Boundary conditions and variable ground state entropy for the antiferromagnetic Ising model on a triangular lattice

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The ground state entropy density of the antiferromagnetic Ising model on a triangular lattice is considered in the infinite volume limit as a function of boundary conditions on a finite triangular domain. The ground states of this domain do not map to a dimer covering and so cannot be classified into string sectors. A parametrized boundary condition is identified that allows the entropy density to be tuned to values between nondegeneracy and maximal degeneracy. The results are compared to those for a rectangular periodic domain for which the ground states can be classified into string sectors.

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I. INTRODUCTION

Frustrated systems are of considerable interest, in part because of their lack of order at zero temperature [1–3]. They possess a highly degenerate ground state and the entropy density of the bulk system does not vanish as the temperature approaches zero. Geometric frustration has recently been applied in diverse areas such as coding theory, spin glasses, superconducting networks, quantum dynamics, high-density chip design, protein folding, and neural computation [3–7], and is increasingly being recognized as an organizing principle in a wide variety of physical systems. We describe here a parametrized boundary condition for an archetypical frustrated system, the classical antiferromagnetic Ising model on a triangular lattice (AIT), that allows the ground state entropy to be varied.

The entropy density at $T=0$ in the thermodynamic (infinite volume) limit S_0 is defined by [8]

$$S_0 = \lim_{T\to 0}\ \lim_{V\to\infty} S(V,T), \tag{1}$$

where $S(V,T)$ denotes the entropy density for the system at volume V and temperature T. Implicit in Eq. (1) is some boundary condition, and we denote by $V(B)$ the volume of the domain with regular (as $V\to\infty$) boundary condition B. The thermodynamic limit $S(T)=\lim_{V\to\infty}S(V,T)$ is known to exist and to be independent of the boundary conditions for $T>0$ [8,9]. However, convergence at $T=0$ is unclear and the order of the limits in Eq. (1) is important [8,9]. For example, the AIT has a finite ground state entropy density in the thermodynamic limit, despite the fact that boundary conditions can be chosen for a finite system such that it is nondegenerate at $T=0$ [10], implying zero entropy density in the thermodynamic limit. An incorrect result is therefore obtained by reversing the order of the limits in Eq. (1). However, there are some advantages to calculating the zero-temperature entropy based on finite-volume ensembles as a means of studying infinite systems. Aizenman and Lieb [8] showed that the order of the limits in Eq. (1) can be reversed and the correct value for S_0 obtained if it is calculated as

$$S_0 = \max_B \left\{ \lim_{V\to\infty} \left\{ \lim_{T\to 0} S(V(B),T) \right\} \right\}, \tag{2}$$

i.e., by considering boundary conditions *that give maximal degeneracy*.

We have shown previously that the finite AIT on a parallelogram domain with free boundary spins is nondegenerate and that finite size scaling calculations indicate that a triangular domain with free boundary spins is maximally degenerate [10]. We identify in this paper boundary conditions on a triangular domain that give variable degeneracy.

II. ENTROPY DENSITY AS A FUNCTION OF BOUNDARY CONDITIONS

The AIT with nearest neighbor interactions is fully frustrated, leading to ground state configurations whose number grows as $O(e^N)$ for N spins, and to a finite entropy density at $T=0$. Wannier [11] and Houtappel [12] computed the ground state entropy density as $\sim 0.3231R$ (note that the numerical value given in Ref. [11] is incorrect). We define the normalized entropy density at absolute zero for a finite system of N spins with boundary conditions $B, S_0(N,B)$, by

$$S_0(N,B) = \frac{\ln W(N,B)}{0.3231N}, \tag{3}$$

where $W(N,B)$ is the number of ground state configurations, so that

$$\max_B \left[\lim_{N\to\infty} S_0(N,B) \right] = 1. \tag{4}$$

We address in this paper the thermodynamic limit for *particular* boundary conditions, i.e., the nature of

$$S_0(B) = \lim_{N\to\infty} S_0(N,B). \tag{5}$$

For the AIT it is known that boundary conditions exist such that $S_0(B)=0$ (the nondegenerate case) [10], and boundary conditions must exist such that $S_0(B)=1$. However, do

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boundary conditions exist such that $S_0(B)=\gamma$ for any $0<\gamma<1$? This question has been answered in the affirmative by Dhar *et al.* [13] as follows. For a finite system on a rectangular domain with periodic boundary conditions, the ground states of the AIT can be mapped to dimer coverings on the dual (hexagonal) lattice [14]. Superposing the dimers of a particular ground state configuration with the dimers of the *standard configuration* (alternate rows of up and down spins) gives contiguous *strings* of dimers for that ground state. The ground states are classified into *string sectors*, each sector being specified by the number of strings. The normalized entropy density, denoted by $\alpha(p)$, in a sector with string density (number of strings divided by the number of sites in a row) p is given by [13]

$$S_0(\mathrm{RP}(p)) = \alpha(p) = \frac{1}{0.3231}\left(p \ln 2 + \frac{2}{\pi}\int_0^{\pi p/2} \ln[\cos(x)]dx\right), \tag{6}$$

where $\mathrm{RP}(p)$ denotes a rectangular periodic boundary condition with string density p. The function $\alpha(p)$ is zero for $p=0$ and $p=1$, and peaks at unity (maximal degeneracy) for $p=2/3$. The sectors therefore represent manifolds of ground states that have different degeneracies, the degeneracy being parametrized by the string density. Strings intersect the two opposite edges of the boundary of the domain between each pair of adjacent opposite spins. For a ground state configuration the strings are constrained to occur in pairs that are tightly packed (pass through adjacent sites of the dual lattice). Therefore, for regular boundary conditions in which the spins on one boundary edge are fixed such that adjacent spins are identical or triples of sites contain opposite adjacent spins, the string density, and thus the entropy density, can be calculated.

Not all boundary conditions allow a dimer covering, however [14]. The dimer covering as described above results from each elementary triangle for a ground state having only one unfavorable edge (an edge joining like spins). For the triangular domain, however, referring to Fig. 1(a) shows that a ground state requires only that the elementary triangles labeled "a" in the figure have one unfavorable edge. An example of a ground state configuration in which one of the other triangles has three unfavorable edges is shown in Fig. 1(b). The ground states therefore do not admit a dimer covering and this domain presents a distinct case that cannot be analyzed within the analytical framework of strings.

Consider a triangular domain on which the spins are fixed to be identical on one edge and free on the other two edges [Fig. 1(a)], which we denote by T1I. It is easy to show that this system is nondegenerate. The lattice is decomposed into individual triangles [labeled "a" in Fig. 1(a)], and the minimum energy corresponds to only one unfavorable edge for each triangle. The bottom row of "a" triangles must therefore have favorable edges on their other two sides, and so the next row of sites has identical spins that are opposite to the spins in the bottom row. Continuing in this manner shows that the configuration in Fig. 1(a) is the only minimum energy configuration and the system is nondegenerate, i.e.,

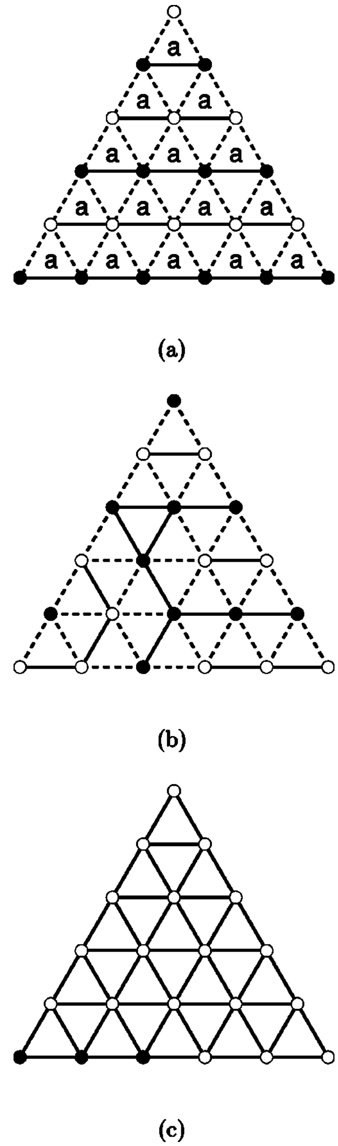

FIG. 1. (a) The minimum energy configuration for the boundary condition T1I. Filled and open circles denote up and down spins, respectively, and favorable and unfavorable interactions are denoted by broken and solid lines, respectively. (b) A ground state configuration that has an elementary triangle with three unfavorable edges. (c) The boundary condition T1I(0.5), where fixed identical spins are shown as filled circles and free spins by open circles.

$$S_0(\mathrm{T1I}) = 0. \tag{7}$$

For free boundary conditions, denoted by TF, the normalized entropy density $S_0(N,\mathrm{TF})$ was calculated by exact enumeration of the number of ground states on domains of size up to $N=325$, and is plotted vs N as the top curve in Fig. 2(a). We used an algorithm [15] that allows exact enumeration up to size $N\sim 300$ for certain boundary conditions, which corresponds to $\sim 10^{50}$ states. By standard finite size scaling arguments,

$$S_0(N,B) \approx S_0(B) + bN^{-1/2}, \quad N\to\infty, \tag{8}$$

for some constant b (which depends on B), which allows $S_0(B)$ to be estimated from the numerical data $S_0(N,B)$. The

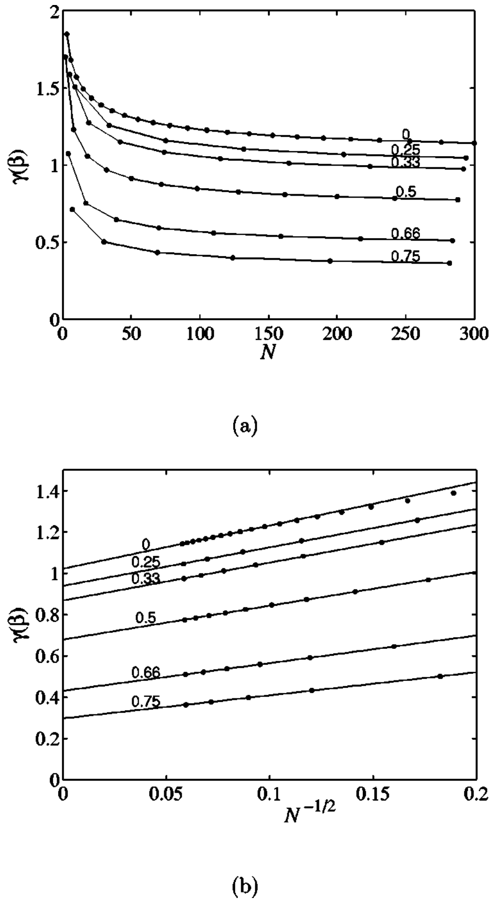

FIG. 2. Normalized entropy density $S_0(N,\mathrm{T1I}(\beta))=\gamma(\beta)$ (a) vs N and (b) vs $N^{-1/2}$ for the values of β as shown. The linear fits are shown in (b). The top curves are for $S_0(N,\mathrm{TF})$.

entropy density $S_0(N,\mathrm{TF})$ is plotted versus $N^{-1/2}$ as the top curve in Fig. 2(b) for the larger values of N, and is seen to be approximately linear for large N (the left portion of the plot). The value of $S_0(\mathrm{TF})$ was estimated by fitting a straight line for $N \geqslant 100$, and the number of data points used is denoted by N_d and the relative rms error in the fit by e. This gives $S_0(\mathrm{TF}) \approx 1.02$ with $N_d=12$ and $e=0.04\%$, providing good evidence that the free boundary case is maximally degenerate, i.e.,

$$S_0(\mathrm{TF}) = 1. \tag{9}$$

TABLE I. Estimated entropy densities $\hat{S}_0(\mathrm{T1I}(\beta))$ for various values of β.

β	$\hat{S}_0(\mathrm{T1I}(\beta))$	N_d	e
0	1.02	12	0.0004
0.25	0.94	5	0.0018
0.33···	0.87	6	0.0011
0.5	0.68	9	0.0010
0.66···	0.43	6	0.0006
0.75	0.30	5	0.0007
1	0		

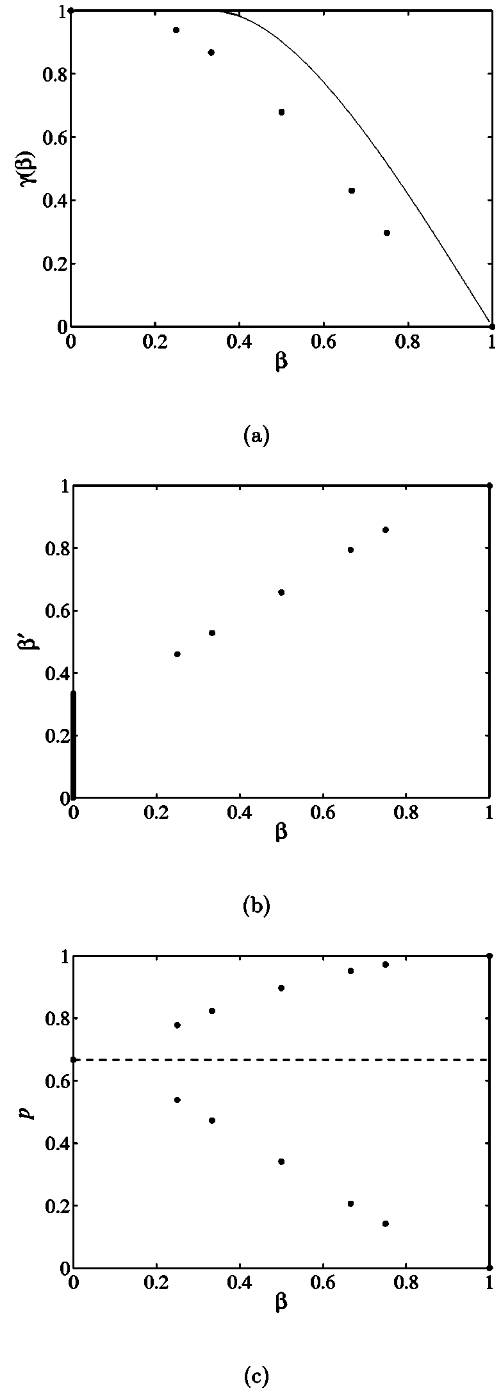

FIG. 3. (a) Normalized entropy density $\gamma(\beta)=S_0(\mathrm{T1I}(\beta))$ vs β (•). The curve shows $S_0(\mathrm{RP1I}(\beta))$. (b) The relationship between β and β' such that $S_0(\mathrm{T1I}(\beta))=S_0(\mathrm{RP1I}(\beta'))$, and (c) the relationship between p and β such that $S_0(\mathrm{T1I}(\beta))=S_0(\mathrm{RP}(p))$.

III. A BOUNDARY CONDITION GIVING VARIABLE DEGENERACY

Since the case T1I is nondegenerate and the case TF is maximally degenerate, we investigate the case, denoted $\mathrm{T1I}(\beta)$, for which βn of contiguous spins on one edge are fixed to identical values and the remaining boundary spins are free, where β is a constant and $0 \leqslant \beta \leqslant 1$ [Fig. 1(c)]. The number of free sites is now $N-\beta n$, which we simply refer to as N since no confusion should arise. The normalized entropy density $S_0(N,\mathrm{T1I}(\beta))$ was calculated for different values of β as above and the results are plotted vs the number of free sites in Fig. 2(a). Inspection of the figure shows that the normalized entropy density for $N\to\infty$ is a decreasing function of β, i.e.,

$$S_0(\mathrm{T1I}(\beta)) = \gamma(\beta), \tag{10}$$

where $\gamma(0)=1$ and $\gamma(1)=0$. Plots of the entropy density versus $N^{-1/2}$ are shown in Fig. 2(b), and values of $\gamma(\beta)$ were estimated (for $N>25$) and are listed in Table I and plotted in Fig. 3(a). Intermediate degeneracy can therefore be obtained on a triangular domain as it can on a rectangular periodic domain. The entropy density for the two domains can be compared by considering both a rectangular domain with boundary condition analogous to $\mathrm{T1I}(\beta)$, and a rectangular periodic domain parametrized by the string density.

Consider first a rectangular periodic domain for which a fraction β of contiguous spins are fixed and the remainder are free on one edge, denoted by $\mathrm{RP1I}(\beta)$, i.e., analogous to the boundary condition $\mathrm{T1I}(\beta)$ for the triangular domain. Since strings intersect the boundary between opposite spins, for the boundary condition $\mathrm{RP1I}(\beta)$ the string density can take any value on the interval $(0,\ 1-\beta)$. Since $\alpha(p)$ is an increasing function of p for $0\leqslant p<2/3$, for $1/3<\beta<1$ the number of states is dominated by that at $p=1-\beta$. For $\beta<1/3$ the sector $p=2/3$ dominates. The normalized entropy density $S_0(\mathrm{RP1I}(\beta))$ is therefore given by

$$\begin{aligned} S_0(\mathrm{RP1I}(\beta)) &= 1, \quad 0\leqslant\beta\leqslant 1/3 \\ &= \alpha(1-\beta), \quad 1/3\leqslant\beta\leqslant 1, \end{aligned} \tag{11}$$

which is shown by the curve in Fig. 3(a). Note the similiar behavior of $S_0(\mathrm{T1I}(\beta))$ and $S_0(\mathrm{RP1I}(\beta))$, although $S_0(\mathrm{T1I}(\beta))$ is strictly less than $S_0(\mathrm{RP1I}(\beta))$. The relationship between β and β' such that $S_0(\mathrm{T1I}(\beta))=S_0(\mathrm{RP1I}(\beta'))$ is plotted in Fig. 3(b). Note that this relationship is multivalued at $\beta=0$ where $\beta'\in(0,1/3)$.

Consider now the rectangular periodic domain in particular string sectors parametrized by the string density p. The relationship between β and p such that $S_0(\mathrm{T1I}(\beta))=S_0(\mathrm{RP}(p))$ is plotted in Fig. 3(c). This relationship is two-valued (except at $\beta=0$), i.e., two distinct boundary conditions on the rectangular domain give the same entropy density as for only one boundary condition on the triangular domain.

IV. CONCLUSIONS

The ground states of the triangular Ising model on a finite triangular domain cannot be mapped to a dimer covering and cannot therefore be classified into string sectors. Boundary conditions exist for the triangular domain that give intermediate degeneracy and show interesting relationships to the rectangular periodic domain. Although it is known that certain boundary conditions on finite frustrated systems can lift the thermodynamic degeneracy, not a lot is known, the results of Dhar *et al.* [13] notwithstanding, about the relationship between boundary conditions and degeneracy for general frustrated systems. For example, the manifold of maximally degenerate boundary conditions corresponds to the string sector with $p=2/3$ *if* one restricts oneself to the set of limiting periodic boundary conditions on a rectangular domain, but other maximally degenerate limiting boundary conditions exist. The same applies to boundary conditions that give intermediate degeneracy.

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