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Critical behaviour of a two-layer Ising system

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Abstract. A two-layer Ising system, in which the coupling strengths within each layer are in general unequal and also differ from the coupling strength between the layers, is studied by means of a mean-field theory, a generalized mean-field theory, a scaling approach, and high-temperature series expansions. A number of predictions regarding the variation of the critical temperature and magnetization within each layer, with J_{12} , the interlayer coupling strength, are made.

1. Introduction

As a result of the considerable amount of work that has been carried out in recent years we now have a rather good understanding of the critical behaviour of the Ising model in its standard form in which the lattice is infinite in extent in all directions. For reviews of the subject the reader is referred to articles by Fisher (1967a) and Domb (1974).

Real crystals of course are not infinite in extent and we can expect modifications to the infinite crystal results due to both: (i) the finite size of the lattice; and (ii) the presence of free surfaces. There exist reviews of such effects (Fisher 1971, Watson 1972).

An early investigation of an Ising system which is of finite extent in one lattice direction is due to Ballentine (1964). Using high-temperature series expansions he studied a system of two infinite quadratic layers coupled together and concluded that this system had two-dimensional critical behaviour. This work was extended by Allan (1970) to films of up to five layers. In both of these investigations it was assumed that all the intralayer exchange constants were equal, although for the case of two layers, Allan (unpublished) has also considered the case where the interlayer coupling differs from the coupling within layers. For the two-layer system where the coupling between layers differs from the coupling within the layers Abe (1970) and Mikulinskii (1971) have developed scaling theories describing the critical behaviour for small interlayer coupling.

A different approach has been to study the effect of a free surface on an otherwise infinite lattice. Mills (1971) has investigated a semi-infinite Heisenberg model using a Landau–Ginsburg approach and has predicted the possible occurrence of long-range order in the surface layer at temperatures above the bulk transition temperature. Such a phenomenon apparently occurs in binary alloys (Højlund Nielsen 1973). The effect of a free surface has also been studied by Binder and Hohenberg (1972) by means of a Landau–Ginsburg theory, series expansions, and a scaling theory. A scaling theory for finite-size and surface effects has been developed independently by Fisher and co-workers (Fisher and Barber 1972, Barber and Fisher 1973).

The aim of the present work is to investigate the critical behaviour of a two-layer Ising system illustrated in figure 1. The system consists of two infinite quadratic lattices with exchange constants J_1 and J_2 (with in general $J_1 \neq J_2$) coupled by interactions of strength J_{12} . We feel that this model is worthy of study for a number of reasons:

(i) It is an obvious generalization of the work of Ballentine and Allan referred to above, to the case where the exchange constants are not all equal. The results may be applicable to experiments (as yet future) on thin films of one material on another.

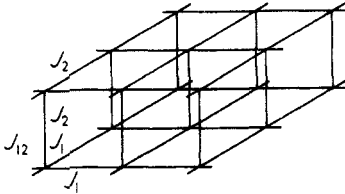


Figure 1. The two-layer Ising system.

(ii) It can also be used, less directly, as a model for general surface effects. It is to be expected that at a free surface the lattice parameters will differ from those of the bulk material. Thus one may expect that the coupling constants both within the surface layer (or layers) and between the surface and the bulk material may differ from the coupling constants in the interior. The significant feature of this model is that it represents a coupling of two subsystems with different critical points. The behaviour of such systems is a question of general theoretical interest and the present model gives some indication of the type of behaviour that might be expected.

(iii) In zero magnetic field the model can also be regarded as a staggered eight-vertex model with an applied electric field proportional to J_{12} . The exponents obtained in § 4 indicate the diverse behaviour that may be expected in such systems.

Since we are mainly concerned with exploring the general consequences of coupling between non-identical sub-systems, the most appropriate system for initial study is an Ising model. This has the advantage of comparative simplicity, an advantage which must however be set against the fact that except in rare-earth systems such as that studied by Hunt and Newman (1969) using a related coupled model, Ising models generally give a poor representation of real magnets.

The Hamiltonian for the system can be written as

$$\mathcal{H} = - \sum_{\langle ij \rangle} J_{ij} S_i S_j - mH \sum_i S_i \quad (1)$$

where the spin variables take values $S_i = \pm 1$, the first summation is over all nearest-neighbour pairs, denoted by $\langle ij \rangle$, m is the magnetic moment per spin, and H is an external magnetic field which we assume to be the same at each site. The exchange constant J_{ij} has the value

$$J_{ij} = \begin{cases} J_1 & \text{if } \langle ij \rangle \text{ is in layer 1} \\ J_2 & \text{if } \langle ij \rangle \text{ is in layer 2} \\ J_{12} & \text{if } \langle ij \rangle \text{ is between layers.} \end{cases} \quad (2)$$

In the absence of an exact solution, which is not known for this model, it would seem

worthwhile to use simple closed-form approximations such as the mean-field approximation (MFA). While it is known that MFA is quantitatively incorrect in the vicinity of a critical point it is nevertheless true that it usually gives a qualitatively correct picture of critical behaviour and we believe that it does so in the present case. In § 2 of the paper we derive and discuss the results of MFA for the two-layer system. We also use MFA and a generalization of MFA to obtain a number of rigorous bounds for this system. In § 3 we develop a scaling theory in which J_{12} is treated as a second symmetry-breaking field. We define a number of new critical exponents, obtain estimates of their values, and provide confirmation for some of the GMFA predictions of the previous section. In § 4 we derive and analyse high-temperature series expansions. This approach again provides confirmation of some of the previous results and allows estimates of the critical temperature to be made for all values of J_2/J_1 and J_{12}/J_1 . Finally in § 5 we summarize our results and present our conclusions.

2. The mean-field approximation

The mean-field approximation replaces the coupling between spins by an interaction of each spin with an average field due to the other spins. It is obtained by replacing the exact Hamiltonian (1) by the effective uncoupled Hamiltonian

$$\mathcal{H}_{\text{MFA}} = -m \sum_i H_i^{\text{eff}} S_i \quad (3)$$

where the effective field H_i^{eff} is given by

$$mH_i^{\text{eff}} = mH + \sum_j J_{ij} \langle S_j \rangle. \quad (4)$$

The thermodynamic average spin $\langle S_i \rangle$ then satisfies the equation

$$\langle S_i \rangle = \tanh(\beta m H_i^{\text{eff}}) = \tanh\left(\beta \sum_j J_{ij} \langle S_j \rangle + \beta m H\right) \quad (5)$$

where $\beta = 1/kT$. We are then left with this set of nonlinear equations to solve for the average spin or magnetization of the system.

In the present context the quantity $\langle S_i \rangle$ can take two values, depending on whether site i is in layer 1 or layer 2. We denote these two values by σ_1 and σ_2 respectively. They are determined by the pair of equations

$$\begin{aligned} \sigma_1 &= \tanh(4\beta J_1 \sigma_1 + \beta J_{12} \sigma_2 + \beta m H) \\ \sigma_2 &= \tanh(\beta J_{12} \sigma_1 + 4\beta J_2 \sigma_2 + \beta m H). \end{aligned} \quad (6)$$

In general this pair of equations must be solved numerically.

The first point we make concerns the existence of a nonzero magnetization, or long-range order in the system in the absence of an external field ($H = 0$). For the special case $J_{12} = 0$, when the two layers are uncoupled, each layer will have its own critical temperature (given in MFA by $T_1 = 4J_1/k$, $T_2 = 4J_2/k$) below which long-range order occurs. If however the two layers are coupled, no matter how weakly, then from equation (6) we see that the two magnetizations σ_1 and σ_2 must be either zero or nonzero together so that it is not possible for long-range order to exist in one layer but not in the other. This behaviour can be understood physically in the following way. We suppose that the system is initially in the high-temperature disordered phase. As the

temperature is lowered to a critical temperature T_c the layer with the stronger exchange interaction (which we will call layer 1) will order. The effect of this on layer 2 will be equivalent to switching on an external field and thus layer 2 will immediately order as well. This can be shown rigorously by means of simple correlation inequalities. If the coupling J_{12} is weak however then the magnetization in layer 2 will be quite small until the temperature gets close to the original critical temperature of layer 2.

We have solved the equations (6) numerically for zero field to obtain the variation of σ_1 and σ_2 with temperature T for various values of the parameters $x_2 = J_2/J_1$ and $x_{12} = J_{12}/J_1$. In figure 2 we show some results for the case $x_2 = 0.5$. We also show the variation with temperature of the total magnetization per spin

$$\sigma = \frac{1}{2}(\sigma_1 + \sigma_2). \tag{7}$$

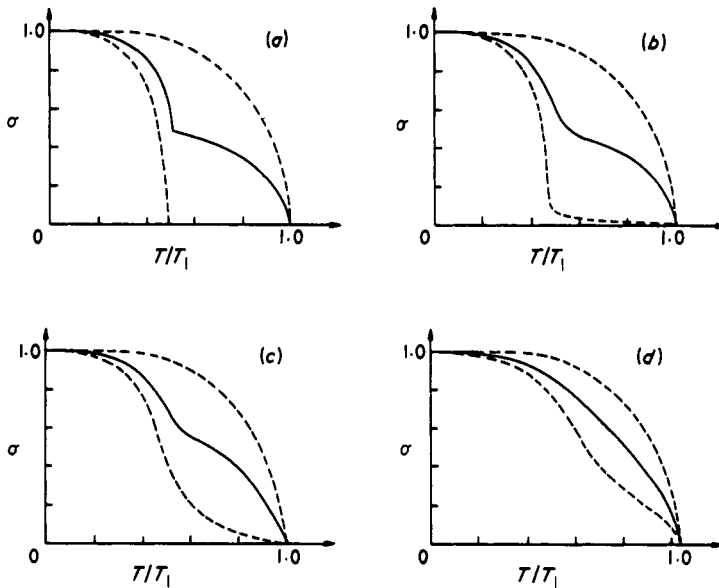


Figure 2. The mean-field approximation for the single-layer magnetizations (broken curves) and total magnetization (full curve) for: (a) $x_2 = 0.5, x_{12} = 0.0$; (b) $x_2 = 0.5, x_{12} = 0.01$; (c) $x_2 = 0.5, x_{12} = 0.1$; (d) $x_2 = 0.5, x_{12} = 0.5$.

We note that for weak interlayer coupling the long-range order in layer 2 decreases rapidly in the vicinity of T_2 , the critical temperature of this layer in the uncoupled case. The total magnetization σ has a sharp kink near this temperature. This shows up well in figure 2(b).

The critical temperature T_c in MFA is given by

$$\frac{kT_c}{J_1} = 2 + 2x_2 + [4(1 - x_2^2)^2 + x_{12}^2]^{1/2}. \tag{8}$$

This shows that T_c increases with increasing interlayer coupling J_{12} .

The dimensionless susceptibility in zero field

$$\chi_0 = \frac{kT}{m} \left(\frac{\partial \sigma}{\partial H} \right)_{H=0} \tag{9}$$

is shown in figure 3, again for the case $x_2 = 0.5$ and a series of values of x_{12} . For $x_{12} = 0$ the susceptibility diverges at two critical temperatures T_1 and T_2 . As soon as coupling between the layers is introduced the low-temperature peak becomes rounded and the high-temperature peak, which represents the true critical point, moves to higher temperatures in accordance with equation (8).

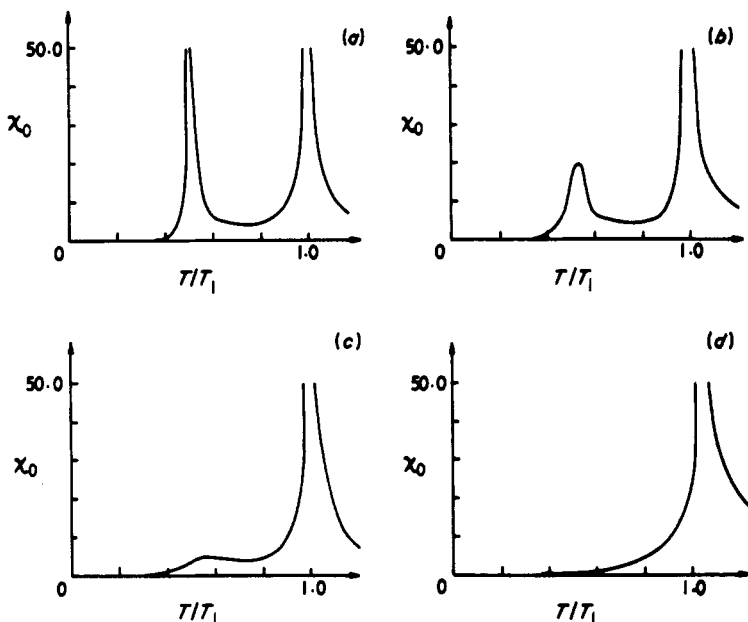


Figure 3. The mean-field solution for the zero-field susceptibility for: (a) $x_2 = 0.5$, $x_{12} = 0.0$; (b) $x_2 = 0.5$, $x_{12} = 0.01$; (c) $x_2 = 0.5$, $x_{12} = 0.1$; (d) $x_2 = 0.5$, $x_{12} = 0.5$.

Although the unusual thermodynamic behaviour shown in figures 2 and 3 is obtained from an approximate theory we believe that MFA gives a correct qualitative picture of the true behaviour of the model.

It is known that MFA provides rigorous upper bounds for various thermodynamic quantities and for the true critical temperature (Fisher 1967b, Thompson 1971). The solutions σ_1 , σ_2 of the MFA equations (6) are upper bounds for the magnetization of layer 1 and layer 2 respectively. The MFA critical temperature (8) is an upper bound for the true critical temperature and the high-temperature susceptibility obtained from equation (9)

$$\chi_0 = \frac{1 - 2\beta J_1 - 2\beta J_2 + \beta J_{12}}{(1 - 4\beta J_1)(1 - 4\beta J_2) - (\beta J_{12})^2} \quad (10)$$

is an upper bound for the true high-temperature susceptibility.

A lower bound on the critical temperature

$$\frac{kT_c}{J_1} > 2.269$$

follows from the work of Griffiths (1967).

Better bounds can be obtained by treating only some of the interactions by the mean-field approximation (Enting 1973a). In the remainder of this section we will

consider this approach. In particular we will treat the interlayer interactions J_{12} by MFA.

Within this approximation we write the magnetizations σ_1 and σ_2 as

$$\begin{aligned}\sigma_1 &= \sigma_{\text{sq}}(\beta J_1, \beta mH + \beta J_{12}\sigma_2) \\ \sigma_2 &= \sigma_{\text{sq}}(\beta J_2, \beta mH + \beta J_{12}\sigma_1)\end{aligned}\quad (11)$$

where $\sigma_{\text{sq}}(\beta J, \beta mH)$ is the true magnetization of the simple quadratic lattice Ising model. The solution of this pair of equations gives upper bounds for the magnetization on each layer.

From the equations (11) and the standard result

$$\sigma_{\text{sq}}(K_c, h) \sim h^{1/\delta} \quad (12)$$

we obtain the following results for the dependence of σ_1 and σ_2 on J_{12} at the true critical temperatures T_1 and T_2 of the uncoupled quadratic layers.

If $J_1 > J_2$ we find

$$\left. \begin{aligned}\sigma_2 &\sim J_{12}^{1/\delta} = J_{12}^{1/15} && \text{at } T = T_2 \\ \sigma_1 &\sim J_{12}^{2/(\delta-1)} = J_{12}^{1/7} \\ \sigma_2 &= J_{12}^{(\delta+1)/(\delta-1)} = J_{12}^{8/7}\end{aligned}\right\} \text{at } T = T_1. \quad (13)$$

If $J_1 = J_2$ we find

$$\sigma \sim J_{12}^{1/(\delta-1)} = J_{12}^{1/14} \quad (14)$$

at $T = T_1 = T_2$.

These expressions for σ_1 , σ_2 , σ are all upper bounds for the appropriate subsystem magnetizations once the appropriate amplitudes are included and so the exponents obtained from this generalized mean-field approximation are lower bounds for the true values.

The high-temperature susceptibility in this generalized mean-field approximation can be obtained from equations (11) as

$$2\chi_{\text{GMFA}} = \frac{\chi_{\text{sq}}(\beta J_1) + \chi_{\text{sq}}(\beta J_2) + 2\beta J_{12}\chi_{\text{sq}}(\beta J_1)\chi_{\text{sq}}(\beta J_2)}{1 - (\beta J_{12})^2 \chi_{\text{sq}}(\beta J_1)\chi_{\text{sq}}(\beta J_2)} \quad (15)$$

where $\chi_{\text{sq}}(\beta J)$ is the true high-temperature susceptibility for the quadratic lattice. The temperature T^* at which χ_{GMFA} diverges is an upper bound for the true critical temperature T_c .

Setting the denominator of (15) equal to zero and using the limiting form

$$\chi_{\text{sq}}(\beta J_1) \sim (K_c k T^* / J_1 - 1)^{-7/4} \quad (16)$$

we obtain the results

$$\begin{aligned}T^* - T_1 &\sim J_{12}^{8/7}; && J_1 \neq J_2 \\ T^* - T_1 &\sim J_{12}^{4/7}; && J_1 = J_2.\end{aligned}\quad (17)$$

If we define an exponent ϕ by

$$T_c - T_1 \sim J_{12}^{1/\phi} \quad (18)$$

then since $T_c < T^*$ we obtain an upper bound for ϕ :

$$\begin{aligned} \phi &\leq \frac{7}{8}; & J_1 &\neq J_2 \\ \phi &\leq \frac{7}{4}; & J_1 &= J_2. \end{aligned} \tag{19}$$

We have calculated T^* from the equation

$$(kT^*)^2 = J_{12}^2 \chi_{sq}(J_1/kT^*) \chi_{sq}(J_2/kT^*) \tag{20}$$

using the representation of $\chi(K)$ given by Sykes *et al* (1972). The results are plotted in figure 4. As $J_2 \rightarrow J_1$ the region of validity of the $\phi = \frac{7}{8}$ behaviour decreases. Outside this region the T^* variation can be described by a $\frac{7}{4}$ behaviour.

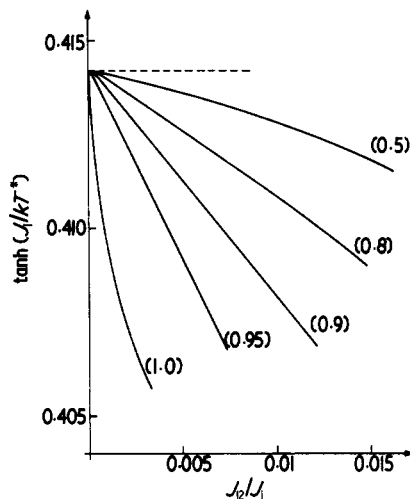


Figure 4. Estimates of critical temperature T^* from generalized mean-field approximation for various values of x_2 (in brackets).

In terms of the susceptibility exponent $\gamma = \frac{7}{4}$ we have

$$\phi = \begin{cases} \frac{1}{2}\gamma & J_1 \neq J_2 \\ \gamma & J_1 = J_2 \end{cases}$$

from GMFA. This result also follows from MFA (equation (8)) with $\gamma = 1$. Scaling theory predicts the same connection between the exponents ϕ and γ .

3. Scaling theory

The scaling approach to critical phenomena has been successfully used in many papers since the pioneering work of Widom (1965), Domb and Hunter (1965), Kadanoff (1966) and others. The recent extensive discussion by Hankey and Stanley (1972) is based on the use of generalized homogeneous functions. The assumption is that the free energy satisfies the equation

$$\lambda G(t, H) = G(\lambda^a t, \lambda^b H) \tag{21}$$

for any λ , where $t = T - T_c$. From this it is simple to relate a and b to the usual critical

exponents α and δ , and for the two-dimensional Ising model it follows that $a = \frac{1}{2}$, $b = \frac{15}{16}$.

For the two-layer model, in addition to the field H , it is convenient to regard J_{12} as a second symmetry-breaking field. This is reasonable since the type of ordering changes discontinuously as J_{12} passes through zero. The order parameter conjugate to J_{12} is the interplane correlation function.

$$Q = \langle S_1 S_2 \rangle$$

where S_1 is a spin on layer 1 and S_2 the nearest-neighbour spin on layer 2.

We thus generalize equation (21) and make the assumption that we can represent the most singular part of the free energy by a generalized homogeneous function :

$$\lambda G(t, H, J_{12}) = G(\lambda^a t, \lambda^b H, \lambda^c J_{12}) \quad \text{near } T_2, \text{ with } t = T - T_2 \quad (22)$$

and

$$\lambda \bar{G}(\bar{t}, H, J_{12}) = \bar{G}(\lambda^{a\bar{t}}, \lambda^b H, \lambda^c J_{12}) \quad \text{near } T_1, \text{ with } \bar{t} = T - T_1. \quad (23)$$

We expect that G and \bar{G} will be different functions, and in general $c \neq \bar{c}$. For $J_{12} = 0$ both the transitions are two-dimensional Ising model transitions so the exponents a and b will take the same values as in (21). We note that in (22) and (23) the exponents describe only the singular part of the behaviour, for instance at $T = T_2$ the magnetization does not go to zero but it does have a singularity with exponent $\beta = (1-b)/a = \frac{1}{8}$.

The notation to be used for the exponents follows that used by Enting (1973b) in connection with the modified F -model. In that model an applied electric field corresponds to a two-spin interaction which couples two subsystems and is thus closely related to J_{12} of the present model. Exponents obtained by considering derivatives of G with respect to J_{12} are distinguished by the subscript e whereas exponents obtained from the field H are given the subscript m .

We first consider the behaviour of the system near $T = T_2$. Defining an exponent β_e by

$$Q \sim (-t)^{\beta_e} \quad (24)$$

and using the result that for $J_{12} = 0$

$$Q = \sigma_1 \sigma_2 \sim \text{constant} \times (-t)^{1/8}$$

gives $\beta_e = \frac{1}{8}$. From (24) on the other hand we get by differentiating with respect to J_{12}

$$Q(t, H, J_{12}) = \lambda^{c-1} Q(\lambda^a t, \lambda^b H, \lambda^c J_{12}).$$

Putting $H = J_{12} = 0$ and $\lambda = (-1/t)^{1/a}$ gives

$$Q(t, 0, 0) = (-t)^{(1-c)/a} Q(-1, 0, 0)$$

whence

$$\frac{1-c}{a} = \frac{1}{8} \quad \text{ie } c = \frac{15}{16}.$$

Having determined the value of c we can now use the scaling form (21) to determine the behaviour of other quantities near and at $T = T_2$. We find that

$$\left(\frac{\partial^2 G}{\partial J_{12}^2} \right)_{J_{12}=0} \sim |t|^{-\gamma_e} \quad \text{with } \gamma_e = \frac{7}{4}$$

and at $t = 0$

$$Q \sim J_{12}^{1/\delta_e}$$

with

$$\delta_e = \frac{c}{1-c} = 15. \tag{25}$$

This last result is in agreement with equation (13) of the previous section.

In order to determine the behaviour of the system near $T = T_1$ we need to determine first the exponent \bar{c} in equation (23). Putting $H = 0$ and $\lambda = J_{12}^{-1/\bar{c}}$ in (23) gives

$$\bar{G}(\bar{t}, 0, J_{12}) = \lambda^{-1} \bar{G}(J_{12}^{-a/\bar{c}} \bar{t}, 0, 1).$$

If a singularity occurs in \bar{G} for nonzero J_{12} it must be at one particular value of $J_{12}^{-a/\bar{c}} \bar{t}$, ie at

$$T_c = T_1 = \text{constant} \times J_{12}^{a/\bar{c}}. \tag{26}$$

Comparing this with equation (18) gives $\bar{c}/a = \phi$, and assuming the value of $\phi = \frac{7}{8}$ for the crossover exponent gives

$$\bar{c} = \frac{7}{16}. \tag{27}$$

The result $\phi = \frac{7}{8}$ can be obtained by generalizing the renormalization group arguments of Grover (1973). One takes a system of two independent layers and treats J_{12} as a perturbation. One then considers how the perturbation must behave under the renormalization transformation if a sequence of transformations is to approach a fixed point. For $J_1 = J_2$ one has, in common with the anisotropic Ising model, the requirement that the perturbation $S(k)S(k)J_{12}$ approaches a fixed point and the transformation of the $S(k)$ is that appropriate to the two-dimensional Ising model. If $J_1 \neq J_2$ the $S(k)$ for one layer is essentially constant under the renormalization transformation and we require a fixed point for $S(k)J_{12}$, which implies that ϕ is half the anisotropic Ising model value.

Having obtained the exponent \bar{c} we can at once obtain from the scaling form (23) the following results:

$$\left(\frac{\partial^2 \bar{G}}{\partial J_{12}^2} \right)_{J_{12}=0} \sim \begin{cases} \bar{t}^{-\gamma_e} \\ (-\bar{t})^{-\gamma_e} \end{cases} \quad \text{with } \gamma'_e = \gamma_e = -\frac{1}{4} \tag{28}$$

and at $\bar{t} = 0$

$$Q \sim J_{12}^{1/\delta_e}$$

with

$$\delta_e = \frac{\bar{c}}{1-\bar{c}} = \frac{7}{9}. \tag{29}$$

This last result is again in agreement with equation (13) of the previous section.

The temperature dependence of derivatives of the susceptibility with respect to J_{12}

$$\chi^{(n)} = \left(\frac{\partial^n \chi}{\partial J_{12}^n} \right)_{J_{12}=0} \sim |t|^{-g(n)} \tag{30}$$

is also of interest. From (23) we find

$$g(n) = \gamma_m + n\phi. \tag{31}$$

For $\bar{t} > 0$, at least, this seems to hold only for even n , and for $n = 2j + 1$ one has, in agreement with the expansion of (18)

$$g(2j + 1) = g(2j). \tag{32}$$

In fact for $n = 1, 2, 3$ the values $\frac{7}{4}, \frac{7}{2}, \frac{7}{2}$ can be shown to be upper bounds for the exponents by generalizing the work of Liu and Stanley (1972).

The fact that this prediction of $g(2n + 1) = g(2n)$ is the same as obtained from GMFA shows that this type of stepwise increase is not inconsistent with the generalized homogeneous function hypothesis that we have used to formulate scaling theory. This is because, as shown by Enting (1973a), this type of susceptibility approximation can be derived from a variational free energy. Simple algebraic manipulation shows that if the two-dimensional Ising model free energy is a generalized homogeneous function then the GMFA free energy is a generalized homogeneous function of the type assumed above and with exponents $a = \frac{1}{2}, b = \frac{15}{16}, \bar{c} = \frac{7}{16}$ as above.

4. High-temperature series

A different approach, which has been used with considerable success for many years in the study of cooperative lattice models, is the method (or methods) of exact series expansions. For reviews of this approach we refer the reader to the article by Fisher (1967a) and the recent book by Domb and Green (1974) in which methods of series derivation and analysis are discussed.

The derivation of high-temperature series for the two-layer system follows completely standard lines and we omit details here. In zero applied field the logarithm of the partition function becomes

$$\frac{1}{N} \ln Z = \ln 2 + \ln \cosh \beta J_1 + \ln \cosh \beta J_2 + \frac{1}{2} \ln \cosh \beta J_{12} + \sum_{l,m,n} a_{lmn} v_1^l v_2^m v_{12}^n \tag{33}$$

where

$$\begin{aligned} v_1 &= \tanh \beta J_1 \\ v_2 &= \tanh \beta J_2 \\ v_{12} &= \tanh \beta J_{12}. \end{aligned} \tag{34}$$

The dimensionless susceptibility, defined by

$$\chi_0 = \left(\frac{kT}{m} \right)^2 \lim_{H \rightarrow 0} \frac{\partial^2}{\partial H^2} \left(\frac{1}{N} \ln Z \right)$$

is given by

$$\chi_0 = 1 + \sum_{l,m,n} b_{lmn} v_1^l v_2^m v_{12}^n. \tag{35}$$

By computer counting of graphs we have evaluated the coefficients a_{lmn} for $l + m + n < 12$ and b_{lmn} for $l + m + n < 11$. The values are given in the appendix. The coefficients a_{lm2} for $l + m = 12$ can be obtained indirectly, as indicated below, and are included in the table.

A number of checks on the correctness of our results are available. For $J_{12} = 0$ the series should reduce to the known result for the simple quadratic lattice, which it does.

For $J_1 = J_2 = J_{12}$ the model reduces to the case for which series expansions have been previously derived by Ballentine (1964) and Allan (1970). Again exact agreement is obtained with the first ten terms of χ_0 given by Ballentine and the 11th term supplied by M E Fisher (private communication).

A number of other checks, related to the derivatives of the free energy with respect to J_{12} (the gap exponent series) are available. In particular using the result

$$\left(\frac{\partial^2 \ln Z}{\partial(\beta J_{12})^2} \right)_{J_{12}=0} = N \sum_i \langle S_0 S_i \rangle_{\text{layer 1}} \langle S_0 S_i \rangle_{\text{layer 2}}$$

and the correlation function series of Fisher and Burford (1967) we can obtain the coefficients a_{lm2} for $m+n \leq 12$. From a simple generalization of the work of Liu and Stanley (1972) we obtain the result

$$b_{lm1} = 4b_l b_m$$

where b_l is the susceptibility coefficient for the simple quadratic lattice. Another check is obtained from the quantities

$$s_{m,j} = \sum_n b_{n,m-n,j}.$$

The sums s_{m2} and s_{m3} can be derived from the coefficients given by Oitmaa and Enting (1972) for the anisotropic Ising model, using correlation expressions of the type given by Liu and Stanley (1972) and Enting (1974).

We have performed all these checks and in fact in so doing discovered several minor errors in the anisotropic Ising model coefficients given by Oitmaa and Enting (1972). The correct values are $b_{92} = 2784352$, $b_{83} = 5440200$. While these checks do not completely eliminate the possibility of errors their likelihood is certainly small.

Having obtained the series in three variables the procedure adopted is to choose particular values for the parameters $x_2 = J_2/J_1$ and $x_{12} = J_{12}/J_1$ and expand the series in a single variable $v \equiv v_1$. This yields a susceptibility series of the form

$$\chi_0 = 1 + \sum_r b_r v^r \quad (36)$$

with coefficients up to and including b_{11} known.

In view of the complex behaviour which this system can apparently show, as indicated in the previous sections, one can probably expect only limited success from series analysis. In particular the nature of the singularity, especially for $J_1 \simeq J_2$ is expected to be rather complex. We therefore simplify our problems by using the 'universality hypothesis' (Kadanoff 1970) to assume that $\gamma = \frac{7}{4}$ for this model, independent of x_2 and x_{12} . We then use the ratio and Padé approximant methods to obtain estimates for the critical temperature $v_c = \tanh(J/kT_c)$.

In the ratio method, which has been extensively discussed by Gaunt and Guttmann (1974) one initially considers the ratios of successive coefficients $\mu_n = b_n/b_{n-1}$. If the asymptotic form of the susceptibility is of the form $(v_c - v)^{-\gamma}$ then

$$\mu_n = \frac{1}{v_c} \left[1 + \frac{\gamma-1}{n} + O\left(\frac{1}{n^2}\right) \right].$$

Since we are making the assumption $\gamma = \frac{7}{4}$ it is better to use the modified ratios

$$\mu_n^* = \frac{\mu_n}{[1 + (\gamma - 1/n)]} \sim v_c^{-1} \left[1 + O\left(\frac{1}{n^2}\right) \right]. \tag{37}$$

In loose-packed lattices, such as the present case, the occurrence of an antiferromagnetic singularity on the circle of convergence introduces odd-even oscillations into the ratios μ_n and μ_n^* . This difficulty can be partially overcome by considering the geometric mean of successive ratios (Stanley 1967). These are

$$g_n^{(2)} = \left(\frac{\mu_n^*}{\mu_{n-1}^*} \right)^{1/2} \sim v_c^{-1} \left[1 + O\left(\frac{1}{n^2}\right) \right]. \tag{38}$$

More refined estimates are obtained by taking pairs of $g_n^{(2)}$ and eliminating successively higher powers of $(1/n)$. If

$$g_n^{(k)} \sim v_c^{-1} [1 + O(1/n^k)] \tag{39}$$

then

$$g_n^{(k+1)} = \frac{n^k g_n^{(k)} - (n-2)^k g_{n-2}^{(k)}}{n^k - (n-2)^k} \sim v_c^{-1} [1 + O(1/n^{k+1})]. \tag{40}$$

We have used the quantities $g_n^{(k)}$ for $k = 2, 3, 4$ to obtain sequences of estimates for v_c^{-1} . The results for the case $x_2 = 0.5, x_{12} = 0.2$ are shown in table 1. It appears that we do not have enough terms for these sequences to have settled down to their limiting behaviour.

Table 1. Ratio method estimates of v_c^{-1} for the case $x_2 = 0.5, x_{12} = 0.2$

n	b_n	$g_n^{(2)}$	$g_n^{(3)}$	$g_n^{(4)}$
1	3.20000			
2	8.70000	1.9015		
3	25.2840	2.1441		
4	70.4390	2.3355	2.4801	
5	196.713	2.3869	2.5234	
6	537.387	2.4284	2.5027	2.5121
7	1459.64	2.4408	2.4969	2.4817
8	3906.74	2.4502	2.4783	2.4605
9	10391.3	2.4511	2.4671	2.4405
10	27374.6	2.4529	2.4577	2.4361
11	71747.1	2.4521	2.4540	2.4382

The other techniques that were used are based on the use of Padé approximants. We have followed the standard procedures of considering Padé approximants to the series for

(i) $\frac{d}{dv} \ln \chi(v)$

(ii) $\chi(v)^{1/\gamma}$

which should both have simple poles at $v = v_c$ if $\chi(v)$ has the limiting form $(v_c - v)^{-\gamma}$.

We have also looked at the 'exponent renormalized' series

$$(iii) \quad \chi^*(v) = 1 + \sum_r b_r v^r / (-\gamma).$$

This technique, due to Hunter and Baker (1973), will, for the case $J_{12} = 0$, transform a sum of two divergent terms with equal exponents γ to two simple poles.

In general the Padé approximant analysis did not yield satisfactory results. A useful test is the case $x_{12} = 0$ for which the critical points are known exactly. For $x_2 \neq 1$ these cases give a test of how well the various techniques can separate the effect of the two peaks. Padé approximant analysis using the series (ii) gave the best results of the three approaches. The method worked quite well for all cases with $x_2 = 1.0$, where there is only one singularity. The method also worked quite well for small values of x_2 , where the two peaks are well separated.

The overall estimates of v_c obtained from the methods described above are presented in table 2. For $J_1 \neq J_2$ it is apparent that there is a variation of T_c as $(T_c - T_1) \sim \eta^{1/\phi}$ with $\phi < 1$ but the T_c estimates are not sufficiently precise for us to be able to estimate ϕ . For $J_1 = J_2$ we have plotted $v_c(J_{12}) - v_c(0)$ against $J_{12}^{4/7}$. This is shown in figure 5 and appears to confirm the scaling prediction of Abe (1970). The choice of v for the temperature variable follows Enting (1974) where it was found that a similar choice of variables minimized the rate at which the larger J_{12} behaviour deviated from its limiting form.

Table 2. Estimates of v_c^{-1} for various values of x_2, x_{12} obtained from: (1) ratio estimates using $g_n^{(3)}$ given by equation (40); (2) ratio estimates using $g_n^{(4)}$ given by equation (40); (3) Padé approximants to exponent renormalized series; (4) Padé approximants to logarithmic derivative series; (5) Padé approximants to $\chi^{4/7}$. Blanks indicate cases where no reasonably consistent estimates could be obtained

x_2	x_{12}	(1)	(2)	(3)	(4)	(5)
1.0	1.0	3.312 ± 0.007	3.305 ± 0.01	3.30	3.3	3.33
1.0	0.5	3.025 ± 0.005	3.02 ± 0.01	3.02	—	3.03
1.0	0.1	2.64 ± 0.01	2.66 ± 0.01	2.63	2.68	2.63
1.0	0.05	2.55 ± 0.01	2.57 ± 0.03	—	2.57	2.57
1.0	0.01	2.45 ± 0.01	2.45 ± 0.01	—	—	2.44
1.0	0	2.416 ± 0.005	2.415 ± 0.01	—	2.41	2.41
0.9	0.5	2.905 ± 0.01	2.90 ± 0.01	—	2.9	—
0.9	0.1	2.56 ± 0.01	2.57 ± 0.01	—	2.60	—
0.9	0.05	2.48 ± 0.01	2.49 ± 0.01	—	2.51	—
0.9	0.01	2.40 ± 0.01	2.415 ± 0.01	—	2.42	—
0.9	0	2.39 ± 0.03	2.39 ± 0.03	—	2.39	—
0.5	0.5	2.554 ± 0.007	2.55 ± 0.05	2.55	—	2.56
0.5	0.2	2.45 ± 0.01	2.44 ± 0.05	2.45	—	2.47
0.5	0.1	2.43 ± 0.01	2.418 ± 0.01	2.42	—	2.42
0.5	0.05	2.425 ± 0.01	2.413 ± 0.01	2.415	—	2.42
0.5	0.01	2.423 ± 0.01	2.413 ± 0.01	2.415	—	2.42
0.5	0	2.423 ± 0.01	2.413 ± 0.01	—	—	2.42
0.2	0.2	2.420 ± 0.005	2.42 ± 0.01	2.42	—	2.42
0.2	0.1	2.417 ± 0.005	2.416 ± 0.01	2.42	—	2.42
0.2	0.05	2.415 ± 0.003	2.416 ± 0.01	2.42	—	2.42
0.2	0.01	2.415 ± 0.004	2.416 ± 0.01	—	—	2.42
0.2	0	2.415 ± 0.004	2.416 ± 0.01	—	—	2.42

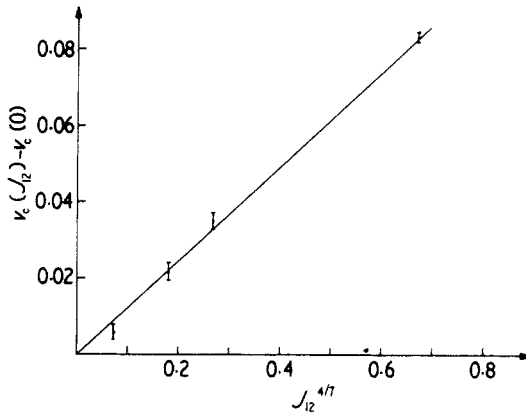


Figure 5. Plot of $v_c(J_{12}) - v_c(0)$ against $J_{12}^{4/7}$ for the case $J_1 = J_2$. Scaling theory predicts a straight line through the origin.

We have also attempted to estimate gap exponents in order to test the scaling hypothesis of § 4.

For $J_1 = J_2$ we have $\gamma_c = \frac{3}{2}$ and the series are equivalent to those considered by Enting (1973c). For $J_1 \neq J_2$ scaling predicts $\gamma_c = -\frac{1}{4}$ at T_1 and as might be expected this singularity was too weak to be separated from the generally complicated behaviour, and no useful estimates could be obtained.

Since the series for $\chi^{(0)}$, $\chi^{(1)}$ can be expressed in terms of the square lattice susceptibility we have $\gamma_m = g(1) = \frac{7}{4}$ ($J_1 \neq J_2$). Attempts to estimate $g(2)$, $g(3)$ by using the ratio method and constructing higher extrapolants using equation (40) met with only limited success. The estimates were somewhat irregular being consistent with $g(3) = \frac{7}{2}$ but indicating $g(2) < \frac{7}{2}$. The series are really too short to give any reliable indication of whether the stepwise scaling predictions of (31), (32) are correct or not.

5. Discussion and conclusions

In this paper we have studied the critical behaviour of a two-layer Ising system in which the coupling strengths in each layer are in general unequal and also differ from the strength of the interlayer coupling J_{12} .

When $J_{12} = 0$ the system has two critical points and the susceptibility will diverge at two temperatures T_1 and T_2 (we take $T_1 > T_2$). For any non-zero value of J_{12} the critical point at T_2 will vanish, although the susceptibility may still show a rounded peak, while the critical point at T_1 will become the only critical point and will shift to higher temperatures. This behaviour is clearly seen in the mean-field solution.

Using a generalized mean-field theory, in which the interactions within layers are treated exactly while the interlayer interactions are treated by a mean-field approximation we have obtained a number of results for the variation of T_c and the magnetizations in each layer with J_{12} . These predictions are in agreement with results obtained from a scaling approach. Using the scaling theory we have also investigated the temperature dependence of derivatives of the free energy and susceptibility with respect to J_{12} .

We have also used the technique of high-temperature series expansions to study the behaviour of this model. Although the series analysis has not been as successful as we had originally hoped some useful results have nevertheless been obtained. In particular we have been able to obtain the critical temperature for various values of the exchange constant ratios J_2/J_1 , J_{12}/J_1 . For $J_1 = J_2$ and $J_{12} = \eta J_1$ we have confirmed the scaling result of Abe (1970) for the variation of T_c with η . We have also obtained estimates for the susceptibility and free energy gap exponents which, while somewhat irregular, are consistent with the scaling predictions.

The most interesting behaviour of this system occurs below the critical temperature. Since low-temperature series are in practice almost always more irregular than high-temperature series it seems unlikely that series expansions will yield satisfactory results below T_c . The situation is particularly difficult for lattices of low coordination number where a large number of high-field polynomials are needed to give a reasonable number of terms in the temperature grouping. It is expected that long series will be needed to represent the rapid changes near T_2 and then to continue to represent the approach to the true critical temperature. The simplest approximation to the rounded peaks that are expected to occur in the specific heat and susceptibility is $[(x-a)^2 + \delta^2]^{-1}$ with δ small. This is a product of two poles at a $\pm i\delta$ and it would seem to be extremely difficult to extrapolate between two closely spaced poles to obtain any indication of the true critical behaviour. On the other hand it should be possible to obtain some information concerning the heights of the peaks near T_2 since the poles can be readily represented by Padé approximants. We hope to investigate this model by low-temperature series in future work.

In our view the question of what happens when two subsystems, which each have a critical point, are coupled together is one of general theoretical importance and we believe the present work is the first investigation of such behaviour. Even when the two subsystems have the same critical point interesting effects can result, as exemplified by the eight-vertex model. The eight-vertex model can be regarded as two identical Ising models coupled by a four-spin interaction (Wu 1971, Kadanoff and Wegner 1971). It is in fact fairly simple to set up a correspondence between the present model and a staggered eight-vertex model. The details and consequences of this correspondence will be presented elsewhere.

The work presented in this paper, although based on a simple and somewhat artificial model, shows that coupled cooperative systems are likely to exhibit a number of quite interesting effects. Although our motivation for this work has been primarily theoretical we have indicated several types of experimental systems in which such behaviour may occur. We hope that this work will act as a stimulus to experimentalists to investigate critical behaviour of coupled systems.

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Appendix

Zero-field free energy coefficients a_{lmn}

l	m	n	a_{lmn}	l	m	n	a_{lmn}
4	0	0	$\frac{1}{2}$	12	0	0	$18\frac{2}{3}$
1	1	2	1	9	1	2	42
6	0	0	1	8	2	2	110
3	1	2	2	7	3	2	258
2	2	2	5	6	4	2	508
8	0	0	$2\frac{1}{4}$	5	5	2	653
5	1	2	4	6	2	4	-4
4	2	2	14	5	3	4	-76
3	3	2	23	4	4	4	$-168\frac{1}{2}$
2	2	4	$-2\frac{1}{2}$	3	3	6	$9\frac{1}{3}$
10	0	0	6	11	1	2	164
7	1	2	12	10	2	2	394
6	2	2	36	9	3	2	818
5	3	2	86	8	4	2	1714
4	4	2	121	7	5	2	2956
4	2	4	-7	6	6	2	3607
3	3	4	-24				

Coefficients for $m > l$ are obtained from the symmetry relation

$$a_{lmn} = a_{mln}$$

Initial susceptibility coefficients b_{lmn}

l	m	n	b_{lmn}	l	m	n	b_{lmn}
1	0	0	2	7	0	0	986
0	0	1	1	6	0	1	740
2	0	0	6	5	1	1	1104
1	0	1	4	4	2	1	1200
3	0	0	18	3	3	1	1296
2	0	1	12	5	0	2	138
1	1	1	16	4	1	2	1036
1	0	2	2	3	2	2	1472
4	0	0	50	3	1	3	232
3	0	1	36	2	2	3	408
2	1	1	48	2	1	4	4
2	0	2	6	8	0	0	2586
1	1	2	24	7	0	1	1972
5	0	0	138	6	1	1	2960
4	0	1	100	5	2	1	3312

Initial susceptibility coefficients b_{lmn} —continued

l	m	n	b_{lmn}	l	m	n	b_{lmn}
3	1	1	144	4	3	1	3600
2	2	1	144	6	0	2	370
3	0	2	18	5	1	2	3108
2	1	2	100	4	2	2	4664
1	1	3	8	3	3	2	5152
6	0	0	370	4	1	3	872
5	0	1	276	3	2	3	1824
4	1	1	400	3	1	4	52
3	2	1	432	2	2	4	132
4	0	2	50	9	0	0	6746
3	1	2	324	8	0	1	5172
2	2	2	420	7	1	1	7888
2	1	3	56	6	2	1	8880
5	3	1	9936	11	0	0	44882
4	4	1	10000	10	0	1	34876
7	0	2	986	9	1	1	53968
6	1	2	9172	8	2	1	62064
5	2	2	14312	7	3	1	70992
4	3	2	16972	6	4	1	74000
5	1	3	2936	5	5	1	76176
4	2	3	6912	9	0	2	6746
3	3	3	8584	8	1	2	74500
4	1	4	236	7	2	2	121464
3	2	4	964	6	3	2	153924
10	0	0	17438	5	4	2	173864
9	0	1	13492	7	1	3	29048
8	1	1	20688	6	2	3	77184
7	2	1	23664	5	3	3	118552
6	3	1	26640	4	4	3	136024
5	4	1	27600	6	1	4	3252
8	0	2	2586	5	2	4	19204
7	1	2	26308	4	3	4	34468
6	2	2	42024	4	2	5	1424
5	3	2	51708	3	3	5	2528
4	4	2	55692	3	2	6	4
6	1	3	9464				
5	2	3	23840				
4	3	3	33752				
5	1	4	932				
4	2	4	4752				
3	3	4	7032				
3	2	5	184				

The result $b_{lmn} = b_{min}$ is used to obtain coefficients for $m > l$.

References

- Abe R 1970 *Prog. Theor. Phys.* **44** 339–47
- Allan G A T 1970 *Phys. Rev. B* **1** 352–6
- Ballentine L E 1964 *Physica* **30** 1231–7
- Barber M N and Fisher M E 1973 *Ann. Phys., NY* **77** 1–78
- Binder K and Hohenberg P C 1972 *Phys. Rev. B* **6** 3461–87
- Domb C 1974 *Phase Transitions and Critical Phenomena*, vol 3 eds C Domb and M S Green (New York: Academic Press) pp 357–484
- Domb C and Green M S (eds) 1974 *Phase Transitions and Critical Phenomena*, vol 3 (New York: Academic Press)
- Domb C and Hunter D L 1965 *Proc. Phys. Soc.* **86** 1147–51
- Enting I G 1973a *J. Phys. A: Math., Nucl. Gen.* **6** 1878–87
- 1973b *J. Phys. C: Solid St. Phys.* **6** L302–3
- 1973c *Phys. Lett.* **44A** 417–8
- 1974 *J. Phys. C: Solid St. Phys.* **7** 1237–41
- Fisher M E 1967a *Rep. Prog. Phys.* **30** 615–730
- 1967b *Phys. Rev.* **162** 480–5
- 1971 *Proc. Enrico Fermi Summer School on Critical Phenomena* ed M S Green (New York: Academic Press)
- Fisher M E and Barber M N 1972 *Phys. Rev. Lett.* **28** 1516–9
- Gaunt D S and Guttman A J 1974 *Phase Transitions and Critical Phenomena*, vol 3 eds C Domb and M S Green (New York: Academic Press) pp 181–243
- Griffiths R B 1967 *J. Math. Phys.* **8** 478–83
- Grover M K 1973 *Phys. Lett.* **44A** 253
- Hankey A and Stanley H E 1972 *Phys. Rev. B* **6** 3515–42
- Højlund Neilsen P E 1973 *Phys. Lett.* **42A** 468
- Hunt B A and Newman D J 1969 *J. Phys. C: Solid St. Phys.* **2** 75–83
- Hunter D L and Baker G A 1973 *Phys. Rev. B* **7** 3346–76 3377–92
- Kadanoff L P 1966 *Physics* **2** 263–72
- Kadanoff L P and Wegner F J 1971 *Phys. Rev. B* **4** 3989–93
- Liu L L and Stanley H E 1972 *Phys. Rev. Lett.* **29** 927–30
- Mikulinskii M A 1971 *Sov. Phys.—JETP* **33** 782–5
- Mills D L 1971 *Phys. Rev. B* **3** 3887–95
- Oitmaa J and Enting I G 1972 *J. Phys. C: Solid St. Phys.* **5** 231–44
- Stanley H E 1967 *Phys. Rev.* **158** 546–51
- Sykes M F, Gaunt D S, Roberts P D and Wyles J A 1972 *J. Phys. A: Gen. Phys.* **5** 624–39
- Thompson C J 1971 *Commun. Math. Phys.* **24** 61–6
- Watson P G 1972 *Phase Transitions and Critical Phenomena*, vol 2 eds C Domb and M S Green (New York: Academic Press) pp 101–59
- Widom B 1965 *J. Chem. Phys.* **43** 3892–7
- Wu F Y 1971 *Phys. Rev. B* **4** 2312–4