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Upper bound on the critical temperature in the 3D Ising model

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Abstract. The upper bound on the critical temperature in the Ising model, recently derived from Callen's correlation equalities by Sá Barreto and O'Carroll and improved by Monroe, is further improved by a more economical use of Messager and Miracle-Sole inequalities, starting from a different Callen correlation equality.

1. Introduction

In two recent papers, Sá Barreto and O'Carroll (1983) and subsequently Monroe (1984) showed how upper bounds on the critical temperature of the Ising model in two and three dimensions can be derived from Callen's correlation equalities (Callen 1963). These correlation equalities in their simplest form hold for Ising spin variables S_i, distributed according to the canonical law

$$\begin{aligned} &\mathrm{Prob}(\{S_i\}) = Z^{-1} \exp\Big(\beta \sum_{i<j} J_{ij} S_i S_j\Big) \\ &Z = \sum_{\{S_i\}} \exp\Big(\beta \sum_{i<j} J_{ij} S_i S_j\Big), \qquad \beta = 1/kT, \end{aligned} \tag{1}$$

and are as follows

$$\langle S_i f(S_j, \ldots)\rangle = \langle f(S_j, \ldots) \tanh(\beta E_i)\rangle. \tag{2}$$

f is an arbitrary function of the spins which is independent of S_i and has a finite expectation value, E_i denotes the factor of S_i in the sum $\Sigma J_{ij} S_i S_j$, and $\langle\ \rangle$ denotes the expectation value with respect to the probability distribution (1), allowing only the values ± 1 for each of the spins $\{S_n\}$. The equality (2) is easily proved by writing the probability distribution (1) as the product of a conditional distribution, conditioned on the values of all spins other than S_i, and the probability distribution of these other spins, and then averaging over S_i explicitly.

Sá Barreto and O'Carroll (1983) considered the particular equality

$$\langle S_i S_j\rangle = \langle S_j \tanh(\beta E_i)\rangle \tag{3}$$

and, by estimating the right-hand side, established the necessary conditions for using a theorem of Simon (1980) to prove the exponential decay of $\langle S_i S_j\rangle$ with the distance

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between the sites i and j in the square and cubic lattices with ferromagnetic nearest-neighbour interactions ($J_{ij}=J>0$, for nearest neighbours), on the provision that β was less than a certain limit, which thus gives a bound on the critical temperature. For the cubic lattice they obtained $\beta_c J \geqslant 0.1844$. Their method was improved by Monroe (1984), who did a more economical estimate of the right-hand side of (3). He obtained $\beta_c J \geqslant 0.1976$. A standard assessment of the true value of $\beta_c J$ is 0.2217 (see, e.g. Domb 1974, Pawley *et al* 1984), whereas the mean-field approximation gives the bound $\beta_c J \geqslant 0.1667$ (Griffiths 1967a).

The purpose of this paper is to contribute a further improvement of the bound by what essentially corresponds to a better method of estimating the right-hand side of (3). However, in order to achieve a simpler self-contained treatment, we actually use a different Callen correlation equality together with a different criterion for the disordered phase (not using Simon's theorem). We thus use the equality

$$\langle S_i \rangle = \langle \tanh(\beta E_i) \rangle \tag{4}$$

and determine a bound β_0, below which there can be no $\langle S_i \rangle \neq 0$. We then obtain

$$\beta_c J \geqslant \beta_0 J = 0.199\,96. \tag{5}$$

On the way, we show that already a crude estimate of the right-hand side of (4) leads to a bound as good as $\beta_c J \geqslant 0.1955$.

The bound (5) is an improvement over several rigorous bounds that have been established in the literature. (In addition to the references above, see, e.g., Holley and Stroock 1976, Brydges *et al* 1982.) It, however, is *not* the best rigorous bound known. The relatively old result of Fisher and Sykes (1959) and Fisher (1967), $\beta_c J \geqslant 0.2085$, obtained from a comparison of the high-temperature expansion graphs with self-avoiding random walks, is still the closest to the estimated 'true' value $\beta_c J = 0.2217$. Also, by exploiting a correlation equality due to Thompson (1971), Krinsky (1975) has obtained the bound $\beta_c J \geqslant 0.2027$. However, the methods that led to these results in both cases depend decisively on special properties of the $S^2=1$ Ising model, while the method described in the present paper does hold the promise of being generalisable to other statistical models.

2. The upper bound

We evaluate Callen's correlation equality (4) for a fixed but arbitrary spin S_0 in the simple cubic lattice with translation invariant ferromagnetic nearest-neighbour interactions, denoting the nearest neighbours of S_0 by $S_1, S_2, \ldots, S_6$:

$$\begin{aligned}\langle S_0 \rangle &= \langle \tanh(\beta E_0) \rangle \\ &= \langle \tanh(\beta J(S_1+S_2+\ldots+S_6)) \rangle \\ &= \tfrac{1}{6}\tanh(6\beta J)\sum_{i=1}^{6}\langle S_i \rangle + [\tfrac{1}{4}\tanh(4\beta J)-\tfrac{1}{6}\tanh(6\beta J)]\langle g \rangle \\ &\quad + [\tfrac{1}{2}\tanh(2\beta J)-\tfrac{1}{6}\tanh(6\beta J)]\langle h \rangle,\end{aligned} \tag{6}$$

where

$$g = \tfrac{1}{2}(S_1+\ldots+S_6)\left(1-\prod_{i=1}^{6} S_i\right) \tag{7}$$

$$h = -\tfrac{9}{16}\left(1 - \tfrac{1}{36}\left(\sum_{i=1}^{6} S_i\right)^2\right) \sum_{\neq} S_i S_j S_k, \tag{8}$$

and the summation $\Sigma_{\neq}$ is over all (non-ordered) sets of three different indices. g and h play the role of indicator functions, taking the value of the sum of the spins if this is ± 4 or ± 2, respectively, and the value 0 otherwise. Note that the expressions in the curly brackets are both non-negative. The expectation values $\langle\ \rangle$ are the infinite volume limits of expectation values taken with respect to (1) for a finite subsystem of spins (e.g. a cube of N^3 spins and $N \to \infty$), fixing the boundary spins to $+1$.

Our strategy is to use correlation inequalities to bound the right-hand side of (6) from above by $\langle S_0 \rangle$ times an explicit function of β, and check whether the ensuing inequality can be satisfied with a positive $\langle S_0 \rangle$. Here we shall indeed be dealing with an increasing function of β that leads to a lower limit for β_c.

The translation and (discrete) rotation symmetries of the infinite lattice allow us to greatly simplify the notation. Thus we can drop the indices and write

$$\langle g \rangle = 3(\langle S \rangle - \langle SSSSS \rangle), \tag{9}$$

where the second expectation value contains any five of the nearest neighbours of the spin chosen for consideration. The expectation value of h can be written as

$$\begin{aligned}\langle h \rangle &= -\tfrac{9}{16}\left\langle \left[\sum_{\neq} S_i S_j S_k - \tfrac{1}{36}\left(6 + 2\sum_{\neq} S_i S_j\right) \sum_{\neq} S_i S_j S_k \right]\right\rangle \\ &= \tfrac{9}{16}\left\{ \tfrac{1}{18}\left\langle \left(\sum_{\neq} S_i S_j\right)\left(\sum_{\neq} S_i S_j S_k\right)\right\rangle - \tfrac{5}{6}\sum_{\neq} \langle S_i S_j S_k \rangle \right\},\end{aligned} \tag{10}$$

where the summations are over all different sets of two, resp. three, of the indices of the six nearest-neighbour spins to the spin S_0. There are two kinds of three-spin correlation functions that occur that we denote by $\langle SSS \rangle_{\parallel}$, if the three spins lie in a plane containing S_0, and by $\langle SSS \rangle_{\perp}$, if this is not the case. Using Messager and Miracle-Sole inequalities (Messager and Miracle-Sole 1977), we show in the appendix that

$$\langle SSS \rangle_{\perp} \geq \langle SSS \rangle_{\parallel} \geq \langle SSSSS \rangle. \tag{11}$$

Carrying out the multiplication in (10), we obtain

$$\begin{aligned}\langle h \rangle &= \tfrac{1}{32}\left(60\langle S \rangle + 60\langle SSSSS \rangle - 6\sum_{\neq} \langle S_i S_j S_k \rangle\right) \\ &= \tfrac{3}{8}(5\langle S \rangle + 5\langle SSSSS \rangle - 6\langle SSS \rangle_{\parallel} - 4\langle SSS \rangle_{\perp}),\end{aligned} \tag{12}$$

so that using (11), we have

$$\langle h \rangle \leq \tfrac{15}{8}(\langle S \rangle - \langle SSS \rangle_{\parallel}). \tag{13}$$

The easiest way to get the desired condition on the critical temperature is to entirely neglect the negative contributions to (9) and (13) and also replace $\frac{15}{8}$ by 2. From (6), one then has

$$\langle S \rangle \leq [\tfrac{1}{6}\tanh(6\beta J) + \tfrac{3}{4}\tanh(4\beta J) + \tanh(2\beta J)]\langle S \rangle \tag{14}$$

and $\langle S \rangle$ can be larger than zero only if the expression in the square brackets is larger than or equal to one. There follows that

$$\beta_c J \geq 0.1955, \tag{15}$$

which already is considerably better than the bound 0.1844 obtained by Sá Barreto and O'Carroll (1983). An improvement of (15) is achieved by using, instead of the zeros, non-zero lower bounds to the 3- and 5-spin correlation functions in (9) and (13) (and of course retaining the $\frac{15}{8}$ factor in (13)). Using Griffiths inequalities (Griffiths 1967b, Kelly and Sherman 1967), we have

$$\langle S_iS_jS_k\rangle \geqslant \langle S_i\rangle\langle S_jS_k\rangle \tag{16}$$

and

$$\langle S_iS_jS_kS_lS_m\rangle \geqslant \langle S_i\rangle\langle S_jS_kS_lS_m\rangle. \tag{17}$$

Furthermore, by Griffiths inequalities, the values of the two- and four-spin correlation functions are reduced by calculating them for small finite lattices, instead of the infinite lattice. Sá Barreto and O'Carroll in a similar step in their calculation used $\langle S_iS_j\rangle \geqslant \langle S_iS_j\rangle_1$, where the right-hand side is the next-nearest-neighbour correlation in a one-dimensional chain. Monroe substituted this with a better bound using $\langle S_iS_j\rangle_8$, which is the correlation calculated for the spins belonging to a finite system of eight spins located at the corners of an elementary cube with the two particular spins sitting diagonally in a face. Although in our calculation, this choice for the pair correlation, together with a simple lower bound for the 4-spin correlation (using a planar subsystem of nine spins), already brings about the main improvement (0.1996) over Monroe's bound, we shall advance the result slightly more by using a larger subsystem. Thus we calculate both the two-spin and the four-spin correlation in a subsystem of 12 spins located at the corners of two elementary cubes that share a common face. The two spins of the pair correlation function occupy diagonal sites in the shared face, and for the four-spin correlation function, the additional two spins are situated at both ends of the double cube. (The 4-spin configuration was kindly suggested to us by J Monroe (private communication).) A straightforward calculation of the correlation functions yields

$$\langle SS\rangle_{12} = \{C(4)^2C(3)^4 + C(3)^2C(1)^2[4C(4)C(2)-2] + C(1)^4[2C(4)+4C(2)-1] - 8C(3)C(2)C(1)^3\}/D \tag{18}$$

$$\langle SSSS\rangle_{12} = \{C(4)^2C(3)^4 - C(3)^2C(1)^2[4C(2)^2-2] + C(1)^4[2C(4)-4C(2)^2+3]\}/D, \tag{19}$$

where

$$D = C(4)^2C(3)^4 + C(3)^2C(1)^2[4C(4)C(2)+2+4C(2)^2] + C(1)^4[2C(4)+4C(2)+4C(2)^2+3] + 8C(3)C(2)C(1)^3 \tag{20}$$

and $C(n)$ denotes $\cosh(n\beta J)$.

Using (18) and (19) with (9), (13), (16) and (17), we obtain from (6) the inequality

$$\langle S\rangle \leqslant \{\tanh(6\beta J) + [\tfrac{3}{4}\tanh(4\beta J) - \tfrac{1}{2}\tanh(6\beta J)](1-\langle SSSS\rangle_{12}) + \tfrac{15}{16}[\tanh(2\beta J) - \tfrac{1}{3}\tanh(6\beta J)](1-\langle SS\rangle_{12})\}\langle S\rangle, \tag{21}$$

which cannot be satisfied with a strictly positive $\langle S\rangle$, when β is less than a certain value β_0, which thus is our lower bound on the critical value β_c,

$$\beta_cJ \geqslant \beta_0J = 0.199\,96. \tag{22}$$

With $\beta = 1/kT$, (22) provides an upper bound on the critical temperature for the three-dimensional ferromagnetic nearest-neighbour Ising model.

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Appendix. Proof of the inequalities (11)

The inequalities (11) are consequences of a general set of inequalities, which were derived by Messager and Miracle-Sole (1977) for Ising systems that have a reflection symmetry. Consider a ferromagnetic nearest-neighbour Ising spin system with the Hamiltonian $H=-\frac{1}{2}\Sigma_{i,j} J_{ij}S_iS_j$ on a lattice Λ, and let the map $\varphi: \Lambda\to\Lambda$ be a reflection symmetry of the system with respect to some fixed plane. Let Λ_1 denote the part of the lattice that is on one side of the plane, including whatever sites that happen to lie in the symmetry plane itself. Thus

$$\Lambda=\Lambda_1\cup\varphi(\Lambda_1), \text{ while } \Lambda_1\cap\varphi(\Lambda_1)=N=\{i|i=\varphi i\}. \tag{A1}$$

For any $A\subset\Lambda$, denote $S_A=\Pi_{i\in A} S_i$.

Theorem. (First Messager and Miracle-Sole (1977) inequality): Let $A\subset\Lambda_1$ and $B\subset\Lambda_1\backslash N$. Then

$$\langle S_AS_B\rangle\geqslant\langle S_AS_{\varphi(B)}\rangle. \tag{A2}$$

Remark. The original proof of this theorem (Messager and Miracle-Sole 1977) did not allow A to contain spins from within the reflection plane. It requires only a minor change, however, to include that situation. This is in fact necessary for our application of the theorem. Thus one shows that $S_A(S_B-S_{\varphi(B)})$, written in terms of the variables $\mu_i=\frac{1}{2}(S_i+S_{\varphi i})$ and $\sigma_i=\frac{1}{2}(S_i-S_{\varphi i})$, $i\in\Lambda_1$, is a sum of product terms $\Pi_{i\in\Lambda_1}\mu_i^{n_i}\Pi_{k\in\Lambda_1}\sigma_k^{m_k}$, n_i, $m_k\in\{0, 1, 2\}$, multiplied by positive coefficients. Written in the new variables, the Hamiltonian H still has ferromagnetic pair couplings, and the non-negativity of the expectation values of the products follows by a series expansion of $\exp(-\beta H)$, as in the standard duplicate variables proof of the Griffiths inequalities (see, e.g., Glimm and Jaffe 1981, p 55).

In order to prove the inequalities (11), we denote the pairs of nearest-neighbour spins of S_0 in opposite directions by (S_1, S_6), (S_2, S_5) and (S_3, S_4), and consider the symmetry plane that contains S_1, S_0 and S_6 and has S_2 and S_3 on the same side (S_4 and S_5 are the spins on their mirror image sites). Then, using (A2) with $A=(S_1, S_6, S_2, S_3\}$ and $B=\{S_3\}$, we have

$$\langle S_1S_6S_2\rangle\geqslant\langle S_1S_6S_2S_3S_5\rangle, \tag{A3}$$

and choosing $A=\{S_1, S_2\}$ and $B=\{S_3\}$, we have

$$\langle S_1S_2S_3\rangle\geqslant\langle S_1S_2S_5\rangle. \tag{A4}$$

In our simplified notation, however, $\langle S_1S_6S_2S_3S_5\rangle=\langle SSSSS\rangle$, $\langle S_1S_6S_2\rangle=\langle S_1S_2S_5\rangle=\langle SSS\rangle_\parallel$ and $\langle S_1S_2S_3\rangle=\langle SSS\rangle_\perp$, so that (11) follows.

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