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A Remark on the Residual Entropy of the Antiferromagnetic Ising Model in the Maximal Critical Field

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Abstract By means of a transfer matrix method, we show that the residual entropy S of the two-dimensional square lattice antiferromagnetic Ising model in the maximal critical field satisfies $(\ln\lambda_n)/(n+1) \le S \le (\ln\lambda_n)/n$, where λ_n is the largest eigenvalue of the transfer matrix F_n on a strip of width n. Using these bounds, we numerically calculate the value of S, with precise estimates on the errors, namely, $S = 0.394198 \pm 0.020747$.

Keywords Residual entropy · Antiferromagnetic Ising model · Critical magnetic field · Transfer matrix

Formally, the Hamiltonian of the two-dimensional square lattice critical field antiferromagnetic Ising (CFAI) model is given by

$$H(\sigma) = -J \sum_{\langle i,j\rangle} \sigma_i \sigma_j - h_c \sum_i \sigma_i, \tag{1}$$

where $J < 0$, $h_c = 4|J|$, $\langle i, j\rangle$ denotes nearest-neighbor pairs in $\mathbb{Z}^2$ and $\sigma \in \{-1, 1\}^{\mathbb{Z}^2}$ is a spin configuration. An interesting feature of the above model is that it exhibits bond frustration, leading to an infinite number of ground state configurations where two neighboring spins are not allowed to point downward. In this model, frustration leads to a nonzero residual entropy. The residual entropy is the entropy which is present even after a substance is cooled to absolute zero. One of the first examples of residual entropy was pointed out by Pauling [1] to describe ice, which is an example of geometrically frustrated material. Other well-known examples of frustrated spin models are, for instance, the Sherrington–Kirkpatrick model [2], the ANNNI model [3] and the Blume–Emery–Griffiths (BEG) model [4], for certain values of the Hamiltonian's parameters, see [5].

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According to [6], the residual entropy S is given by the limit

$$\lim_{\Lambda\uparrow\infty}\sup_{b_\Lambda\in\Omega_{\Lambda^c}}\frac{\ln N_{b_\Lambda}(\Lambda)}{|\Lambda|},$$

where $N_{b_\Lambda}(\Lambda)$ denotes the degeneracy of the minimum energy configurations (ground states) of the Hamiltonian restricted to $\Lambda\subset\mathbb{Z}^2$ and with boundary conditions $b_\Lambda\in\Omega_{\Lambda^c}\equiv\{-1,1\}^{\Lambda^c}$ and $|\Lambda|$ is the cardinality of Λ. For the antiferromagnetic Ising model described by (1), $N_{b_\Lambda}(\Lambda)$ is maximized by free (or plus) boundary condition (see paragraph after (3)), which we denote by $N(\Lambda)$. Therefore

$$S=\lim_{|\Lambda|\to\infty}\frac{\ln N(\Lambda)}{|\Lambda|},\qquad(2)$$

where the limit is taken in any reasonable sense (van Hove, for instance). Its existence follows from subadditivity arguments. Then, S is the exponential rate of growth of $N(\Lambda)$ as $|\Lambda|\to\infty$ and it is an open problem to find the exact value of S for the CFAI model.

Brooks and Domb [7] were the first to estimate the value of S for the CFAI model, half a century ago. Of course, the limit (2) allows for the numerical approximation of S in terms of $\ln N(\Lambda)/|\Lambda|$ as $|\Lambda|$ gets large, although this approximation is not computationally efficient because $N(\Lambda)$ grows exponentially fast with $|\Lambda|$. Since the work of Brooks and Domb, many researchers (see [8] and references therein) have been working on more efficient methods for computing S which, at the same time, would provide higher numerical precision although, as far as the authors know, without analytical bounds on the errors. In [8], the transfer matrix approach was applied with success to compute S and it was observed numerically that: (a) $(\ln\lambda_n)/n$, where λ_n is the highest eigenvalue of the transfer matrix F_n defined by (4), approaches S at the rate $1/n$; (b) $\ln(\lambda_n/\lambda_{n-1})$ approaches S at a rate faster than $1/n$.

The aim of this short note is to point out that the above numerical observation (a), reformulated as $S=(\ln\lambda_n)/n+O(1/n)$ as $n\to\infty$, can actually be obtained analytically by using the transfer matrix approach developed in [5] for the BEG model (see Theorem 1). As a consequence, it will follow that $0\le(\ln\lambda_n)/n-S\le(\ln 2)/n$ and this inequality allows for computing the value of S with the precision one wishes. Of course, higher precision implies larger values of n and, since the sizes of the matrices F_n grow exponentially fast with n, it becomes a technical problem to find λ_n for large values of n. In this note we fix attention to the values of n used in [8]. Regarding the numerical observation (b), it indicates that $S=\ln(\lambda_n/\lambda_{n-1})+o(1/n)$, as $n\to\infty$ but at the moment we do not know how to prove this conjecture.

In order to define the transfer matrix, we rewrite the Hamiltonian (1) in terms of a sum of nearest neighbor pairs, each pair appearing only once, and, without loss of generality, we take $J=-1$ to obtain

$$H_\Lambda(\sigma)=\sum_{\langle i,j\rangle\in\Lambda}(\sigma_i\sigma_j-\sigma_i-\sigma_j).\qquad(3)$$

Ground state configurations are found by minimizing the Hamiltonian (3) over all spin configurations $\sigma\in\{-1,1\}^\Lambda$, which is equivalent to minimizing the spin pair energy $h(\sigma_i,\sigma_j)\equiv\sigma_i\sigma_j-\sigma_i-\sigma_j$. Since $h(-,-)>h(+,+)=h(+,-)$, we conclude that a spin configuration is a ground state of H_Λ if it does not contain pairs of downward-oriented neighboring spins. Also, imposing free boundary condition is the same as imposing $+$ boundary condition.

Let $\Lambda_{m,n}$ be a $m \times n$ box in $\mathbb{Z}^2$ and $N(m,n)$ the number of ground state configurations in $\Lambda_{m,n}$. Let G_n be the collection of all ground state configurations in $\Lambda_{1,n}$. We say that two configurations σ and σ' in G_n are *compatible* if for all $i = 1, \dots, n$ the pair of spins $\sigma_i \sigma_i'$ is of the following form: $++$, $+-$ or $-+$. Then, we construct the ground states in $\Lambda_{m,n}$ by gluing together the compatible elements of G_n. Let F_n be the following $N(1,n) \times N(1,n)$ symmetric matrix defined by

$$F_n(\sigma, \sigma') = \begin{cases} 1, & \text{if } \sigma \text{ and } \sigma' \text{ are compatible,} \\ 0, & \text{otherwise,} \end{cases} \tag{4}$$

which also appeared in [8] and it is known in the literature as a Fibonacci matrix. It gives us an alternative way of determining the number of ground states in $\Lambda_{m,n}$. For instance, $N(2,n) = \sum_{\sigma,\sigma'} F_n(\sigma,\sigma')$ and, in general, $N(m+1,n)$ can be expressed by a similar sum with F_n replaced by F_n^m, the mth power of the matrix F_n.

The set G_n can be ordered so that a suitable representation for F_n is at hand. We will represent the set G_n as a $N(1,n) \times n$ matrix with $+$ or $-$ entries, so that each of its rows corresponds to a unique ground state of G_n. We begin by considering the disjoint union $G_{n,-} \cup G_{n,+} = G_n$, where $G_{n,\rho}$, for $\rho = \pm$, consists of those rows of G_n whose spin value at the column position n is ρ. Given a $m \times n$ matrix A and $\rho = \pm$, let $B = (A|\rho)$ denote the following $m \times (n+1)$ matrix: $B_{i,j} = A_{i,j}$ for $i = 1, \dots, m,\ j = 1, \dots, n$, and $B_{i,n+1} = \rho$ for all i. Then, we construct the matrix G_n recursively as follows

$$G_1 = \begin{pmatrix} + \\ - \end{pmatrix} \quad \text{and} \quad G_n = \begin{pmatrix} G_{n,+} \\ G_{n,-} \end{pmatrix}, \quad n = 2, 3, \dots,$$

where $G_{n,+} = (G_{n-1}|+)$ and $G_{n,-} = (G_{n-1,+}|-)$. Then $|G_{n,+}| = |G_{n-1}| = N(1,n-1)$ and $|G_{n,-}| = |G_{n-1,+}| = |G_{n-2}| = N(1,n-2)$, from which we get the following relation

$$N(1,n) = N(1,n-1) + N(1,n-2),$$

which can be used, together with $N(1,1) = 2$ and $N(1,2) = 3$, to obtain (see the generating functions approach in [5]) that

$$N(1,n) = \frac{1}{\sqrt{5}} \frac{1}{2^{n+2}} \left[(1+\sqrt{5})^{n+2} - (1-\sqrt{5})^{n+2} \right].$$

We enumerate the rows of G_n from $i = 1$ to $N(1,n)$ so that to each i there corresponds a unique ground state in $\Lambda_{m,n}$, namely the ith row of G_n. According to this order, we will denote the entries of F_n by $F_n(i,j)$. We notice that $i = 1$ represents the ground state where all spins are $+$, which implies that $F_n(1,k) = F_n(k,1) = 1$ for all k. For each i, j, $F_n^m(i,j)$ corresponds to the number of ground states in $\Lambda_{m+1,n}$ such that their restrictions to the first and the $(m+1)$th rows are the ground states corresponding to i and j, respectively. The number $N(m+1,n)$ is then given by (see the comments below (4))

$$N(m+1,n) = \sum_{i,j=1}^{N(1,n)} F_n^m(i,j).$$

Here we approach the thermodynamic limit through strips of width n and write the residual entropy as the following limit

$$S = \lim_{n\to\infty} \left[\lim_{m\to\infty} \frac{\ln \sum_{i,j} F_n^m(i,j)}{(m+1)n} \right]. \tag{5}$$

Using the same ideas as in [5] (see (8) with $i = j = 1$), it follows from the Spectral Theorem and the Perron–Frobenius Theorem [9], applied to F_n^2 (since $F_n^2(i, j) \geq 1$), that

$$\lim_{m\to\infty} \frac{\ln F_n^m(1,1)}{m+1} = \ln \lambda_n, \tag{6}$$

where λ_n is the largest eigenvalue of F_n. It will also follow that

$$\sqrt{N(1,n)} \leq \lambda_n \leq N(1,n).$$

Since $0 \leq F_n^m(i, j) \leq F_n^m(1, 1)$, it will hold that

$$F_n^m(1,1) \leq \sum_{i,j=1}^{N(1,n)} F_n^m(i,j) \leq F_n^m(1,1)[N(1,n)]^2.$$

The above inequalities and (6) imply

$$\lim_{m\to\infty} \frac{\ln \sum_{i,j} F_n^m(i,j)}{(m+1)} = \ln \lambda_n. \tag{7}$$

From (5) and (7), S can be written as the limit

$$S = \lim_{n\to\infty} (\ln \lambda_n)/n, \tag{8}$$

which also appears in [8]. Using (8), we now state our result.

Theorem 1 *The residual entropy S of the two dimensional square lattice antiferromagnetic Ising model in the maximal critical field given by* (3) *satisfies the following bounds*:

$$\frac{\ln \lambda_n}{n+1} \leq S \leq \frac{\ln \lambda_n}{n}. \tag{9}$$

Proof For fixed n and for any positive integers k, m, consider only those ground-state configurations in $\Lambda_{2m+1,k(n+1)}$, having +'s in all the columns with index which is a multiple of $n+1$. The number of such configurations is $[N(2m+1,n)]^k$. Therefore

$$N(2m+1, k(n+1)) > [N(2m+1,n)]^k \geq [F_n^{2m}(1,1)]^k,$$

which, together with (6) and (8), imply that

$$S = \lim_{m,k\to\infty} \left[\frac{\ln[N(2m+1,k(n+1))]}{(2m+1)k(n+1)}\right] \geq \frac{1}{n+1} \lim_{m\to\infty} \left[\frac{\ln(F_n)^{2m}(1,1)}{(2m+1)}\right] = \frac{\ln \lambda_n}{n+1}.$$

On the other hand, notice that

$$N(2m+1, kn) < [N(2m+1,n)]^k \leq [N(1,n)]^{2k}[(F_n^2)^m(1,1)]^k,$$

where the second inequality follows from

$$N(m+1,n) = \sum_{i,j=1}^{N(1,n)} F_n^m(i,j) \leq F_n^m(1,1)[N(1,n)]^2.$$

Table 1 Numerical calculations based on the values of λ_n given in [8]

n	λ_n	$\frac{\ln \lambda_n}{n}$	$\frac{\ln \lambda_n}{n+1}$	$\overline{S}_n$	ϵ_n
1	1.618033989	0.481212	0.240606	0.306909	0.120303
2	2.414213562	0.440687	0.293791	0.367239	0.073448
3	3.631381260	0.429871	0.322403	0.376137	0.053734
4	5.457705396	0.424257	0.339406	0.381831	0.042426
5	8.203259194	0.420906	0.350755	0.385831	0.035076
6	12.32988222	0.418671	0.358861	0.388766	0.029905
7	18.53240738	0.417074	0.364940	0.391007	0.026067
8	27.85509910	0.415877	0.369668	0.392773	0.023104
9	41.86755332	0.414946	0.373451	0.394198	0.020747

Then, from (6) and (8), we obtain

$$S = \lim_{m,k\to\infty}\left[\frac{\ln N(2m+1,kn)}{(2m+1)kn}\right] \leq \frac{1}{n}\lim_{m\to\infty}\left[\frac{\ln (F_n)^{2m}(1,1)}{(2m+1)}\right] = \frac{\ln \lambda_n}{n}. \qquad \square$$

It then follows from (9) that $S = (\ln \lambda_n)/n + O(1/n)$ as $n \to \infty$. Besides, the arithmetic mean $\overline{S}_n = [(\ln \lambda_n)/(n+1) + (\ln \lambda_n)/n]/2$ is an approximation for S within an error of at most $\epsilon_n = [(\ln \lambda_n)/n - (\ln \lambda_n)/(n+1)]/2$. Table 1 lists the values of this approximation for $n = 1, \ldots, 9$, from where we obtain

$$S = 0.394198 \pm 0.020747.$$

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