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Upper bounds on T_c for classical Ising models using correlation inequalities

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Abstract. Following closely the work of Sá Barreto and O'Carroll (1983) we improve the upper bounds they derive for the critical temperature of classical Ising ferromagnets. The improvement is achieved by a more critical use of Griffith's inequalities at one point along with a completely new use of Messager and Miracle–Sole inequalities at another stage of the proof.

In this paper we establish some improvements on the upper bounds on the critical temperature for classical Ising systems presented in a recent paper in this journal by Sá Barreto and O'Carroll (1983). Their initial bounds were obtained using correlation equalities along with correlation inequalities and as stated in their paper these upper bounds are lower than those obtained by Simon (1980) and Brydges *et al* (1982) using somewhat similar methods. The improvements established in this work result from a slightly more critical use of correlation inequalities for the case of both the two- and three-dimensional systems considered as well as a new use of a previously proven inequality for the three-dimensional system.

We begin by stating the pertinent results from Sá Barreto and O'Carroll who consider Ising lattice systems with Hamiltonian

$$H = -J \sum_{\langle ij \rangle} S_i S_j \qquad J \geqslant 0 \tag{1}$$

where the sum is over nearest-neighbour sites located on a lattice Λ of d dimension and where each $S_i = \pm 1$. The thermal average is defined in the usual manner as

$$\langle \ldots \rangle = Z^{-1} \sum_{\{S\}} (\ldots) \, e^{-\beta H} \qquad Z = \sum_{\{S\}} e^{-\beta H} \tag{2}$$

where $\beta = 1/kT$ and T is the temperature.

For such systems one can find a T' such that for $T \geqslant T'$

$$\langle S_0 S_l \rangle \leqslant \sum_{|j|=1} a_j \langle S_j S_l \rangle \qquad 0 \leqslant a_j \leqslant 1 \qquad l \neq 0 \tag{3}$$

for the two-point function where the coefficients a_j depend on the specific system under consideration. The inequality in equation (3) when iterated (see Simon 1980) implies exponential decay for $T > T'$. Hence T' is an upper bound on the critical temperature T_c defined to be that temperature at which the two-point function no longer falls off exponentially.

Our major starting point, theorem 3 of Sá Barreto and O'Carroll (1983), is the following.

Theorem 1. (a) For the square lattice

$$\langle S_0 S_l \rangle = A \sum_i \langle S_i S_l \rangle + B \sum_{i<j<k} \langle S_i S_j S_k S_l \rangle \tag{4}$$

where

$$A = \tfrac{1}{8}[\tanh(4\beta J) + 2\tanh(2\beta J)]$$
$$B = \tfrac{1}{8}[\tanh(4\beta J) - 2\tanh(2\beta J)].$$

(b) For the simple cubic lattice

$$\langle S_0 S_l \rangle = A \sum_i \langle S_i S_l \rangle + B \sum_{i<j<k} \langle S_i S_j S_k S_l \rangle + C \sum_{i<j<K<m<n} \langle S_i S_j S_k S_m S_n S_l \rangle \tag{5}$$

where

$$\begin{aligned} A &- \tfrac{1}{32}[\tanh(6\beta J) + 4\tanh(4\beta J) + 5\tanh(2\beta J)] \\ B &= \tfrac{1}{32}[\tanh(6\beta J) - 3\tanh(2\beta J)] \\ C &= \tfrac{1}{32}[\tanh(6\beta J) - 4\tanh(4\beta J) + 5\tanh(2\beta J)]. \end{aligned} \tag{6}$$

The sums over *i,j,k,m*, and *n* are over the nearest neighbours of O to which we have given a numerical ordering.

Sá Barreto and O'Carroll use correlation inequalities to find an upper bound on the right-hand side of equations (4) and (5) which then results in an inequality of the form of equation (3) and hence an upper bound on T_c. We also use correlation inequalities but differ in our use of these inequalities. We consider separately the two cases covered in the above theorem. Now rather than using $\langle S_i S_j \rangle \geqslant \langle S_i S_j \rangle_{1D}$ where the subscript 1D denotes the correlation between S_i and S_j on a one-dimensional chain, it is better to use $\langle S_i S_j \rangle \geqslant \langle S_i S_j \rangle_4$ where the subscript denotes that the correlation is with respect to a system of 4 spins each located on the corner of a unit square of the lattice. Both inequalities follow from the second Griffiths (1967) inequality. With the use of $\langle S_i S_j \rangle \geqslant \langle S_i S_j \rangle_{1D}$ Sá Barreto and O'Carroll obtained the bound $\beta_c J = 0.331\,79$ with $\langle S_i S_j \rangle_{1D} = 0.102\,48$. At the same βJ value $\langle S_i S_j \rangle_4 = 0.202\,83$ almost double the $\langle S_i S_j \rangle_{1D}$ value. A still better bound for $\langle S_i S_j \rangle$ is $\langle S_i S_j \rangle \geqslant \langle S_i S_j \rangle_9$ where the subscript nine denotes a 3×3 square lattice. Then for $\beta J = 0.331\,79$ one has $\langle S_i S_j \rangle_9 = 0.224\,26$ more than double $\langle S_i S_j \rangle_{1D}$. Clearly choosing larger systems allows for better bounds, however the difficulty of calculating the $\langle S_i S_j \rangle$ quickly increases and the increase in the value of $\langle S_i S_j \rangle$ quickly decreases. Simon (1980) also points out a similar approach and with it similar problems. Stopping at the nine-site system we get the following theorem.

Theorem 2. For the square lattice $\beta_c J \geqslant 0.344\,78$.

Proof. Using $\langle S_i S_j \rangle \geqslant \langle S_i S_j \rangle_9$ we have

$$\langle S_0 S_l \rangle \leqslant \sum_{\substack{|j|=1 \\ j \neq l}} \bar{a}_j \langle S_j S_l \rangle \tag{7}$$

with $\bar{a}_j = A - |B|\langle S_i S_j \rangle_9$ and where

$$\langle S_i S_j \rangle_9 = \frac{\cosh(12\beta J) + 4\cosh(8\beta J) + 7\cosh(4\beta J) - 12}{\cosh(12\beta J) + 4\cosh(8\beta J) + 16\cosh(6\beta J) + 23\cosh(4\beta J) + 48\cosh(2\beta J) + 36}. \tag{8}$$

Then one can find a T' such that for all $T > T'$, $\Sigma_{|j|=1}\, \bar{a}_j \leq 1$ and $\bar{a}_j \geq 0$ from which following Simon (1980) and Sá Barreto and O'Carroll (1983), leads to the bound on the critical temperature. The exact value for $\beta_c J$ is given by the Onsager solution as $\beta_c J = 0.4407$.

Now turning to the simple cubic lattice and equation (5) we follow the same basic approach to bound the middle term of this equation as was used for the square lattice. The one difference being that instead of the next-nearest-neighbour correlation on a 3×3 square lattice we get a better bound using an 8 spin system with the spins located on the corners of a cube.

Also for the three-dimensional simple cubic lattice there is now a third term in equation (5) which we need to bound. Since C, the coefficient of the third term is positive we need an upper bound on $\langle S_i S_j S_k S_m S_n S_l \rangle$. Sá Barreto and O'Carroll use an inequality of Newman (1975) and the fact that $\langle S_A \rangle \leq 1$, where

$$\langle S_A \rangle = \left\langle \prod_{i \in A} S_i \right\rangle \qquad A \subset \Lambda. \tag{9}$$

Their bound is five times larger than the bound we obtain using inequalities of a type established by Messager and Miracle-Sole (1977). Messager and Miracle-Sole prove

$$\langle S_A S_B \rangle \geq \langle S_A S_{\bar{B}} \rangle \tag{10}$$

where S_A and S_B are defined as in equation (9) and $S_{\bar{B}}$ is the reflection of the sites in B about any diagonal plane through the site 0.

Third term of equation (5) consists of terms of the form $\langle S_i S_j S_k S_m S_n S_l \rangle$ where i,j,k,m, and n are any five of the six nearest neighbours of the site 0. Four of these five sites will always lie in either the xy, yz, or zx plane of the simple cubic lattice. Two of these four sites will be the reflection of the other two sites about a diagonal plane through site 0. Hence if we select $A = i,j,n,l$ and $B = i,j$ such that i and j reflected about the suitable diagonal plane become k and m then using equation (9) and that $S_i^2 = 1$ for any $i \in \Lambda$ gives

$$\langle S_i S_j S_n S_l S_i S_j \rangle = \langle S_n S_l \rangle \geq \langle S_i S_j S_n S_l S_{\bar{i}} S_{\bar{j}} \rangle = \langle S_i S_j S_n S_l S_k S_m \rangle. \tag{11}$$

Therefore we have, since we can do this for each of the six terms in the sum,

$$\sum_{i<j<k<m<n} \langle S_i S_j S_k S_m S_n S_l \rangle \leq \sum_{|j|=1} \langle S_j S_l \rangle \tag{12}$$

and we can obtain the following bound.

Theorem 3. For the simple cubic lattice $\beta_c J \geq 0.1976$.

Proof. Using the reasoning just presented we have $\langle S_0 S_l \rangle$ bounded as in equation (7) where $\bar{a}_j$ for the simple cubic lattice is

$$\bar{a}_j = A - \tfrac{20}{6}|B|\langle S_i S_j \rangle_B + C \tag{13}$$

with A, B, and C given in equation (6). The next-nearest-neighbour correlation needed in equation (13) is

$$\langle S_i S_j \rangle_8 = \frac{\cosh(12\beta J) + 4\cosh(6\beta J) - \cosh(4\beta J) - 4\cosh(2\beta J)}{\cosh(12\beta J) + 8\cosh(6\beta J) + 15\cosh(4\beta J) + 24\cosh(2\beta J) + 16}. \tag{14}$$

Using the value $\beta J = 0.1976$ in the evaluation of equations (13) and (14) we find $\Sigma_{|j|=1}\, \bar{a}_j \leqslant 1$ and $\bar{a}_j \geqslant 0$ from which again following Simon (1980) and Sá Barreto and O'Carroll (1983) leads to the bound on the critical temperature. Sá Barreto and O'Carroll obtained as their bound $\beta_c J \geqslant 0.1844$. The best estimate for the value of $\beta_c J$ is 0.2216 see Burley (1972).

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