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Bounds for Ising systems

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Abstract. Ising systems are approximated by a generalized mean-field approximation in which only some of the interactions are replaced by their expectation values. If all the interactions are positive then it is shown that a self-consistent solution exists for the magnetization in this model and that it gives an upper bound for the true magnetization. Using this mean-field approximation, a generalization of the random-phase approximation is obtained. This is shown to give an upper bound for the two-spin correlation functions.

1. Introduction

One of the most widely used approximations in statistical mechanics is the mean-field approximation. As well as being used frequently in the interpretation of experimental results, it is also of interest for a number of purely theoretical reasons. The mean-field approximation becomes exact for certain long range forces. In the present work the concept that will be considered is that the mean-field approximation gives rigorous bounds for various thermodynamic quantities. There are a number of results of this type in the literature (Fisher 1967, Thompson 1971). The following work generalizes some of these earlier results by considering a model in which only some of the interactions are treated by their mean-field approximations while the remainder of the interactions are treated exactly. One of the earliest applications of this type of approximation was by Stout and Chisholm (1962). This approximation has also been used to obtain bounds for the anisotropic Ising system (Enting 1973a, b).

Section 2 gives the proof, in full, of the basic result that if all interactions in a system are ferromagnetic then replacing any of the interactions by its mean-field equivalent will increase the expectation value of any of the spins. In § 3 this result is related to the generalized mean-field approximation. It is shown that this generalized approximation will actually have self-consistent solutions for the expectation values of the spins and that these solutions are upper bounds for the true expectation values. The relationship between these results and the work of Thompson (1971) is discussed. In § 4, expressions are obtained for the approximate two-spin correlation functions. These approximations, which are shown to correspond to a generalized random-phase approximation, give upper bounds for the exact two-spin correlation functions. Summing these correlation functions, one recovers bounds for the susceptibility of the type considered by Enting (1973a, b).

In § 5 a number of systems for which these bounds are useful, are considered. Since the susceptibility bounds sometimes predict a variation of critical temperature of the type obtained from scaling theory it is of interest to consider the circumstances under which this scaling result may be expected to hold.

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2. Bounds for a single replacement

The basic hamiltonian that will be considered is

$$H = -\sum_{\{a,a'\}} J_{aa'}\sigma_a\sigma_{a'} - \sum_{\{a\}} \mathscr{H}_a\sigma_a. \tag{1}$$

The σ_a are a set of Ising spins, ± 1 indexed by $\{a\}$. $\{a, a'\}$ is the set of all pairs of indices. In all the sums over this set that will be used, it is sufficient to sum only over those pairs for which $J_{aa'}$ is nonzero.

The thermodynamic quantities are regarded as being functions of the variables $J_{aa'}/T \geqslant 0$ and $\mathscr{H}_a/T \geqslant 0$. The proof following is only valid when these quantities are non-negative. In the special case of all $\mathscr{H}_a$ equal they will be denoted by the variable $\mathscr{H}$.

The main result that will be proved in this section is that if hamiltonian (1) is modified by replacing one interaction $-J_{aa'}\sigma_a\sigma_{a'}$ by $-J_{aa'}(\langle\sigma_a\rangle\sigma_{a'} + \langle\sigma_{a'}\rangle\sigma_a)$ then the expectation value of every spin is increased. The expectation values above are calculated from a hamiltonian in which neither $J_{aa'}\sigma_a\sigma_{a'}$ nor its mean-field equivalent is present.

To concentrate attention on only one interaction, we write (1) in the form

$$H = \bar{H} - J\sigma_r\sigma_s \tag{2}$$

and put

$$G = \bar{H} - J\langle\sigma_r\rangle\sigma_s - J\langle\sigma_s\rangle\sigma_r \tag{3}$$

where

$$\langle \quad \rangle \equiv \langle \quad \rangle_{\bar{H}}. \tag{4}$$

Using the expression used by Thompson (1971) one has

$$\langle\sigma_a\rangle_H = \frac{\langle\sigma_a\rangle + v\langle\sigma_a\sigma_r\sigma_s\rangle}{1 + v\langle\sigma_r\sigma_s\rangle} \tag{5}$$

$$\langle\sigma_a\rangle_G = \frac{\langle\sigma_a\rangle + q_s\langle\sigma_a\sigma_s\rangle + q_r\langle\sigma_a\sigma_r\rangle + q_rq_s\langle\sigma_a\sigma_r\sigma_s\rangle}{1 + q_s\langle\sigma_s\rangle + q_r\langle\sigma_r\rangle + q_rq_s\langle\sigma_r\sigma_s\rangle} \tag{6}$$

where

$$q_r = \tanh(\beta J\langle\sigma_s\rangle) \tag{7}$$

$$q_s = \tanh(\beta J\langle\sigma_r\rangle) \tag{8}$$

$$v = \tanh(\beta J). \tag{9}$$

For any hamiltonian of type (1) it can be proved that

$$\langle\sigma_a\rangle_H \geqslant 0 \tag{10}$$

and

$$\frac{1}{\beta}\frac{\partial\langle\sigma_a\rangle_H}{\partial\mathscr{H}_b} = \langle\sigma_a\sigma_b\rangle_H - \langle\sigma_a\rangle_H\langle\sigma_b\rangle_H \geqslant 0 \tag{11}$$

$$\frac{1}{\beta}\frac{\partial\langle\sigma_a\rangle_H}{\partial J_{bb'}} = \langle\sigma_a\sigma_b\sigma_{b'}\rangle_H - \langle\sigma_a\rangle_H\langle\sigma_b\sigma_{b'}\rangle_H \geqslant 0. \tag{12}$$

These results have been proved (for more general hamiltonians than (1)) by Kelly and Sherman (1968).

Another result that will be needed is that given by Griffiths *et al* (1970):

$$\langle\sigma_a\sigma_r\sigma_s\rangle - \langle\sigma_a\sigma_r\rangle\langle\sigma_s\rangle - \langle\sigma_r\sigma_s\rangle\langle\sigma_a\rangle - \langle\sigma_s\sigma_a\rangle\langle\sigma_r\rangle + 2\langle\sigma_a\rangle\langle\sigma_r\rangle\langle\sigma_s\rangle \leqslant 0. \tag{13}$$

It is also necessary to use the obvious fact that

$$\langle\sigma_a\rangle \leqslant 1. \tag{14}$$

Returning to the 'mean-field' form defined by (3) we have

$$q_s - v\langle\sigma_r\rangle \geqslant 0 \tag{15}$$

$$q_r - v\langle\sigma_s\rangle \geqslant 0. \tag{16}$$

These are merely particular cases of the relation:

$$\tanh ab - a\tanh b \geqslant 0, \qquad 0 \leqslant a \leqslant 1, \qquad b \geqslant 0. \tag{17}$$

The equality holds for $b = 0$ and the derivative of (17) with respect to b is $a(\tanh b - \tanh ab)(\tanh b + \tanh ab)$ which is positive if $0 \leqslant a \leqslant 1$ and $b > 0$, and so (17) is true in this range. Multiplying (15) and (16) gives

$$q_r q_s \geqslant \langle\sigma_s\rangle v q_s + \langle\sigma_r\rangle v q_r - v^2\langle\sigma_r\rangle\langle\sigma_s\rangle. \tag{18}$$

This result now enables us to prove the basic assertion that

$$\langle\sigma_a\rangle_G \geqslant \langle\sigma_a\rangle_H. \tag{19}$$

From (5), (6),

$$\begin{aligned} Q &= (\langle\sigma_a\rangle_G - \langle\sigma_a\rangle_H)(1 + v\langle\sigma_r\sigma_s\rangle)(1 + q_s\langle\sigma_s\rangle + q_r\langle\sigma_r\rangle + q_r q_s\langle\sigma_r\rangle\langle\sigma_s\rangle) \\ &= ((\langle\sigma_a\sigma_s\rangle - \langle\sigma_a\rangle\langle\sigma_s\rangle)q_s + ((\langle\sigma_a\sigma_r\rangle - \langle\sigma_r\rangle\langle\sigma_a\rangle)q_r + ((\langle\sigma_a\sigma_r\sigma_s\rangle \\ &\quad - \langle\sigma_a\rangle\langle\sigma_r\sigma_s\rangle)q_r q_s + v(\langle\sigma_a\rangle\langle\sigma_r\sigma_s\rangle - \langle\sigma_a\sigma_r\sigma_s\rangle) + vq_s(\langle\sigma_a\sigma_s\rangle\langle\sigma_r\sigma_s\rangle \\ &\quad - \langle\sigma_s\rangle\langle\sigma_a\sigma_r\sigma_s\rangle) + vq_r(\langle\sigma_a\sigma_r\rangle\langle\sigma_r\sigma_s\rangle - \langle\sigma_r\rangle\langle\sigma_a\sigma_r\sigma_s\rangle). \end{aligned} \tag{20}$$

In the first line, q_r, q_s, $q_r q_s$ multiply quantities that are non-negative, by (11), and (12). Replacing q_s by $v\langle\sigma_r\rangle$, q_r by $v\langle\sigma_s\rangle$ and $q_r q_s$ by the right-hand side of (18) will then give a quantity less than Q:

$$\begin{aligned} Q \geqslant{} & (\langle\sigma_a\sigma_s\rangle\langle\sigma_r\rangle + \langle\sigma_a\sigma_r\rangle\langle\sigma_s\rangle - 2\langle\sigma_a\rangle\langle\sigma_r\rangle\langle\sigma_s\rangle + \langle\sigma_a\rangle\langle\sigma_r\sigma_s\rangle - \langle\sigma_a\sigma_r\sigma_s\rangle) \\ & - v^2(\langle\sigma_a\sigma_r\sigma_s\rangle - \langle\sigma_a\rangle\langle\sigma_r\sigma_s\rangle)\langle\sigma_r\rangle\langle\sigma_s\rangle v \\ & + v\langle\sigma_r\sigma_s\rangle[q_r(\langle\sigma_a\sigma_r\rangle - \langle\sigma_a\rangle\langle\sigma_r\rangle) + q_s(\langle\sigma_a\sigma_s\rangle - \langle\sigma_a\rangle\langle\sigma_s\rangle)]. \end{aligned} \tag{21}$$

One can find a lower bound for this expression by again replacing q_r, q_s to give

$$\begin{aligned} Q \geqslant{} & -v(1 + v\langle\sigma_r\rangle\langle\sigma_s\rangle)(\langle\sigma_a\sigma_r\sigma_s\rangle - \langle\sigma_a\sigma_r\rangle\langle\sigma_s\rangle \\ & - \langle\sigma_a\sigma_s\rangle\langle\sigma_r\rangle - \langle\sigma_r\sigma_s\rangle\langle\sigma_a\rangle + 2\langle\sigma_a\rangle\langle\sigma_r\rangle\langle\sigma_s\rangle) \\ \geqslant{} & 0 \end{aligned} \tag{22}$$

by (13). Referring back to (20) it is apparent that

$$\langle\sigma_a\rangle_G \geqslant \langle\sigma_a\rangle_H. \tag{23}$$

3. Generalized mean-field solutions

In general, mean-field solutions are obtained by means of a self-consistent equation. For the replacement considered in the previous section, the self-consistent equation would be found by calculating expectation values from the hamiltonian

$$G' = \bar{H} - J\langle\sigma_r\rangle_{G'}\sigma_s - J\langle\sigma_s\rangle_{G'}\sigma_r. \tag{24}$$

To examine this bound, we construct a sequence of hamiltonians

$$G(0) = G$$
$$G(n) = \bar{H} - J\langle\sigma_r\rangle_{G(n-1)}\sigma_s - J\langle\sigma_s\rangle_{G(n-1)}\sigma_r. \tag{25}$$

For all spins σ_a, $\langle\sigma_a\rangle_G \geqslant \langle\sigma_a\rangle_H$ and by (11) which implies that all expectation values are increasing functions of the interaction strengths, one has by induction,

$$\langle\sigma_a\rangle_{G(n)} \geqslant \langle\sigma_a\rangle_{G(n-1)}. \tag{26}$$

Since the sequence of $\langle\sigma_a\rangle_{G(n)}$ is increasing and is bounded above by 1·0, it must have a limit:

$$\langle\sigma_a\rangle_{G(\infty)} = \lim_{n\to\infty} \langle\sigma_a\rangle_{G(n)}. \tag{27}$$

The values $\langle\sigma_r\rangle_{G(\infty)}$, $\langle\sigma_s\rangle_{G(\infty)}$ are self-consistent solutions of (24) (a formal proof of this based on the definition of the limit of a sequence is trivial) and so the arguments above have proved the existence of a solution of (24) and have shown that $\langle\sigma_a\rangle_{G'}$ gives an upper bound for $\langle\sigma_a\rangle_H$.

What is really interesting is to consider a succession of replacements of the type considered in the previous section.

Rewriting hamiltonian (1) as

$$H = H_0 - \sum_{\{b,b'\}\subseteq\{a,a'\}}^{*} J_{bb'}\sigma_b\sigma_{b'} = H_0 - \sum_{k=1}^{m} J(k)\sigma_{b(k)}\sigma_{b'(k)} \tag{28}$$

k is an integer used as an index for the m interactions considered explicitly in (28).

(28) is taken to be the basic or 'true' hamiltonian. It is convenient to consider the following 'approximate' hamiltonians that give bounds for spin expectation values:

$$H(n) = H_0 - \sum_{k=1}^{n} J(k)(\langle\sigma_{b(k)}\rangle_{H(k)}\sigma_{b'(k)} + \langle\sigma_{b'(k)}\rangle_{H(k)}\sigma_{b(k)})$$
$$- \sum_{k=n+1}^{m} J(k)\sigma_{b(k)}\sigma_{b'(k)}, \qquad 0 \leqslant n < m \tag{29}$$

so

$$H(0) = H \tag{30}$$

$$H^*(n) = H_0 - \sum_{k=1}^{m} J(k)(\langle\sigma_{b(k)}\rangle_{H^*(n-1)}\sigma_{b'(k)} + \langle\sigma_{b'(k)}\rangle_{H^*(n-1)}\sigma_{b(k)}) \tag{31}$$

$$H^*(0) = H(m). \tag{32}$$

The results above show that $\langle\sigma_a\rangle_{H(n)}$, which is defined by self-consistent equations, exists and

$$\langle\sigma_a\rangle_{H(n)} \geqslant \langle\sigma_a\rangle_H. \tag{33}$$

In a manner completely analogous to the proof of (26) one has

$$\langle\sigma_a\rangle_{H^*(n+1)} \geqslant \langle\sigma_a\rangle_{H^*(n)} \tag{34}$$

and since the sequence of $\langle\sigma_a\rangle_{H^*(n)}$ is bounded and increasing there is a limit $\langle\sigma_a\rangle_{H^*(\infty)}$ which corresponds to self-consistent solutions of

$$H' = H_0 - \sum_{k=1}^{m} J(k)(\langle\sigma_{b(k)}\rangle_{H'}\sigma_{b'(k)} + \langle\sigma_{b'(k)}\rangle_{H'}\sigma_{b(k)}). \tag{35}$$

In the end, combining the inequalities gives

$$\langle\sigma_a\rangle_{H'} \geqslant \langle\sigma_a\rangle_{H}. \tag{36}$$

In the proof given by Thompson (1971) it is not possible to consider replacing only some interactions by their mean-field equivalents, so the present proof still represents a significant advance. Firstly it has been possible to prove the existence of self-consistent solutions of the generalized mean-field hamiltonians. Secondly, in establishing (36) it has not been necessary to appeal to the translational invariance of the system. Since one does not have to have all spins equivalent, the result (36) will apply to the analogue system defined by Griffiths (1969) to represent spins other than $\frac{1}{2}$. This makes it straightforward to generalize most of the results presented here to the case of Ising systems with arbitrary spin.

The main limitation on the range of validity of these bounds comes from equation (13). In particular this equation has not been proved for systems with four-spin interactions. In principle one can find bounds for such systems by a simple generalization of the graphical expressions obtained by Fisher (1967). It is, however, not possible in general to express these bounds as closed form expressions.

4. Generalized random-phase approximation

Referring back to hamiltonian (1) we note that it is a function of the independent variables $J_{aa'}/T$, $\mathscr{H}_a/T$. Denoting derivatives with respect to $\mathscr{H}_a$ with the other independent variables fixed, by $\mathrm{d}/\mathrm{d}\mathscr{H}_a$ and using $\partial/\partial\mathscr{H}_a$ to denote differentiating only the explicit $\mathscr{H}_a$ dependence, ie $\{\langle\sigma_s\rangle\}$ fixed, one has from (31)

$$\frac{\mathrm{d}}{\mathrm{d}\mathscr{H}_a}\langle\sigma_b\rangle_{H^*(m)} = \frac{\partial}{\partial\mathscr{H}_a}\langle\sigma_b\rangle_{H^*(m)} + \sum_{\{c,c'\}} \frac{\partial\langle\sigma_b\rangle_{H^*(m)}}{\partial\mathscr{H}_c} J_{cc'} \frac{\mathrm{d}\langle\sigma_{c'}\rangle_{H^*(m-1)}}{\mathrm{d}\mathscr{H}_a} \tag{37}$$

$$= \beta\langle\sigma_a\sigma_b\rangle_{H^*(m)} + \sum_{\{c\},\{c'\}} \langle\sigma_b\sigma_c\rangle_{H^*(m)}\beta J_{cc'} \frac{\mathrm{d}\langle\sigma_{c'}\rangle_{H^*(m-1)}}{\mathrm{d}\mathscr{H}_a}. \tag{38}$$

In the high temperature region at $\mathscr{H} = 0$ one has

$$\langle\sigma_a\rangle_H = \langle\sigma_a\rangle_{H^*(m)} = 0 \tag{39}$$

(38) becomes

$$\frac{\mathrm{d}}{\mathrm{d}\mathscr{H}_a}\langle\sigma_b\rangle_{H^*(m)} = \beta\langle\sigma_a\sigma_b\rangle_{H_0} + \sum_{\{c\},\{c'\}} \langle\sigma_b\sigma_c\rangle_{H_0}\beta J_{cc'} \frac{\mathrm{d}\langle\sigma_c\rangle_{H^*(m-1)}}{\mathrm{d}\mathscr{H}_a}. \tag{40}$$

The derivatives are investigated by putting $\mathscr{H}_a = \delta\mathscr{H}_a$ so

$$\langle\sigma_b\rangle_H|_{\delta\mathscr{H}_a} \leqslant \langle\sigma_b\rangle_{H^*(m)}|_{\delta\mathscr{H}_a} \leqslant \langle\sigma_b\rangle_{H^*(m+1)}|_{\delta\mathscr{H}_a}. \tag{41}$$

So dividing by $\delta\mathscr{H}_a \to 0$, one has for high temperatures,

$$\left.\frac{\mathrm{d}\langle\sigma_b\rangle_H}{\mathrm{d}\mathscr{H}_a}\right|_{\mathscr{H}=0} \leqslant \left.\frac{\mathrm{d}\langle\sigma_b\rangle_{H^*(m)}}{\mathrm{d}\mathscr{H}_a}\right|_{\mathscr{H}=0} \leqslant \left.\frac{\mathrm{d}\langle\sigma_b\rangle_{H^*(m-1)}}{\mathrm{d}\mathscr{H}_a}\right|_{\mathscr{H}=0}. \tag{42}$$

Assuming that

$$\lim_{m\to\infty}\lim_{\delta\mathscr{H}_a\to 0}\left.\frac{\langle\sigma_b\rangle_{H^*(m)}}{\delta\mathscr{H}_a}\right|_{\mathscr{H}=0} = \lim_{\delta\mathscr{H}_a\to 0}\lim_{m\to\infty}\left.\frac{\langle\sigma_b\rangle_{H^*(m)}}{\delta\mathscr{H}_a}\right|_{\mathscr{H}=0}, \tag{43}$$

one can take the limit of (40) and find

$$\begin{aligned}\beta\langle\sigma_a\sigma_b\rangle_H &= \left.\frac{\mathrm{d}}{\mathrm{d}\mathscr{H}_a}\langle\sigma_b\rangle_H\right|_{\mathscr{H}=0}\\ &\leqslant \left.\frac{\mathrm{d}}{\mathrm{d}\mathscr{H}_a}\langle\sigma_b\rangle_{H^*(\infty)}\right|_{\mathscr{H}=0} = \beta\langle\sigma_a\sigma_b\rangle_{\mathrm{GRPA}}\\ &= \beta\langle\sigma_a\sigma_b\rangle_{H_0} + \sum_{\{c\},\{c'\}}\langle\sigma_a\sigma_c\rangle_{H_0}\beta J_{cc'}\left.\frac{\mathrm{d}}{\mathrm{d}\mathscr{H}_a}\langle\sigma_{c'}\rangle_{H^*(\infty)}\right|_{\mathscr{H}=0}.\end{aligned} \tag{44}$$

The right-hand side of (44) corresponds to a generalized random-phase approximation GRPA.

If one has hamiltonian (1) in the form

$$H = H_0 - \sum_{\boldsymbol{r}_i}\sum_{\boldsymbol{a}_j} J(\boldsymbol{a}_j)\sigma(\boldsymbol{r}_i)\sigma(\boldsymbol{r}_i+\boldsymbol{a}_j) \tag{45}$$

then it is possible to solve equation (44) in reciprocal space, if one has translational invariance. (This necessitates taking a thermodynamic limit $N \to \infty$ at this point.)

Putting

$$\langle\sigma(\boldsymbol{r})\sigma(\boldsymbol{r}')\rangle_{\mathrm{GRPA}} = C(\boldsymbol{r}'-\boldsymbol{r}) \tag{46}$$

and

$$\langle\sigma(\boldsymbol{r})\sigma(\boldsymbol{r}')\rangle_{H_0} = C_0(\boldsymbol{r}'-\boldsymbol{r}) \tag{47}$$

equation (40) becomes

$$\beta C(\boldsymbol{r}) = \beta C_0(\boldsymbol{r}) + \sum_{\boldsymbol{r}',\boldsymbol{a}_j} C_0(\boldsymbol{r}')\beta J(\boldsymbol{a}_j)\beta C(\boldsymbol{r}-\boldsymbol{r}'-\boldsymbol{a}_j) \tag{48}$$

in reciprocal space,

$$\bar{C}(\boldsymbol{q}) = \bar{C}_0(\boldsymbol{q}) + \sum_{\boldsymbol{a}} \bar{C}_0(\boldsymbol{q})\bar{C}(\boldsymbol{q})\beta J(\boldsymbol{a}_j)\exp(\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{a}_j) \tag{49}$$

or

$$\bar{C}(\boldsymbol{q}) = \frac{\bar{C}_0(\boldsymbol{q})}{1-\Sigma_{\boldsymbol{a}_j}\beta J(\boldsymbol{a}_j)\exp(\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{a}_j)\bar{C}_0(\boldsymbol{q})}. \tag{50}$$

Because the $\exp(\mathrm{i}\boldsymbol{q}\,.\,\boldsymbol{r})$ are not positive numbers in general, the $\bar{C}(\boldsymbol{q})$ is not a bound for the true value, except in the case of $\boldsymbol{q} = \boldsymbol{0}$ where one has the zero-field susceptibility which is given by a sum over equation (44).

The bound (44) is a generalization of the result due to Fisher (1967) that the random-phase approximation gives an upper bound for the two-spin correlation functions. The susceptibility bound obtained by summing (44) or putting $\boldsymbol{q} = \boldsymbol{0}$ in (50) corresponds to the susceptibility bounds quoted by Enting (1973a, b).

5. Applications

5.1. The anisotropic Ising model

In equation (45) H_0 corresponds to L two-dimensional layers each of which is a simple quadratic Ising system. The vectors $\boldsymbol{a}_j$ are given by (0, 0, 1) for an anisotropic SC lattice and $(0, \frac{1}{2}, \frac{1}{2})$, $(0, -\frac{1}{2}, \frac{1}{2})$, $(\frac{1}{2}, 0, \frac{1}{2})$ and $(-\frac{1}{2}, 0, \frac{1}{2})$ for an anisotropic FCC lattice. In this latter case the layers are staggered with respect to each other. The limit $L \to \infty$ is taken and the layers are taken to the limit of an infinite two-dimensional system. Summing the correlation bounds of the previous section, ie taking $\boldsymbol{q} = \boldsymbol{0}$ in (50) gives

$$\chi(T, \eta) \leqslant \frac{\chi_{2\mathrm{D}}(T)}{1 - \eta J z \chi_{2\mathrm{D}}(T)/N} \tag{51}$$

where N is the number of spins per layer. z is the number of interlayer bonds from each site, 2 in SC, 8 in FCC. ηJ is the interplane interaction strength.

Since one has that the two-dimensional susceptibility

$$\chi_{2\mathrm{D}} \sim (T - T_{\mathrm{c}}(2\mathrm{D}))^{-7/4} \tag{52}$$

from Fisher (1959), the expression (51) will diverge at T^* where

$$(T^*(\eta) - T_{\mathrm{c}}(\eta = 0)) \sim \eta^{4/7}. \tag{53}$$

Since the bound (51) is valid above the critical point (equation (42) uses $\langle \sigma_a \rangle = 0$), the bound implies that the singularity in $\chi(T, \eta)$ must be at some temperature below $T^*(\eta)$

$$T_{\mathrm{c}}(\eta) - T_{\mathrm{c}}(\eta = 0) \leqslant T^*(\eta) - T_{\mathrm{c}}(\eta = 0) \sim \eta^{4/7} \tag{54}$$

so that if

$$T_{\mathrm{c}}(\eta) - T_{\mathrm{c}}(\eta = 0) \sim \eta^{1/\phi} \tag{55}$$

then

$$\phi \leqslant \tfrac{7}{4}. \tag{56}$$

If one actually has $\phi = \frac{7}{4}$ as indicated by the latest series analysis results (Krasnow *et al* 1973) then equation (54) can be used to obtain a bound for the amplitude of the singularity in $T_{\mathrm{c}}(\eta)$ (Enting 1973c).

5.2. Two-layer systems

Taking $L = 2$ for the number of layers in systems described in the previous section gives a two-layer system. Scaling theory predictions (Abe 1970, Mikulinskii 1971) suggest that the variation of T_{c} should be of the form (55) with $\phi = \frac{7}{4}$.

If one considers a system with $L = \infty$ as in the previous section and treats the coupling between alternate pairs of layers by a mean-field approximation then one has, using (12)

$$\phi_{L=2} \leqslant \phi_{L=\infty} \leqslant \tfrac{7}{4} \quad \text{and} \quad \phi_{L=\infty} \leqslant \gamma_{L=2} = \tfrac{7}{4}. \tag{57}$$

5.3. Second-neighbour Ising systems

On the FCC lattice, the $L = 2$ system described above is isomorphic to a second-neighbour Ising system in two dimensions. The nearest-neighbour interaction J_1, corresponds to ηJ while the second-neighbour interaction J_2 corresponds to the intraplane interaction of the two layer system.

The bound on critical temperature becomes

$$T_c(J_1) - T_c(J_1 = 0) \leqslant T^*(J_1) - T_c(J_1 = 0) \sim J_1^{4/7}. \tag{58}$$

$T_c(J_1 = 0)$ is given by Kramers and Wannier (1941): $\tanh(J_2/kT_c(J_1 = 0)) = \sqrt{2}-1$.

It is also possible to treat the J_1 interaction exactly and the J_2 interaction by a mean-field approximation so that

$$T_c(J_2) - T_c(J_2 = 0) \leqslant T^*(J_2) - T_c(J_2 = 0) \sim J_2^{4/7} \tag{59}$$

so that if

$$T_c(J_2) - T_c(J_2 = 0) \sim J_2^{1/\phi} \tag{60}$$

then

$$\phi \leqslant \tfrac{7}{4}. \tag{61}$$

In this case the actual behaviour seems to be that $T_c(J_2)$ varies analytically through $J_2 = 0$ so that

$$\phi = 1. \tag{62}$$

The smoothness postulate (Griffiths 1971) provides a ready explanation of why this last case has an analytic $T_c(J_2)$ while all previous examples appeared to have singularities in T_c. The argument treats a line of critical points as the boundary of a first-order transition surface and predicts changes in the behaviour of the critical properties only when the nature of the first-order transition changes. The first-order transition here is on varying the applied field $\mathscr{H}$ through $\mathscr{H} = 0$ to reverse the direction of the magnetization. If one has a coupling strength η connecting two independent sublattices then this first-order transition disappears for $\eta < 0$ as there is never any spontaneous magnetization so one cannot have the situation of a finite change in magnetization for an infinitesimal change in field. One would therefore expect singularities of the scaling law type only when the scaling parameter represents a coupling between two independent sublattices.

In the three-dimensional second-neighbour system $J_1 = 0$ corresponds to two independent FCC lattices so it would be expected that the bound

$$T_c(J_1) - T_c(J_1 = 0) \leqslant T^*(J_1) - T_c(J_1 = 0) \sim J_1^{4/5} \tag{63}$$

may actually describe the singularity in T_c.

6. Conclusions

In the preceding sections a generalized mean-field approximation has been discussed. It has been shown that self-consistent solutions exist for this approximation and that these solutions give upper bounds for the true solutions. These bounds have been used to obtain bounds for the exponent describing the variation of critical temperature. The formal definition of these exponents involves defining them in terms of limits, a procedure which is quite straightforward. From (50),

$$1-\sum_{\boldsymbol{a}_j}\beta J(\boldsymbol{a}_j)\bar{C}_0(\boldsymbol{q}=\boldsymbol{0}, T^*)=0 \tag{64}$$

at T^* an upper bound for T_c

$$\ln \bar{C}_0(\boldsymbol{q}=\boldsymbol{0}, T^*) = -\ln\left(\sum_{\boldsymbol{a}_j}\beta J(\boldsymbol{a}_j)\right) \geqslant 0 \tag{65}$$

$$\ln(T_c - T_c(0)) \leqslant \ln(T^* - T_c(0)) < 0, \qquad \text{for small } J(\boldsymbol{a}_j). \tag{66}$$

So

$$-\frac{\ln \Sigma\beta^* J(\boldsymbol{a}_j)}{\ln(T_c(\eta)-T_c(0))} \geqslant \frac{\ln \bar{C}(\boldsymbol{q}=\boldsymbol{0}, T^*)}{\ln(T^*-T_c(0))} \tag{67}$$

and

$$\phi = \lim \frac{\ln \Sigma\beta^* J(\boldsymbol{a}_j)}{\ln(T_c(\eta)-T_c(0))} \leqslant -\lim \frac{\ln \bar{C}(\boldsymbol{q}=\boldsymbol{0}, T^*)}{\ln(T^*-T_c(0))} = \gamma \tag{68}$$

γ is the susceptibility exponent for $J(\boldsymbol{a}_j)=0$.

These bounds on the 'crossover exponent' describing the variation of critical temperature correspond to the scaling-law predictions. It has been pointed out that although these bounds are valid for a number of situations, in many cases the limiting behaviour of the critical temperature may not be of the same form as the bounds. The smoothness postulate can be used to decide if the critical temperature is likely to have a singularity.

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