtain the density of states via the Wang-Landau (WL) Monte Carlo algorithm [54,55] with high precision, which makes it possible to calculate various physical quantities at any temperature. Exact enumeration provides the exact density of states [41] but requires enormous computational time, making it unsuitable to investigate the properties of the specific heat for $R = 1/2$ on a large finite lattice. By using the obtained density of states, we calculate the specific heat and the partition-function zeros [13,27,28,41,56], which lead us to definite conclusions.

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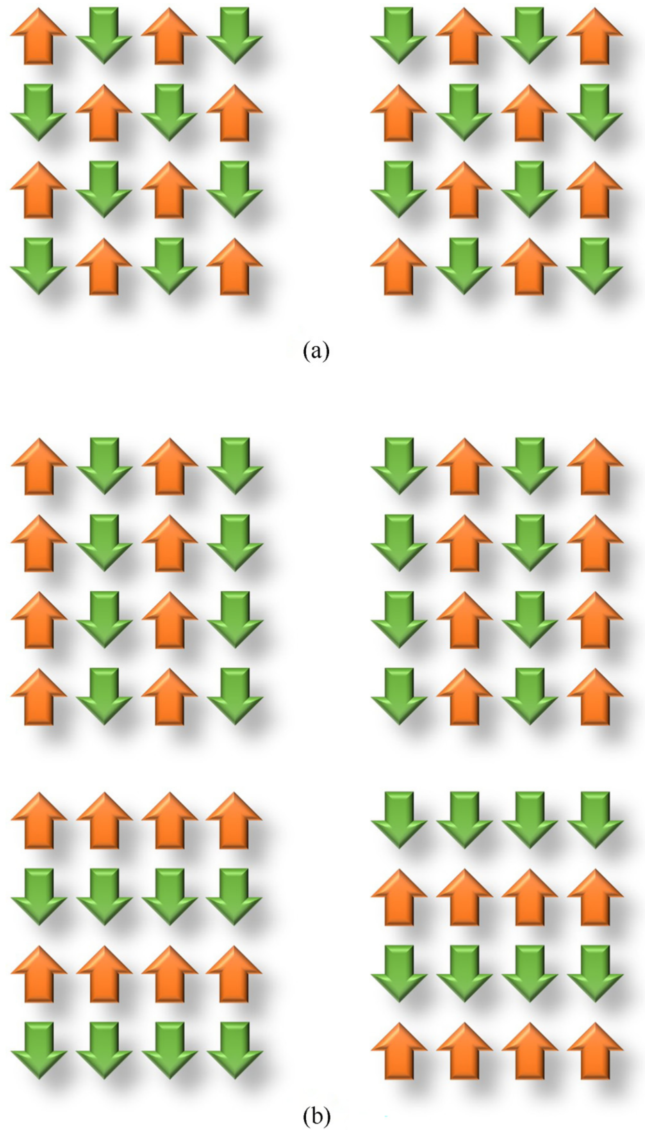

FIG. 1. The ground states of the Ising model with nearest-neighbor and next-nearest-neighbor interactions on a 4×4 square lattice for (a) antiferromagnetic phase ($R < 1/2$) and (b) superantiferromagnetic phase ($R > 1/2$). For $R = 1/2$ this model becomes frustrated because both ground states have the same energy.

II. WAND-LANDAU ALGORITHM

If we define a given energy

$$E \equiv \sum_{\langle i,j \rangle} \sigma_i \sigma_j + \frac{J_2}{J_1} \sum_{\langle i,k \rangle} \sigma_i \sigma_k, \quad (2)$$

the partition function reads

$$Z = \sum_{\{\sigma_n\}} e^{-\mathcal{H}/k_BT} = \sum_{\{\sigma_n\}} e^{-J_1E/k_BT} = \sum_E g(E) e^{-J_1E/k_BT}, \quad (3)$$

where $\{\sigma_n\}$ denotes a sum over all possible configurations, k_B is the Boltzmann constant, T is the temperature, and $g(E)$ is the density of states.

To obtain $g(E)$, the WL method is performed as follows. Initially $g(E) = 1$ and energy histogram $h(E) = 0$ are set for all possible energy states. A spin is placed to each site of $L \times L$ square lattices with periodic boundary conditions, having a value of either $+1$ or -1 at random. The total energy E_i for the current state is calculated first, then E_f is computed after flipping the spin of a randomly selected site. The flipping trial is accepted with the probability

$$p(E_i \to E_f) = \min\left[\frac{g(E_i)}{g(E_f)}, 1\right]. \quad (4)$$

If accepted, the spin is flipped and $E_f \to \tilde{E}$, otherwise the change is rejected and $E_i \to \tilde{E}$: $g(\tilde{E}) \to g(\tilde{E}) \times f_n$ and $h(\tilde{E}) \to h(\tilde{E}) + 1$, where $\tilde{E}$ is the energy value determined after one trial and f_n is a modification factor after the nth satisfaction of the flatness. When the histogram becomes *flat*, $h_{\min}(E) \geqslant 0.99\overline{h}$, all $h(E)$ are reset and the modification factor reduces as $f_{n+1} = f_n^{1/2}$, where $\overline{h}$ is the average histogram of all energy states. In this work the histogram flatness is checked every 10^5 Monte Carlo sweeps. The initial and final modification factors are $f_0 = e \approx 2.718\,28$ and $f_{\text{final}} \approx \exp(10^{-9})$ corresponding to $n = 30$, respectively.

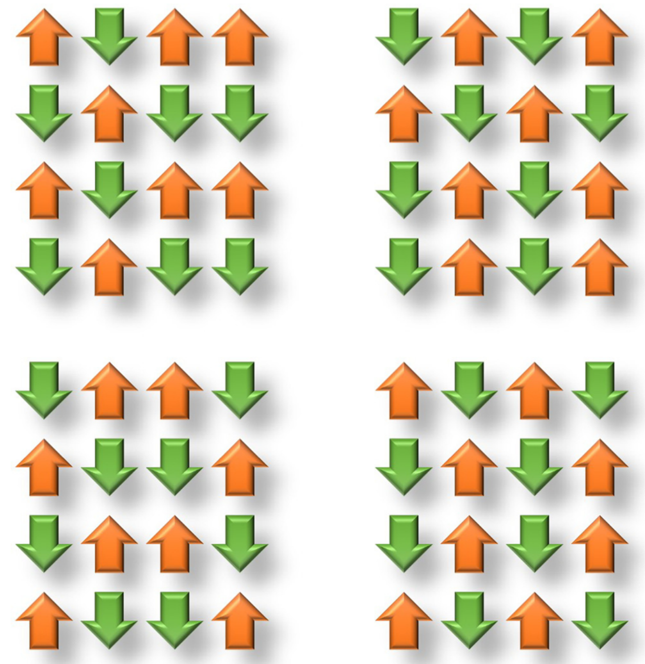

FIG. 2. Several examples of ground states for $R = 1/2$ on a 4×4 square lattice.

III. SPECIFIC HEAT

The internal energy of the system is given as a function of temperature,

$$\langle E^m \rangle_T = \frac{\sum_E E^m g(E) e^{-E/k_BT}}{\sum_E g(E) e^{-E/k_BT}}, \quad (5)$$

where $g(E)$ is the density of states that was sampled by using the WL Monte Carlo simulations and m is a natural number. Figure 3 shows the data for $\langle E \rangle_T / L^2$ that increases monotonically with T. The temperature of the maximum slope decreases gradually as the system size increases, and we

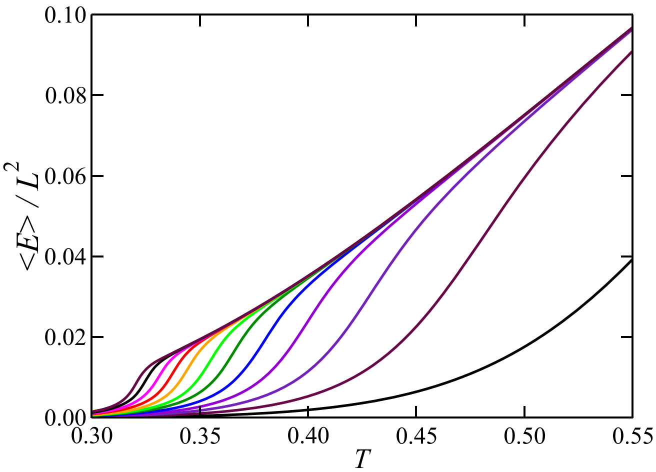

FIG. 3. The internal energies per site on systems of sizes for $L = 10, 20, \ldots, 120$ from right to left.

TABLE I. Peak values and temperature of the round peaks for $L = 40, 50, \ldots, 120$.

L	C_{peak}	Temperature
40	0.437	0.530
50	0.436	0.540
60	0.435	0.542
70	0.436	0.541
80	0.435	0.542
90	0.436	0.542
100	0.436	0.543
110	0.435	0.542
120	0.436	0.541

assume such a temperature to be the critical temperature T^* for a finite system.

In order to estimate the critical temperature accurately, we calculate the specific heat as a function of T using the definition

$$C(T) = \frac{\langle E^2\rangle_T - \langle E\rangle_T^2}{L^2T^2}. \tag{6}$$

Figure 4(a) shows the specific heat for various system sizes. Data for larger systems show double peaks: one sharper at a low temperature and the other round at a higher temperature.

The round peak is observed near $T = 0.5$ irrespective of the size of system for $L \geqslant 50$, as shown in Fig. 4(b). The round-peak value (Table I) does not diverge even in the limit of $L \to \infty$. It has been suggested that such a peak is the main peak of the specific heat [23,30,31,44], and it is similar to the specific heat of the one-dimensional Ising model [30,31,44], which corresponds to the well-known Schottky anomaly [49–53]: $C(T) \sim T^{-2}\exp(-b/T)$. In the case of previous studies or smaller systems, the round peak and sharp peak may be mixed, and the resulting critical temperature might be measured inaccurately. Excluding the data for small sizes, we try to fit this round peak to the following equation:

$$C(T) = \frac{c_1}{T^{c_2}} e^{-c_3/T}, \tag{7}$$

with fitting coefficients $c_1 = 2.100(22)$, $c_2 = 4.062(26)$, and $c_3 = 2.201(14)$ [shown in Fig. 4(b)]. The value of $c_2 \approx 4$ is distinctly different from $c_2 = 2$ for the one-dimensional Ising model. Our result for the round peak is rather similar to the specific heat of a disordered system such as spin glass [43], whose ground states are infinitely degenerate.

For the sharp-peak temperature T^* decreasing as the size of system increases, we plot $\ln T^*$ as a function of $\ln(1/L)$ in Fig. 5(a), in which the data are represented by a curved line. This suggests that $T^*(L)$ for a finite-size system may not follow the well-known power-law behavior $T^* \sim L^{-1/\nu}$ [35], where ν is the correlation-length critical exponent, which is typical for continuous phase transitions. Instead, we plot T^* against $1/(\ln L + c)$ in Fig. 5(b), where c is a constant. It shows that T^* approaches 0 as the system size L increases, implying that $T_c = 0$. This critical behavior fits well with an assumption $\xi \sim \exp(c'/T)$ [23,28], where ξ is the spatial correlation length and c' is a constant.

The peak value of the specific heat $C_{\max}$ increases slowly with the system size, as shown in Fig. 4(a). For $T_c = 0$ and $L \sim \exp(c'/T)$, the typical relation $C_{\max} \sim (T - T_c)^{-\alpha}$

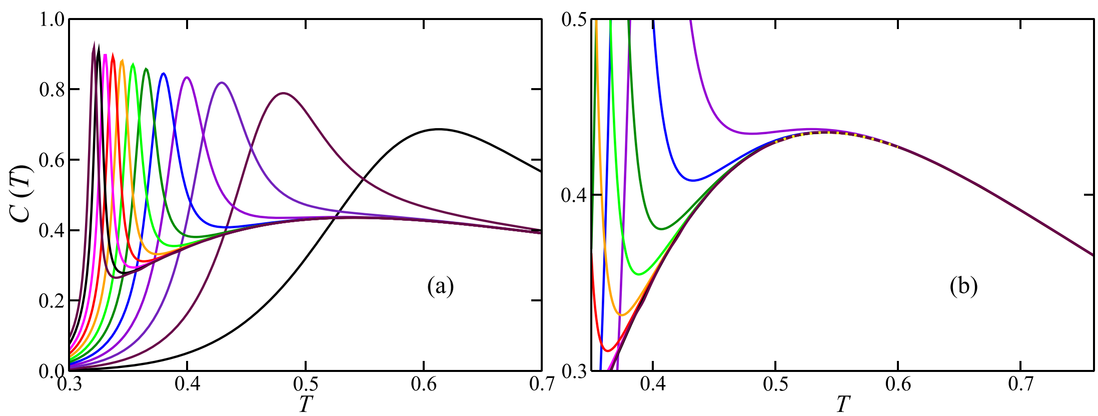

FIG. 4. (a) The specific heat per site for $L = 10, 20, \ldots, 120$ from right to left. The peak temperature T^* gradually decreases as the system size increases. (b) Same plot as (a) for $L = 40, 50, \ldots, 120$ with ranges adjusted to highlight the round peak on the right in (a), where all peaks almost overlap. The dotted line corresponds to the fitting curves of Eq. (7).

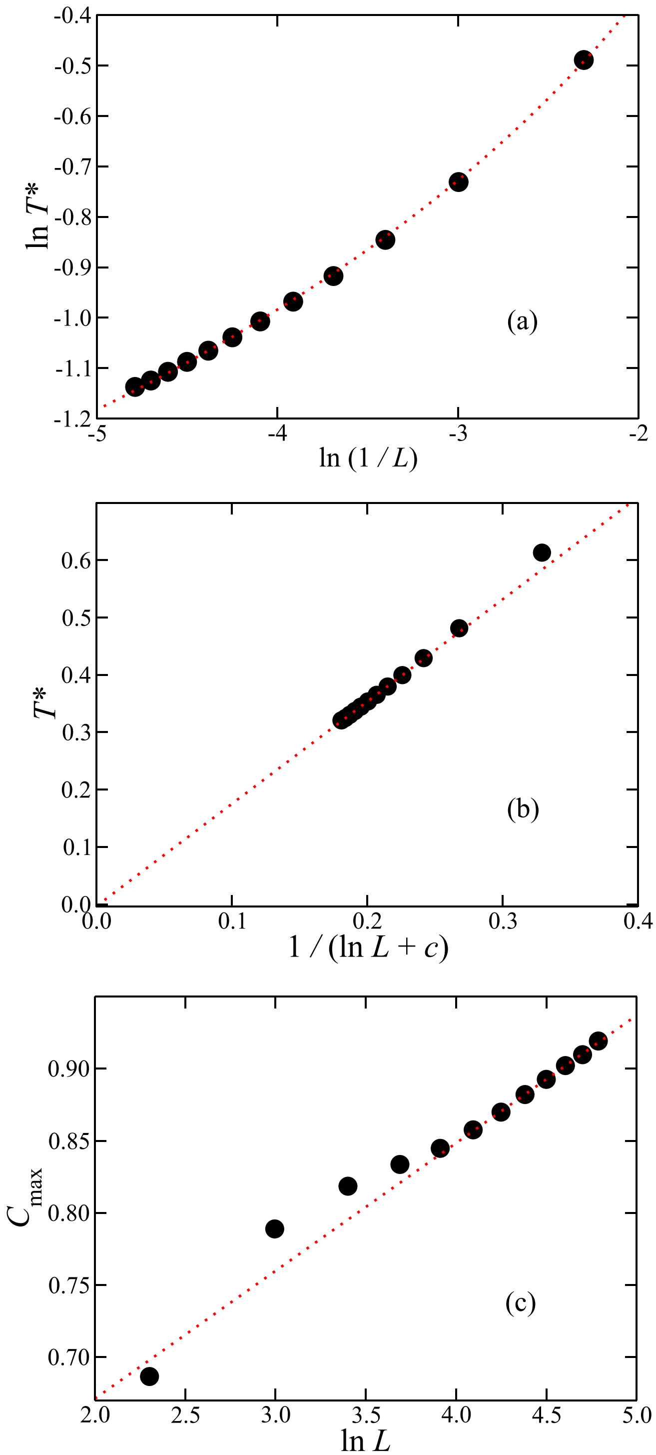

FIG. 5. (a) The log-log plot of the sharp-peak temperature T^* as a function of $1/L$. (b) The peak temperature T^* as a function of $1/(\ln L + c)$ with $c = 0.736$, indicating $T^* \to 0$ in the thermodynamic limit. (c) The peak value of the specific heat, $C_{\max}$, as a function of $\ln L$.

becomes $C_{\max} \sim T^{-\alpha} \sim (\ln L)^{\alpha}$. Figure 5(c) shows that $C_{\max}$ increases logarithmically as L increases with $\alpha = 1$. $C_{\max}(L)$ typically diverges as L^d in the first-order transition [57,58]. However, our logarithmic divergences of the specific heat seem to be too weak to support the first-order transition [59]. A similar case using a power-law fit to the specific heat appears in the study of the antiferromagnetic Ising model for triangular lattices at $T_c = 0$ [60].

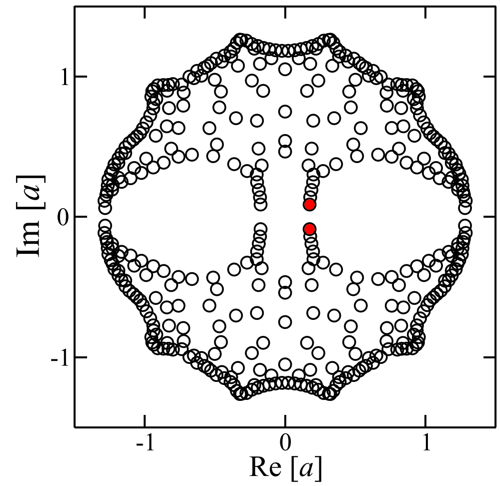

FIG. 6. Distribution of the partition-function zeros in the complex $a = \exp(-J_1/k_BT)$ plane for $R = 1/2$ on 10×10 square lattices. The points closest to the positive real axis (marked as dot) are the first zeros.

To check the possibility of the Berezinskii-Kosterlitz-Thouless (BKT) transition [61], we fit the data of $T^*(L)$ to a formula $T^*(L) = b_1(\ln L + b_2)^{-b_3}$, and then obtain $b_1 = 0.974(17)$, $b_2 = -0.465(30)$, and $b_3 = 0.7608(84)$. If it is a BKT-type transition, b_3 should be 2 with $T^*(L) \sim 1/(\ln L)^2$ for $T_c = 0$. Actually, our data are better fit with $T^*(L) \sim 1/(\ln L + c)$, as shown in Fig. 5(b). Furthermore, the logarithmic divergences of the specific heat [Fig. 5(c)] are inconsistent with the BKT transition.

IV. PARTITION-FUNCTION ZEROS

In the previous section we observed that the Ising model with NN and NNN interactions for $R = 1/2$ undergoes the zero-temperature phase transition. In order to support our observation, we calculated the partition-function zeros and associated critical exponents. The partition function in Eq. (3) can be written as

$$Z = \sum_E g(E) a^E, \tag{8}$$

where $a \equiv \exp(-J_1/k_BT)$. Let the partition-function zeros, i.e., the solutions of the equation $Z = 0$, be a_i. Then, the partition function can be written as the $E_{\max}$-th order polynomial of a,

$$Z = A \prod_{i=1}^{E_{\max}} (a - a_i) = 0, \tag{9}$$

where A is a constant and $E_{\max}$ is the maximum energy.

The partition-function zeros a_i can be calculated with the MATHEMATICA package. Figure 6 shows the partition-function zeros in the complex temperature plane; all data points lie symmetrically with respect to the real axis because of the pairs of complex conjugates. Among them, the zeros closest to the positive real axis are the first zeros a_1. The first zeros will approach the positive real axis as L increases and reach

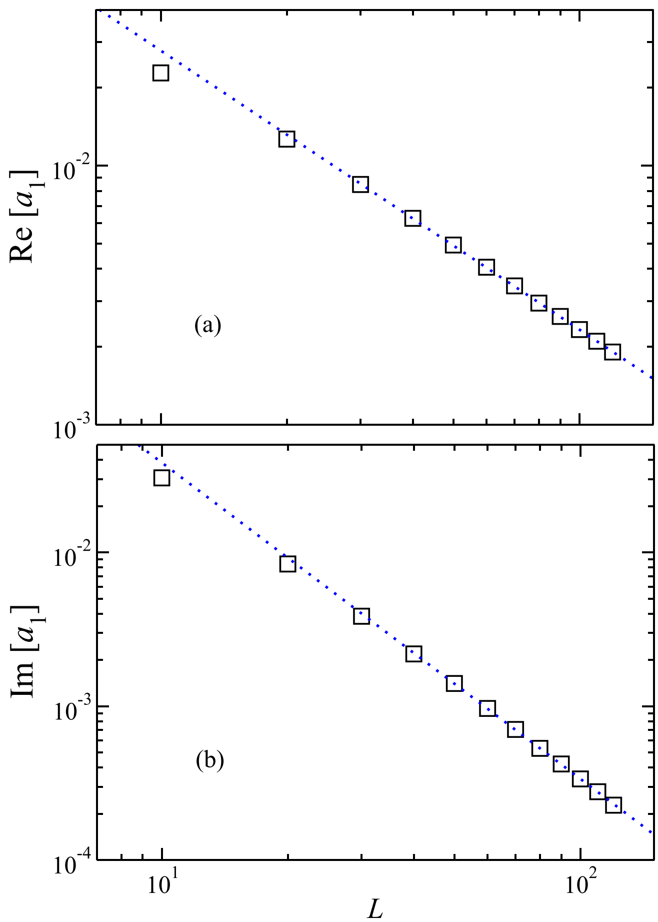

FIG. 7. (a) Double-logarithmic plot of the real part of the first zero Re$[a_1]$ as a function of L. The power-law fit of the dashed line yields $\lambda = 1.0761(65)$. (b) Double-logarithmic plot of the imaginary part of the first zero Im$[a_1]$ as a function of L. The power-law fit along the dashed line gives $y_t = 2.056(19)$.

the value that corresponds to the critical temperature in the thermodynamic limit of $L \to \infty$ if the system shows a phase transition. With the data for finite-size systems, we can estimate the value of the critical point, $a_c = \exp(-J_1/k_B T_c)$, by using the finite-size scaling of the real parts of the first zeros [62],

$$\mathrm{Re}[a_1(L)] - a_c \sim L^{-\lambda}, \tag{10}$$

where λ is the shift exponent [41,63,64]. For given L, we can estimate $T_1(L) = -J_1/k_B \ln a_1(L)$. We confirm that $T_1(L)$ is almost the same with $T^*(L)$ obtained from the sharp-peak of the specific heat within the error bars. Therefore the finite-size scaling analysis of the first zeros supports our earlier analysis for the specific heat. We obtain the power-law decrease of Re$[a_1(L)]$ with $\lambda = 1.0761(65)$ [41] and $a_c = -0.000\,014(9)$, as shown in Fig. 7(a). Because a_c is very small, T_c becomes almost zero.

On the other hand, the imaginary parts of the first zeros follow the finite-size scaling [13],

$$\mathrm{Im}[a_1(L)] \sim L^{-y_t}, \tag{11}$$

where y_t is the thermal scaling exponent. y_t is associated with ν via $y_t = 1/\nu$. From the power-law plot in Fig. 7(b), $y_t = 2.056(19)$ is obtained. It is generally known that $y_t = d$ is a signal for the first-order transition [41,65], which is only valid for the case of nonzero temperature. Using the Taylor expansion, one can expand

$$e^{-1/T} - e^{-1/T_c} = \frac{T - T_c}{T T_c} + \text{higher-order terms.} \tag{12}$$

The left term is proportional to $T - T_c$ for nonzero T_c, but it becomes $\exp(-1/T)$ for $T_c = 0$. Therefore, if the correlation length ξ diverges exponentially $\xi \sim \exp(c'/T)$, y_t controls only the coefficient c'.

V. SUMMARY

We have studied the Ising model with nearest-neighbor and next-nearest-neighbor interactions for the particular case of $R = J_2/J_1 = 1/2$ whose ground states are infinitely degenerate. We calculated the density of states on systems of various sizes by using the WL Monte Carlo algorithm. The internal energy and specific heat were calculated using the density of states, and the critical temperature and critical exponent were estimated from the peak values of the specific heat. The critical temperature for finite systems showed the logarithmic convergence toward $T = 0$ as the size of system increases, and the peak values of the specific heat increased following the logarithmic divergence of the size of the system. We also found the round peak whose height and temperature do not depend on the system sizes. Our result suggests that the second round peak is similar to the specific heat of a disordered system such as spin glass whose ground states are infinitely degenerate.

As an alternative method, we calculated the partition-function zeros and associated critical exponents. The real and imaginary parts of the first zeros of the partition function follow the power-law behaviors. The critical temperature $T_c = 0$ and the thermal scaling exponent $y_t \approx 2$ were extracted from the fits. Therefore our data for the specific heat calculated from the internal energy and those from the partition-function zeros consistently suggested that the Ising model with NN and NNN interactions exhibits the zero-temperature phase transition with the logarithmic divergence of the specific heat for the coupling constant $R = 1/2$.

ACKNOWLEDGMENT

This research was supported by the National Research Foundation of Korea through Grants No. NRF-2017R1D1A3B06035840, No. NRF-2020R1A2C1003971, and No. NRF-2021R1A6A1A03043957.

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