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Ising system bounds for arbitrary spin

I G Enting†

Physics Department, Monash University, Clayton, Victoria, Australia 3168

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Abstract. It is shown that a generalized mean-field approximation can give bounds for Ising systems of arbitrary spin. As a particular example, a spin 1 Ising model which has been used as a model for ^3He–^4He mixtures is considered.

1. Introduction

In a series of recent papers, Enting (1973a, b, c) has given proofs that various generalized mean-field approximations give upper bounds for some thermodynamic quantities in Ising models. As a consequence bounds have been given for critical temperatures and the crossover exponent. These bounds are generalized to Ising systems of spin other than $\frac{1}{2}$ in the present work.

To relate spin greater than $\frac{1}{2}$ to earlier spin $\frac{1}{2}$ work we use the approach of Griffiths (1969) who showed that an Ising system of spin greater than $\frac{1}{2}$ can be represented in terms of a spin $\frac{1}{2}$ Ising system. It will be shown that the results given by Enting can be applied to this spin $\frac{1}{2}$ analogue system to give bounds for the original spin greater than $\frac{1}{2}$ system. The mean-field solution for spin greater than $\frac{1}{2}$ gives upper bounds for magnetization and susceptibility. In addition one can obtain magnetization and susceptibility bounds from generalized mean-field approximations in which only some of the interactions are treated by the mean-field approximation.

The bounds for spin $\frac{1}{2}$ apply only for systems with only one-spin and two-spin interactions, all of which must be ferromagnetic. For most cases these restrictions apply when the bounds are generalized to arbitrary spin. An exception occurs for the special case considered in § 4 where an interaction of the form ΔS^2 can have, under certain conditions, positive or negative values for Δ without invalidating the proofs.

In detail the outline of the paper is as follows: in § 2 it is shown how the bounds on the analogue spin system are transformed into bounds for arbitrary spin. Section three shows how the results of § 2 lead to generalizations of all the bounds obtained for spin $\frac{1}{2}$. As well as this a new exponent bound is given. This is another case in which a scaling theory prediction for an exponent is shown to give an upper bound. It is pointed out that investigation of this exponent would provide a test of scaling predictions for the region below the critical point. Section 4 considers the ^3He–^4He model of Blume *et al* (1972) which has been investigated by Oitmaa (1971, 1972), using high temperature series expansions. This system is used to illustrate the applications of the generalized bounds.

† Present address: King's College, Strand, London, UK.

2. Bounds for arbitrary spin

The basic hamiltonian considered is:

$$H = \bar{H} - \sum_{kk'} J_{kk'} S_k S_{k'}, \qquad J_{kk'} \geqslant 0 \tag{1}$$

where $\bar{H}$ has only one-spin and two-spin interactions, all of which must be ferromagnetic.

If we consider the mean-field hamiltonian:

$$H' = \bar{H} - \sum_{kk'} J_{kk'}(S_k \langle S_{k'} \rangle_H + S_{k'} \langle S_k \rangle_H) \tag{2}$$

then equation (9) shows that taking the expectation value $\langle S_j \rangle_{H'}$ gives an upper bound for $\langle S_j \rangle_H$. However, since (2) is expressed in terms of unknown expectation values it is more useful to consider a self-consistent hamiltonian:

$$H'' = \bar{H} - \sum_{kk'} J_{kk'}(S_k \langle S_{k'} \rangle_{H''} + S_{k'} \langle S_k \rangle_{H''}). \tag{3}$$

The result that $\langle S_j \rangle_{H''} > \langle S_j \rangle_{H'}$ then follows immediately since the spin expectation values are increasing functions of the interaction strengths. The principle is the same as that used by Thompson (1972) in finding bounds for the spin $\frac{1}{2}$ system. A comment by Liu (1973) suggests the need for further justification of this step. The most important aspect of the proof given here (equations (10) to (14)) is that it proves the existence of self-consistent solutions of (3). In constructing these solutions it is necessary to take the limit of an infinite sequence of solutions. There is a certain amount of flexibility in choosing the stage of the argument at which this limit is taken. Enting (1973b, c) give alternative developments.

Following Griffiths (1969) we represent the Ising spins S_k by

$$2S_k = \sum_{j=1}^{p} \sigma_{jk}; \qquad \sigma_{jk} = \pm 1 \tag{4}$$

where the spin S_k is of magnitude $\frac{1}{2}p$; actually the magnitude can be allowed to vary from site to site.

We now use the result due to Griffiths that it is possible to construct analogue hamiltonians $\hat{H}$, $\hat{H}'$ such that

$$\begin{aligned}\langle S_k \rangle_H &= \operatorname*{Tr}_{\{S_j\}} [S_k \exp(-\beta H)] \left(\operatorname*{Tr}_{\{S_j\}} [\exp(-\beta H)] \right)^{-1} = \tfrac{1}{2} \left\langle \sum_{j=1}^{p} \sigma_{jk} \right\rangle_{\hat{H}} \\ &= \tfrac{1}{2} \operatorname*{Tr}_{\{\sigma_{ab}\}} \left(\sum_{j=1}^{p} \sigma_{jk} \exp(-\beta \hat{H}) \right) \left(\operatorname*{Tr}_{\{\sigma_{ab}\}} [\exp(-\beta \hat{H})] \right)^{-1}.\end{aligned} \tag{5}$$

An analogous relation connects H' and $\hat{H}'$. The important point to note is that if the hamiltonians H, H' have only one-spin and two-spin interactions all of which are ferromagnetic, then these properties will also hold in the analogue hamiltonians.

It is now easy to show that each replacement in going from (1) to (2) will increase the expectation value of each spin. The original term is

$$J_{kk'} S_k S_{k'} = \tfrac{1}{4} J_{kk'} \left(\sum_{j=1}^{p} \sigma_{jk} \right) \left(\sum_{j'=1}^{p'} \sigma_{j'k'} \right). \tag{6}$$

It is replaced by

$$J_{kk'}[S_k\langle S_{k'}\rangle_H + S_{k'}\langle S_k\rangle_H] = \tfrac{1}{4}J_{kk'}\sum_{j=1}^{p}\sum_{j'=1}^{p'}[\sigma_{jk}\langle\sigma_{j'k'}\rangle_{\bar{H}} + \sigma_{j'k'}\langle\sigma_{jk}\rangle_{\bar{H}}]. \quad (7)$$

Working in terms of the σ_{jk} variables one can use Enting's results for the generalized mean-field bounds to show that each replacement of the type given above will increase the expectation value of each spin σ_{ab}. This gives

$$\langle\sigma_{ab}\rangle_{\bar{H}} \leqslant \langle\sigma_{ab}\rangle_{\bar{H}'}. \quad (8)$$

Converting back to the original S variables gives

$$\langle S_a\rangle_H \leqslant \langle S_a\rangle_{H'}. \quad (9)$$

To construct self-consistent solutions of (3) we now consider a sequence of hamiltonians

$$H(n) = \bar{H} - \sum_{kk'} J_{kk'}(S_k\langle S_{k'}\rangle_{H(n-1)} + S_{k'}\langle S_k\rangle_{H(n-1)}) \quad (10)$$

$$H(0) = H'.$$

One can then give an inductive proof that

$$\langle S_a\rangle_{H(n)} \geqslant \langle S_a\rangle_{H(n-1)} \quad (11)$$

using (9) as a starting point. The sequence of $\langle S_a\rangle_{H(n)}$ is bounded (by $\tfrac{1}{2}p$) and so must have a limit as $n \to \infty$, denoted $\langle S_a\rangle_{H(\infty)}$. Putting

$$H^* = \bar{H} - \sum_{kk'} J_{kk'}(S_k\langle S_{k'}\rangle_{H(\infty)} + S_{k'}\langle S_k\rangle_{H(\infty)}) \quad (12)$$

one has, so long as the expectation values are continuous functions of the interaction strengths,

$$\lim_{n\to\infty} \langle S_a\rangle_{H(n)} \to \langle S_a\rangle_{H^*} \quad (13)$$

so that

$$\langle S_a\rangle_{H(\infty)} = \langle S_a\rangle_{H^*}. \quad (14)$$

This means that $\langle S_a\rangle_{H(\infty)}$, which has been shown to exist, is a self-consistent solution of the hamiltonian (3).

3. Bounds for exponents

The original application of the generalized mean-field approximation was to the anisotropic Ising model. In that case the interlayer interactions of strength ηJ were treated by a mean-field approximation while the intralayer interactions were treated exactly. Generalizing that treatment to spin greater than $\tfrac{1}{2}$ one obtains the equations:

$$R(S, T, \mathscr{H}, \eta) \leqslant R^*(S, T, \mathscr{H}, \eta) = R_{2D}(S, T, \mathscr{H} + q\eta JR^*) \quad (15)$$

where R is the value of $\langle S_a\rangle$ for spins of magnitude S, R_{2D} is the two-dimensional result for spin S

$$R_{2D}(S, T, \mathscr{H}) = R(S, T, \mathscr{H}, 0) \quad (16)$$

and q is the coordination number for interlayer bonds.

As pointed out by Enting (1973a) bounds for the magnetization can be used to find bounds for the high temperature initial susceptibility so that

$$\chi(S, T, \eta) \leqslant \frac{\chi_{2D}(S, T)}{1-q\eta J\chi_{2D}(S, T)}. \tag{17}$$

These quantities refer to susceptibility per site in each case. One then follows Fisher (1967) in noting that bounds for the susceptibility lead to bounds for the critical temperature so that if the bound (17) diverges at $\bar{T}(S, \eta)$ then

$$T_c(S, \eta) \leqslant \bar{T}(S, \eta) \tag{18}$$

and

$$\bar{T}(S, \eta) - T_c(S, 0) \sim \eta^{1/\gamma}. \tag{19}$$

Since

$$T_c(S, \eta) - T_c(S, 0) \sim \eta^{1/\phi} \tag{20}$$

one could conclude that

$$\phi \leqslant \gamma = \tfrac{7}{4} \tag{21}$$

but it appears that the results given by Grover (1973) extend to spin greater than $\frac{1}{2}$ so that $\phi = \frac{7}{4}$, in which case the bound (18) leads to a bound on the amplitude of the singularity in T_c.

To find a bound for the magnetization at $T_c(S, 0)$ we note that R_{2D} varies as $\mathscr{H}^{1/\delta}$ so that

$$R^* \sim (\eta R^*)^{1/\delta} \tag{22}$$

or

$$R^* \sim \eta^{1/(\delta-1)}. \tag{23}$$

If one has

$$R(S, T_c(S, 0), \mathscr{H} = 0, \eta) \sim \eta^{1/\psi} \tag{24}$$

then

$$\psi \leqslant \delta - 1 = 14.$$

The scaling prediction is $\psi = 14$. This is obtained most easily by following Hankey and Stanley (1972) and assuming that the singular part of the free energy (and hence of the other thermodynamic quantities) is a generalized homogeneous function. In particular putting

$$\epsilon = T - T_c(S, 0) \tag{25}$$

assume

$$R(\lambda^a\epsilon, \lambda^b\mathscr{H}, \lambda^c\eta) = \lambda R(\epsilon, \mathscr{H}, \eta). \tag{26}$$

The well known two-dimensional exponents give

$$a = 8 = \beta^{-1} \tag{27}$$

$$b = 15 = \delta \tag{28}$$

and we also have

$$c = \phi a = 14. \tag{29}$$

The prediction for ψ is obtained by substituting $\epsilon = 0, \mathscr{H} = 0, \lambda^c = \eta^{-1}$ into (26) to give

$$R(0, 0, \eta) = \eta^{1/c} R(0, 0, 1). \tag{30}$$

The generalized homogeneous function assumption is justified by the renormalization group arguments of Grover (1973) so that it appears that $\psi = 14$. In that case by including the appropriate amplitude factors in (22), (23) one could, in principle, find bounds for the amplitude of the singularity in R as $\eta \to 0$.

4. Bounds for a spin one system

As an example of the use of bounds we consider a particular spin one model, described by the hamiltonian (31) proposed by Blume *et al* (1972) as a model for ^{4}He–^{3}He mixtures. References to a number of other applications of this model are given by Oitmaa (1971, 1972) who has analysed the critical behaviour by means of high temperature series expansions.

$$H = -J \sum_{ab}{}' S_a S_b + \Delta \sum_a S_a^2 - \eta \sum_a S_a. \tag{31}$$

The lattice that will be considered is face-centred cubic so that direct comparisons can be made with the results of Oitmaa. The sum Σ' is over all nearest-neighbour pairs. Δ is the difference in chemical potentials for ^{4}He, ^{3}He. η is the conjugate to the superfluid order parameter and will be zero in all the following calculations. The spins are spin 1, so that when the spin (ie the z component) is zero this is interpreted as the presence of ^{3}He at that site. The values ± 1 correspond to ^{4}He, the ordering of these values being interpreted as superfluid ordering. Transforming (31) to an analogue hamiltonian gives, for $\eta = 0$,

$$\hat{H} = -\tfrac{1}{4} J \sum_{ab}{}' (\sigma_a + \sigma_{a'})(\sigma_b + \sigma_{b'}) + \tfrac{1}{4} \Delta \sum_a (2 + 2\sigma_a \sigma_{a'}) + \sum_a k_B T f (1 - \sigma_a \sigma_{a'}) \tag{32}$$

where $S_a = \frac{1}{2}(\sigma_a + \sigma_{a'})$. The sets $\{\sigma_a\}$ and $\{\sigma_{a'}\}$ form two coupled FCC sublattices of spin $\frac{1}{2}$. This has represented the three values of $S_a = 1, 0, -1$ by the four pairs of values of $(\sigma_a, \sigma_{a'})$, ie $(1, 1)$, $(1, -1)$, $(-1, 1)$, $(-1, -1)$. To obtain the correct weighting in the partition function we need a weighting factor on each site which is 1 for $(1, 1)$ and $(-1, -1)$ and $\frac{1}{2}$ for $(1, -1)$ and $(-1, 1)$. This factor is obtained by the final term in hamiltonian (32) so that in $\exp(-\beta \hat{H})$ this term is

$$\exp[-f(1-1)] = 1 \qquad \text{if } S = \pm 1 \tag{33}$$

$$\exp[-f(1+1)] \qquad \text{if } S = 0. \tag{34}$$

The required weighting is given by

$$e^{-2f} = \tfrac{1}{2}$$

$$f = \tfrac{1}{2} \ln 2 = 0.3466\ldots. \tag{35}$$

As pointed out by Griffiths, this hamiltonian is T dependent. We can however treat T as a normal interaction parameter when constructing a partition function and when performing any mathematical operation on that partition function except for differentiating with respect to T. The order parameters and susceptibilities are derivatives with respect to η evaluated at $\eta = 0$.

For $\Delta < 0$ we can use the results of § 2 directly and immediately show that the mean-field critical temperature plotted by Oitmaa (1972) is an upper bound for the true critical temperature. This result can be shown without having to make any detailed study of the T dependent term in (32). One works in terms of mean-field approximations to (31) without ever considering (32).

This particular model is, however, a special case. One can combine the interactions to form an interaction $(k_B Tf - \frac{1}{2}\Delta)\sigma_a\sigma_{a'}$. One can then extend the bounds into the region of positive Δ so long as

$$\Delta < 2k_B T \ln 2. \tag{36}$$

One works within the analogue system (32) and applies bounds for the analogue system to the original spin 1 system by using

$$\langle S_a \rangle = \tfrac{1}{2}(\langle \sigma_a \rangle + \langle \sigma_{a'} \rangle) \tag{37}$$

$$\langle S_a^2 \rangle = \tfrac{1}{2} + \tfrac{1}{2}\langle \sigma_a \sigma_{a'} \rangle. \tag{38}$$

For any strictly positive Δ it is not possible to satisfy (36) for all values of T but this does not prevent one from finding bounds for T_c. If one treats (32) by any generalized mean-field approximation one finds a function $T'(\Delta)$ which is a temperature above which the approximation gives $\langle \sigma_a \rangle_{MFA} = 0$. If $T > \Delta/k_B \ln 2$, $\langle \sigma_a \rangle \leqslant \langle \sigma_a \rangle_{MFA}$ and if $T > T'(\Delta)$, $\langle \sigma_a \rangle_{MFA} = 0$. Since below the actual critical point, T_c, one assumes $\langle \sigma_a \rangle > 0$ one has

$$T_c \leqslant \max(\tfrac{1}{2}\Delta/k_B \ln 2, T'(\Delta)). \tag{39}$$

A number of bounds of this type are plotted on figure 1, there being a number of bounds $T'(\Delta)$ that can be obtained. One finds the bounds $T'(\Delta)$ by treating (32) by a generalized mean-field approximation. Some or all of the interactions in (32) are replaced by their mean-field equivalent.

Replacing all interactions by their mean-field equivalent gives a critical point defined by $k_B T_c$ equal to the sum of interactions on one spin

$$k_B T_c = +\tfrac{1}{4}J2q - \tfrac{1}{2}\Delta + [k_B Tf]_{T=T_c}. \tag{40}$$

q is the coordination number, 12 for the FCC lattice, so

$$k_B T' = \frac{6J - \frac{1}{2}\Delta}{1 - \frac{1}{2}\ln 2}. \tag{41}$$

This is the worst of the bounds that will be given since it is obtained by treating all interactions by their mean-field approximation. Improved bounds are obtained if some interactions are treated exactly. Consider treating the interactions of strength $\frac{1}{4}J$ within each of the FCC sublattices exactly. The other interactions are treated approximated by a mean field of strength $(\frac{1}{4}Jq - \frac{1}{2}\Delta + k_B Tf)\langle \sigma_a \rangle$ at each site.

If on an FCC lattice one has $\langle \sigma_a \rangle = R(T, \mathscr{H})$ for an interaction strength $\frac{1}{4}J$, then

$$\langle \sigma_a \rangle = R[T, (\tfrac{1}{4}Jq - \tfrac{1}{2}\Delta + k_B Tf)\langle \sigma_a \rangle + \mathscr{H}]. \tag{42}$$

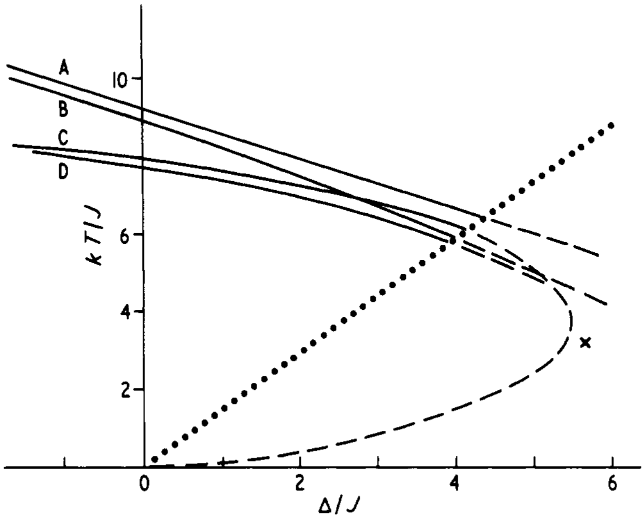

Figure 1. Critical temperature bounds for the ^3He–^4He model. Full curves are bounds, broken curves their analytic continuations. × marks the series estimate of the tricritical point (Oitmaa 1972). The defining equations for bounds are: curve A, (41); curve B, (44); curve C, (45). The dotted line gives the boundary of the region in which the bounds are valid, given by equation (36). Curve D is the T_c obtained from the Bethe approximation to the susceptibility of the analogue system.

The susceptibility $(\mathrm{d}/\mathrm{d}\mathscr{H})\langle\sigma_a\rangle$ is given by

$$\frac{\mathrm{d}}{\mathrm{d}\mathscr{H}}\langle\sigma_a\rangle = \frac{\mathrm{d}R}{\mathrm{d}\mathscr{H}}\left(1+(\tfrac{1}{4}Jq-\tfrac{1}{2}\Delta+k_{\mathrm{B}}Tf)\frac{\mathrm{d}}{\mathrm{d}\mathscr{H}}\langle\sigma_a\rangle\right)$$

$$= \frac{\mathrm{d}R}{\mathrm{d}\mathscr{H}}\left(1-(\tfrac{1}{4}Jq-\tfrac{1}{2}\Delta+k_{\mathrm{B}}Tf)\frac{\mathrm{d}R}{\mathrm{d}\mathscr{H}}\right)^{-1}. \qquad (43)$$

$\mathscr{H}$ is an artificial field introduced to obtain expressions for the susceptibility. In the absence of a field this susceptibility can be given a real interpretation as a sum of two spin correlation functions. $\mathrm{d}R/\mathrm{d}\mathscr{H}$ is the initial susceptibility of an FCC lattice. In this approximation, T' is the temperature at which the denominator of (43) vanishes so that one has

$$\Delta = 2\left[3J+k_{\mathrm{B}}T'f-\left(\frac{\mathrm{d}R}{\mathrm{d}\mathscr{H}}\right)^{-1}\right]. \qquad (44)$$

This bound is evaluated and plotted in figure 1. $\mathrm{d}R/\mathrm{d}\mathscr{H}$ as a function of T' was found by using the representation for the FCC susceptibility given by Sykes *et al* (1972). This bound is quite close to the bound given by (41). This is because an FCC lattice has a large coordination number and so the susceptibility is given to a comparatively close approximation by the mean-field approximation. Treating the sublattice exactly does not give a great improvement.

Another possibility is to treat the interactions between $\sigma_a, \sigma_{a'}$ exactly and all other interactions by mean field. This means that one treats a spin S_a on its own, treating the

Δ term exactly. The Tf term gives the correct weightings to the partition functions of the spin. This approximation is exactly the mean-field approximation of treating one spin exactly but approximating its interactions with other spins by a mean-field approximation, as done by Oitmaa (1972).

The susceptibility expression is, above T_c,

$$\frac{\mathrm{d}}{\mathrm{d}\eta}\langle S\rangle = \frac{2}{2+e^{\beta\Delta}-2\beta qJ}. \tag{45}$$

The critical point is found by equating the denominator to zero. The curve which has been given by Oitmaa (1972) is also plotted on figure 1.

The bounds are valid up to $\Delta/J \simeq 4{\cdot}0$ and so do not apply near the tricritical point which was estimated by Oitmaa to be at $\Delta/J \simeq 5{\cdot}7$. From figure 1 it will be seen that the bound from (45) is the best bound on T_c over most of the values of Δ. There is however a small range of Δ values for which the bound (44) is best.

It is possible to improve these bounds by breaking the lattice into small clusters, treating interactions within each cluster exactly and treating interactions between clusters by the mean-field approximation. This is not attempted here because experience with other systems indicates that the improvement obtained by using clusters of a reasonable size is slight.

Enting (1973c) has shown that a generalized random-phase approximation gives upper bounds for $\langle\sigma_a\sigma_b\rangle$. This would be useful in the present case because of the relation (38) and the interpretation of $\langle S^2\rangle$ as the ^{4}He concentration. The full expression for the bound involves the lattice Green functions for an FCC lattice and is not quoted here.

Since the bound (41) is obtained by treating all the interactions in the analogue system by the mean-field approximation it can be obtained using the results of Fisher (1967) and Thompson (1972). The bound that is obtained for magnetization is not, however, the mean-field solution for spin 1 which is obtained by treating the T-dependent weighting factors and the ΔS^2 interaction exactly.

In a spin $\frac{1}{2}$ system the Bethe approximation gives an upper bound for the susceptibility (Fisher 1967). Figure 1 shows that the T_c bound obtained by applying this result to the analogue system gives a better bound than any of the techniques discussed above. To obtain bounds for the 'magnetization' it is, however, necessary to use one of the mean-field bounds.

5. Conclusions

A number of useful results have been proved in the preceding sections. Earlier generalized mean-field bounds have been extended to the case of arbitrary spin and a new bound has been obtained for an exponent describing crossover behaviour of the magnetization in the anisotropic Ising model. The bound obtained corresponds to the scaling law prediction for this exponent.

The bounds for the ^{4}He–^{3}He model are useful in illustrating the various methods of obtaining bounds for spin one systems. They do not however give a large amount of significant information concerning the ^{4}He–^{3}He model since the proof does not hold near the tricritical point.

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