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 $(\ln \lambda_n)/(n + 1) \leq S \leq (\ln \lambda_n)/n$, where $\lambda_n$ 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

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

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].
According to [6], the residual entropy $S$ is given by the limit
\[
\lim_{\Lambda \uparrow \infty} \sup_{b_\Lambda \in \Omega_{\Lambda'}} \frac{\ln N_{b_\Lambda}(\Lambda)}{|\Lambda|},
\]
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 $b_\Lambda \in \Omega_{\Lambda'} = \{-1, 1\}^{\partial \Lambda}$ and $|\Lambda|$ is the cardinality of $\Lambda$. 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
\[
S = \lim_{|\Lambda| \to \infty} \frac{\ln N(\Lambda)}{|\Lambda|}, \tag{2}
\]
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 $\lambda_n$ 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 $0 \leq (\ln \lambda_n)/n - S \leq (\ln 2)/n$ 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 $\lambda_n$ 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
\[
H_\Lambda(\sigma) = \sum_{\langle i, j \rangle \in \Lambda} (\sigma_i \sigma_j - \sigma_i - \sigma_j). \tag{3}
\]
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 $H_\Lambda$ if it does not contain pairs of downward-oriented neighboring spins. Also, imposing free boundary condition is the same as imposing $+$ boundary condition.