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Upper Bounds on the Critical Temperature for Various Ising Models

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Upper bounds are obtained for spin ± 1 systems. In the case of only nearest-neighbor interactions on, for example, the square lattice we obtain $\beta_c J > 0.3592$. The method's strength is seen when considering systems with longer-range interactions. For example, we obtain $\beta_c J > 0.360$ compared to the previous best bound of $\beta_c J \geqslant 0.345$ for the one-dimensional lattice with $1/r^2$ interactions. The method relies upon an identity between correlation functions and then the use of correlation inequalities to obtain the final bounds.

KEY WORDS: Critical temperature; Ising model; correlation inequalities.

1. INTRODUCTION

Bounds on the critical temperature T_c for various spin systems have been of interest for some time. For the standard Ising model with spins equal to ± 1 and only ferromagnetic nearest-neighbor interactions the best numerical results for the upper bound remain those established by Fisher[1] in 1967 using results from Fisher and Sykes[2] concerning self-avoiding walks. Since 1967 others have established methods which give upper bounds on T_c which, while not as good as Fisher's bound for the standard Ising model, might be applied to systems with other spin variables, e.g., classical rotators,[3] or to systems with more general interactions, e.g., the one-dimensional lattice with $1/r^2$ interactions.[4] The following method is of the latter type. The bounds which one obtains from rather simple calculations are better than the recent bounds of Sá Barreto and O'Carroll,[5] Monroe[6] and the Bethe approximation result of Krinsky,[7]

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but for the nearest-neighbor systems they are not as good as the Fisher–Sykes result.

It should be pointed out that recently Simon[8] has presented a method for computing a sequence of upper bounds on T_c which is guaranteed to converge to the true transition temperature. The method involves the calculation of pair correlation functions as does the method to be presented here. In addition Aizenman[9] has obtained complementary lower bounds on T_c for a general class of spin systems. These methods give one the possibility of getting arbitrarily good bounds on T_c although the amount of calculation needed may be substantial.

In the remainder of this section we introduce the necessary notation and present one identity which is the starting point for the method. The following section consists of the method used on nearest-neighbor interaction systems. This has been done because the use of the method can be most clearly seen when applied to these simpler systems and as stated above the results are good although not the best. Then in Section 3 we conclude by considering those systems with interactions beyond nearest neighbors.

Consider a collection of N lattice sites where on each site there is a spin variable $\sigma = \pm 1$, the spin on the ith site will be labeled σ_i. The spin interactions are given by

$$H(\{\sigma\}) = -\sum_{i<j} J_{ij}\sigma_i\sigma_j - \sum_i h_i\sigma_i \tag{1.1}$$

where $\{\sigma\}$ represents a configuration of the N spins. The thermal average for a product of the spins is

$$\langle \sigma_A \rangle = \sum_{\{\sigma\}} \sigma_A e^{-\beta H} \Big/ \sum_{\{\sigma\}} e^{-\beta H} = Z^{-1} \sum_{\{\sigma\}} \sigma_A e^{-\beta H} \tag{1.2}$$

where $\beta = 1/kt$ and where

$$\sigma_A = \prod_{i \in A} \sigma_i \tag{1.3}$$

with A any subset of the N spins.

One has the identity

$$\exp[\beta J_{kl}\sigma_k\sigma_l] = \cosh(\beta J_{kl})[1 + T_{kl}\sigma_k\sigma_l] \tag{1.4}$$

where $T_{kl} \equiv \tanh(\beta J_{kl})$. Then applying the identity to (1.2) one obtains

$$\langle \sigma_A \rangle = \frac{\langle \sigma_A \rangle_{kl} + T_{kl}\langle \sigma_A\sigma_k\sigma_l \rangle_{kl}}{1 + T_{kl}\langle \sigma_k\sigma_l \rangle_{kl}} \tag{1.5}$$

where the subscript kl on the brackets denoting the thermal averages denotes a thermal average where the interaction J_{kl} has been set to zero. One may use the identity (1.4) again to delete other interactions, this is the starting point for the method discussed in the following sections. A similar starting point was used by Thompson[10] to establish that the mean-field magnetization is an upper bound on the true magnetization and later by Krinsky[7] to prove the Bethe approximation bound for the magnetization.

2. NEAREST-NEIGHBOR INTERACTION SYSTEMS

We now restrict our interactions to nearest-neighbor interactions with all interactions of equal strength and all magnetic field terms of equal strength. Furthermore we specify periodic boundary conditions and consider the square lattice as a specific example although the method works for any regular lattice.

We choose a site and label it as the zeroth site as shown in Fig. 1a.

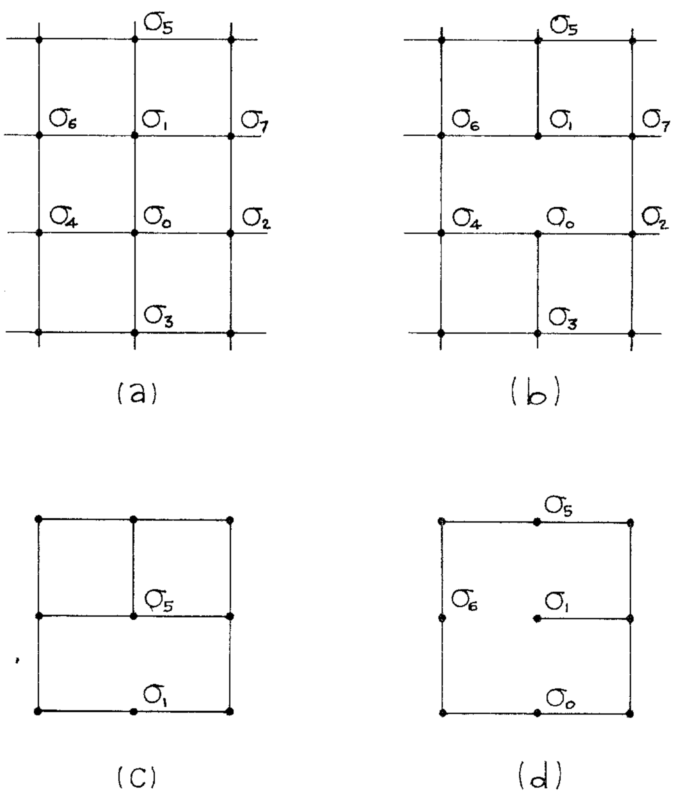

Fig. 1. System and subsystems used in the analysis of the n.n. interaction case.

Then using the identity (1.4) four times so that σ_0 at the end of the four applications is no longer interacting with any other spins, we then have

$$\langle\sigma_0\rangle = \frac{\tau + T\langle\sigma_4\rangle_{01,02,03,04}}{B_1 B_2 B_3 B_4} + \frac{T\langle\sigma_3\rangle_{01,02,03}}{B_1 B_2 B_3} + \frac{T\langle\sigma_2\rangle_{01,02}}{B_1 B_2} + \frac{T\langle\sigma_1\rangle_{01}}{B_1} \tag{2.1}$$

where $T = \tanh(\beta J)$, where $\tau = \tanh(\beta h)$, and where

$$\begin{aligned} B_1 &= 1 + T\langle\sigma_0\sigma_1\rangle_{01}, & B_2 &= 1 + T\langle\sigma_0\sigma_2\rangle_{01,02} \\ B_3 &= 1 + T\langle\sigma_0\sigma_3\rangle_{01,02,03}, & B_4 &= 1 + T\langle\sigma_0\sigma_4\rangle_{01,02,03,04} \end{aligned} \tag{2.2}$$

we want to bound the right-hand side and hence the left-hand side of (2.1). To do so we will use the Griffiths, Kelly, and Sherman (hereafter GKS) inequalities[11,12] which are

$$\langle\sigma_A\rangle \geqslant 0 \tag{2.3}$$

$$\frac{\partial\langle\sigma_A\rangle}{\partial\beta J_B} = \langle\sigma_A\sigma_B\rangle - \langle\sigma_A\rangle\langle\sigma_B\rangle \geqslant 0 \tag{2.4}$$

Using these inequalities we have the bound

$$\langle\sigma_0\rangle \leqslant \tau + \frac{4T}{B_1}\langle\sigma_1\rangle_{01} \tag{2.5}$$

since by (2.3) all B's $\geqslant 1$ and since by (2.4) along with periodicity

$$\langle\sigma_4\rangle_{01,02,03,04} \leqslant \langle\sigma_3\rangle_{01,02,03} \leqslant \langle\sigma_2\rangle_{01,02} \leqslant \langle\sigma_1\rangle_{01} \tag{2.6}$$

We now use the identity (1.4) applying it to the $<\sigma_1>_{01}$ term which already has the interaction between σ_0 and σ_1 deleted as in Fig. 1b. Therefore to free spin σ_1 from the remainder of the lattice we need apply the identity only three more times to get

$$\langle\sigma_0\rangle \leqslant \tau + \frac{4T}{B_1}\left\{\frac{\tau + T\langle\sigma_7\rangle_{01,15,16,17}}{B_5 B_6 B_7} + \frac{T\langle\sigma_6\rangle_{01,15,16}}{B_5 B_6} + \frac{T\langle\sigma_5\rangle_{01,15}}{B_5}\right\} \tag{2.7}$$

where

$$\begin{aligned} B_5 &= 1 + T\langle\sigma_1\sigma_5\rangle_{01,15}, \qquad B_6 = 1 + T\langle\sigma_1\sigma_6\rangle_{01,15,16}, \\ B_7 &= 1 + T\langle\sigma_1\sigma_7\rangle_{01,15,16,17} \end{aligned} \tag{2.8}$$

Using the GKS inequalities as before we have

$$\langle\sigma_0\rangle \leqslant \tau + \frac{4T}{B_1}\{\tau + A\langle\sigma_1\rangle_{01}\} \tag{2.9}$$

where we define A to be

$$A \equiv \frac{2T}{B_5 B_6} + \frac{T}{B_5} \tag{2.10}$$

Now we repeat this procedure on $\langle \sigma_1 \rangle_{01}$ generating the inequality

$$\langle \sigma_0 \rangle \leqslant \tau + \frac{4T}{B_1} \{ \tau + \tau A + \tau A^2 + \cdots + \tau A^{n-1} + A^n \langle \sigma_1 \rangle_{01} \} \tag{2.11}$$

In the limit $n \to \infty$ for $A < 1$ we have

$$\langle \sigma_0 \rangle \leqslant \tau + \frac{4T}{B_1} \tau \frac{1}{1-A} \tag{2.12}$$

This is true for any size lattice and therefore will be true for the infinite lattice. Then for $h \to 0$, i.e., $\tau \to 0$, we have no magnetization for $A < 1$. Therefore for all βJ such that $A < 1$ no phase transition exists.

If we bound B_5 and B_6 by one then we have that there is no phase transition for $\beta J > \tanh^{-1}(1/3)$ which is the Bethe approximation. To go beyond the Bethe approximation we must evaluate B_5 and B_6 more carefully. We must always be getting lower bounds not upper bounds of B. These can be found by explicit calculation of the pair correlation functions involved in the B's using small systems since by the GKS inequality increasing the size of the system only increases the amount of correlation between any two spins. For the $\langle \sigma_1 \sigma_5 \rangle_{01,15}$ we use only the nine-spin system in Fig. 1c and for $\langle \sigma_1 \sigma_6 \rangle_{01,15,16}$ we use the nine-spin system of Fig. 1d. We then get $\beta_c J > 0.3592$. This is to be compared to, for example, the bound of Sa Barreto and O'Carroll[5] of 0.3318, Krinsky's[7] Bethe bound of 0.3466, and the best bound, that of Fisher and Sykes[1,2] of 0.3870.

One could improve these bounds by considering larger systems than those shown in Figs. 1c and 1d although this would quickly involve substantially larger calculations. As mentioned in the introduction, Simon has developed an algorithm using pair correlations to get a sequence of upper bounds converging to the true critical temperature. As in our method to obtain better and better bounds one needs to consider larger and larger systems. The only numerical result of the Simon procedure is his bound[8] of $\beta_c J > 0.3242$ for the system considered in this section.

3. NON-NEAREST-NEIGHBOR INTERACTION SYSTEMS

The procedure discussed in Section 2 is most effective when dealing with systems where interactions beyond nearest-neighbor interactions are present. Here we obtain the best bounds available with a substantial improvement in most cases, e.g., the $1/r^2$ one-dimensional system. We first present results for a square lattice with nearest-neighbor (n.n.) interactions J_1 and next-nearest-neighbor (n.n.n.) interactions $J_2$with periodic boundary conditions. We for simplicity drop the magnetic field from the beginning.

We again label a zeroth site along with its neighboring sites as in Fig. 2a. Using the identity (1.4) eight times and then the GKS inequalities we have

$$\langle \sigma_0 \rangle \leqslant \frac{4T_1}{B_1} \langle \sigma_1 \rangle_{01} + \frac{4T_2}{B_1} \langle \sigma_5 \rangle_{05} \tag{3.1}$$

where $T_1 = T$, with T and B_1 as in the preceding section, and $T_2 = \tanh(\beta J_2)$. Now we reuse the identity (1.4) seven times on $\langle \sigma_1 \rangle_{01}$, three times on the n.n. interactions and four times on the n.n.n. interactions. Also we use (1.4) seven times on $\langle \sigma_5 \rangle_{05}$, four times on the n.n.

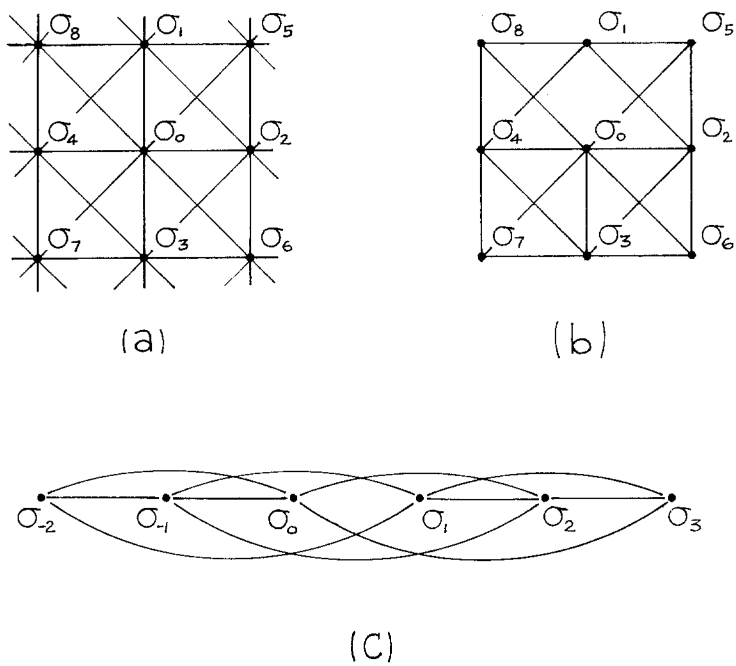

Fig. 2. System and subsystems used in the analysis of systems with interactions beyond n.n. interactions.

interactions and three times on the n.n.n. interactions. This along with the GKS inequalities allows us to obtain

$$\langle\sigma_0\rangle \leqslant \frac{4T_1}{B_1}[3T_1\langle\sigma_1\rangle_{01} + 4T_2\langle\sigma_5\rangle_{05}] + \frac{4T_2}{B_1}[4T_1\langle\sigma_1\rangle_{01} + 3T_2\langle\sigma_5\rangle_{05}] \tag{3.2}$$

We can repeat this procedure as many times as we like but the expressions quickly become very complicated. Thus we will treat two different cases one with $T_1 \neq T_2$ and one with $T_1 = T_2$. For the latter case we can repeat the process $n-1$ times to obtain

$$\langle\sigma_0\rangle \leqslant \frac{8T_1}{B_1}(7T_1)^n\langle\sigma_0\rangle \tag{3.3}$$

Now if $n \to \infty$ we get no phase transition if

$$\tanh(\beta J_1) < \frac{1}{7} \tag{3.4}$$

which gives the bound $\beta_c J_1 > 0.1438$.

When $T_1 \neq T_2$ because of not being able to simplify the expressions we repeat the procedure only three more times after (3.2) obtaining

$$\langle\sigma_0\rangle \leqslant \frac{1}{B_1}[324T_1^5 + 2592T_1^4T_2 + 6688T_1^3T_2^2 + 6688T_1^2T_2^3 + 2592T_1T_2^4 + 324T_2^5]\langle\sigma_0\rangle \tag{3.5}$$

Looking at a particular case of $T_1 \neq T_2$, e.g., $J_1 = 4J_2$, which is the first two terms of a $1/r^2$ interaction, then (3.5) gives the bound $\beta_c J_1 > 0.2361$ where to compute B_1we use the nine spin system as shown in Fig. 2b.

We can make two comparisons of these bounds. First, Domb and Dalton[13] for $J_1 = J_2$ estimate $\beta_c J$ to be 0.1901 and for $J_1 = 4J_2$ Dalton and Wood[14] estimate that $\beta_c J$ is 0.328. Both estimates are based on series expansion methods. Second, Fisher's method can be used to obtain bounds for systems with interactions beyond the n.n. interactions and the result is that there is no phase transition for all βJ such that the following inequality is satisfied:

$$\sum_r \tanh(\beta J_r) - \min[\tanh(\beta J_r)] < 1 \tag{3.6}$$

where the sum is over all sites interacting directly with the zeroth site. For $J_1 = J_2$ one has $\beta_c J > 0.1438$ and for $J_1 = 4J_2$, $\beta_c J > 0.2132$. One word of caution is appropriate at this point. For the case of n.n. interactions only (3.6) gives the Bethe approximation T_c as a bound and not the result mentioned in Section 2. To get the result of Section 2 the self-avoiding walk results of Fisher and Sykes must also be used. Their results, however, do not apply to non-n.n. interaction systems.

We now consider an infinite-range interaction of any form and restrict ourselves to a one-dimensional lattice of N sites with periodic boundary conditions and again choose a zeroth site. We can use the identity (1.4) to obtain

$$\langle\sigma_0\rangle = \frac{T_1\langle\sigma_1\rangle_1}{B_1} + \frac{T_1\langle\sigma_{-1}\rangle_{11}}{B_1 B_{11}} + \frac{T_2\langle\sigma_2\rangle_{112}}{B_1 B_{11} B_{112}} + \cdots + \frac{T_n\langle\sigma_n\rangle_{11223\cdots n}}{B_1 B_{11} B_{112}\cdots B_{11223\cdots n}} + \cdots \tag{3.7}$$

where the subscripts 1, 2, 3,... represent the n.n., n.n.n., third n.n.,... interaction of σ_0 which has been deleted and a repeated number means both interactions at that distance have been deleted. Finally $T_n = \tanh(\beta J_n)$ with n representing the nth nearest neighbor. By the symmetry due to the periodic boundary conditions and the GKS inequalities we have

$$\langle\sigma_0\rangle \leqslant \frac{2T_1}{B_1}\langle\sigma_0\rangle_1 + \frac{2T_2}{B_1}\langle\sigma_0\rangle_2 + \frac{2T_3}{B_1}\langle\sigma_0\rangle_3 \cdots + \frac{2T_n}{B_1}\langle\sigma_0\rangle_n + \cdots \tag{3.8}$$

Now for each term in the above expression we can go through a procedure deleting the remaining interactions with the zeroth site. Then again using the symmetry of the system as well as the GKS inequalities we have

$$\begin{aligned}\langle\sigma_0\rangle \leqslant{}& \frac{2T_1}{B_1}\{T_1\langle\sigma_0\rangle_1 + 2T_2\langle\sigma_0\rangle_2 + 2T_3\langle\sigma_\Omega\rangle_3 + \cdots\} \\ &+ \frac{2T_2}{B_1}\{2T_1\langle\sigma_0\rangle_1 + T_2\langle\sigma_0\rangle_2 + 2T_3\langle\sigma_0\rangle_3 + \cdots\} + \cdots \\ &+ \frac{2T_n}{B_1}\{2T_1\langle\sigma_0\rangle_1 + 2T_2\langle\sigma_0\rangle_2 + \cdots + T_n\langle\sigma_0\rangle_n + \cdots\} + \cdots\end{aligned} \tag{3.9}$$

We repeat this procedure one more time. This time we replace all $\langle\sigma_0\rangle_n$'s with $\langle\sigma_0\rangle$ and then collect terms to get

$$\langle\sigma_0\rangle \leqslant \left\{\frac{8}{B_1}\left(\sum_{n=1}^{\infty} T_n\right)^3 - \frac{8}{B_1}\left(\sum_{n=1}^{\infty} T_n\right)\left(\sum_{n=1}^{\infty} T_n^2\right) + \frac{2}{B_1}\left(\sum_{n=1}^{\infty} T_n^3\right)\right\}\langle\sigma_0\rangle \tag{3.10}$$

For all βJ such that the term in parenthesis is less than 1 we have no phase transition. We now look at the special case where we have specifically the $1/r^2$ interaction. The term in parenthesis is itself bounded above in the following manner: we used the upper bound for the first and third terms found by taking the first three terms in the power series expansion of Th and Th^3 and we used the lower bound of the second term found by taking only the first two terms of Th and Th^2. For B_1we use the six spin system shown in Fig. 2c. We then have $B_c J > 0.360$. Fisher's result gives $\beta_c J > 0.310$. Very recently Siu[4] has proven bounds on the critical temperature and has examined in particular the $1/r^2$ one-dimensional model for which he obtains the bound $\beta_c J > 0.345$ which was the best known result. The best estimate for the critical temperature of this system is $\beta_c J = 0.633$ obtained by Bhattacharjee *et al.*[15]

In conclusion we note that through the calculation of correlation functions in spin systems of small size we have a method of obtaining upper bounds on T_c for many spin ± 1 systems. For the specific systems considered here the bounds obtained are the best numerical bounds we know of except in the nearest-neighbor case. All bounds have been obtained through simple calculations done by hand.

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