

## Exactly solvable model for tricritical phenomena\*

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An  $n$ -component continuous-spin model with a tricritical point is solved exactly in the limit  $n \rightarrow \infty$ . Its properties are derived and are compared with the results of experiments and approximate calculations. The model leads to an analytical description of the features of tricritical points and suggests the use of an approximation procedure for discrete spin systems which is a substantial qualitative and quantitative improvement on mean-field theory.

### I. INTRODUCTION

This paper is concerned with an  $n$ -component continuous-spin model which may be solved exactly in the limit  $n \rightarrow \infty$  and has a tricritical point. It is a generalization of the Blume-Emery-Griffiths<sup>1</sup> (BEG) model, and the tricritical point is obtained by varying a "nonordering" field  $\Delta$  (analogous to a crystal field in a magnetic problem) or its conjugate variable  $x$ , which is comparable to the <sup>3</sup>He concentration in helium mixtures. A simpler version of this model has previously been discussed by Amit and de Dominicis<sup>2</sup> who used the renormalization-group method to determine some of the properties of the disordered phase near to the  $\lambda$  line and the tricritical point. However, we shall obtain an exact solution which not only does not require the fixed-point assumption of the renormalization-group method, but also is valid for all temperatures and, in particular, for the ordered phase and for first-order phase transitions. This is essential for a complete description of the tricritical region.

The following properties are obtained: (1) The critical exponents are spherical along the  $\lambda$  line and Gaussian at the tricritical point for fixed  $\Delta$ . (2) The concentration susceptibility  $(\partial x / \partial \Delta)_T$  diverges at the tricritical point with an exponent of  $\frac{1}{2}$  for constant  $\Delta$  and 1 for constant  $x$  or along the coexistence curve. (3) For  $d=3$ , the phase boundary has a discontinuous slope at the tricritical point in the  $(x, T)$  plane. (4) The tricritical exponents remain Gaussian to order  $n^{-1}$ . (5) There are no logarithmic singularities<sup>3</sup> at  $d=3$ . (6) In general, there is no tricritical point for  $d < 3$ .

The first two results have been obtained by the renormalization-group method<sup>2,4</sup> and the fourth could be derived in the same way. The second and third agree with experiments<sup>5-7</sup> on helium mixtures and FeCl<sub>2</sub>, and with series approximations<sup>8</sup> for the BEG model. They are not obtained from mean-field calculations<sup>1</sup> for the disordered phase, or the classical theory of phase transitions. In addition to these properties the wave-vector-depend

ent concentration susceptibility for the model has the expected scaling form and is in agreement with light-scattering experiments<sup>6</sup> in both the ordered and disordered phases.

The model and the method of solution are described in Sec. II. Upper and lower bounds for the free energy are obtained and shown to become equal to each other in the limit  $n \rightarrow \infty$ . The consequent free energy is a generalization of the Hartree approximation, and it could alternatively have been obtained by making an integral representation for the statistical operator and then using the method of steepest descents.<sup>9</sup> The approach of bounding the free energies is similar in spirit to the Kac-Thompson discussion<sup>10</sup> of the classical Heisenberg model, and it has a number of advantages when compared to the method of steepest descents. It can be made rigorous and, in particular, when there are  $N$  lattice sites, the limits  $n \rightarrow \infty$  and  $N \rightarrow \infty$  can be taken in either order or both together. The self-consistency condition is simpler and also rather more convenient to use in the first-order region where it is necessary to distinguish between two different solutions. This is one of the main practical reasons for giving a more careful discussion of the Hartree approximation, which is not usually shown to provide a bound on the free energy. Expressions for correlation functions are also derived in Sec. II, and the solution of the self-consistency condition leading to properties of the model is given in Sec. III. Finally, in Sec. IV, it is pointed out that there is an approximation method for physically relevant discrete-spin systems, which leads to qualitatively the same results as this exactly solvable model and to a potentially good quantitative determination of phase diagrams and physical properties. It is therefore a substantial improvement on mean-field theory, although it is scarcely more difficult to apply.

### II. DEFINITION AND FORMAL SOLUTION OF THE MODEL

The model has  $n$  spins  $S_{i\alpha}$  ( $\alpha = 1, 2, \dots, n$ ) taken to be the components of a vector  $\vec{S}_i$  at each site  $i$ .

The Hamiltonian is

$$\mathcal{H} = \sum_{i,j} J_{ij} \vec{S}_i \cdot \vec{S}_j + \sum_i n\phi(\Delta, n^{-1}\vec{S}_i^2) + \sum_i \vec{H} \cdot \vec{S}_i. \quad (2.1)$$

The spins vary continuously from  $-\infty$  to  $+\infty$  and the temperature  $T$  is absorbed into  $J_{ij}$  and  $\phi$ , so that the partition function is

$$Z_n = \int_{-\infty}^{\infty} \prod_{\alpha} \prod_i dS_{i\alpha} e^{-\mathcal{H}}. \quad (2.2)$$

The parameter  $\Delta$  plays the role of the crystal-field splitting of the BEG model,<sup>1</sup> and variation of  $\Delta$  is one way of producing a tricritical point. The magnetic field  $\vec{H}$  is assumed to be in the  $(1, 1, \dots, 1)$  direction which is necessary<sup>9</sup> for general  $n$ -component systems for large  $n$ , although it will be seen that, with the model of Eq. (2.1), the more usual convention of having a field of order  $n^{1/2}$  along one direction could also be used. There are two ways of viewing the Hamiltonian. It may be regarded as a generalization of the  $n$ -component continuous-spin model used by Wilson,<sup>11</sup> with the function  $n\phi(\Delta, n^{-1}\vec{S}_i^2)$  replacing the fourth-order form  $[r\vec{S}_i^2 + (u/n)(\vec{S}_i^2)^2]$ . The factors of  $n$  are necessary to obtain a well-defined limit as  $n \rightarrow \infty$ , and both the inclusion of higher-order terms and the parametric dependence on  $\Delta$  are essential for the discussion of tricritical points. Alternatively a one-component version may be obtained from the BEG model<sup>1</sup> by making a Gaussian integral representation of the exchange term, leading to Eq. (2.1) with  $n=1$  and a particular choice of  $\phi$ . The derivation is given in the appendix. In either case,  $J_{ij}$  is taken to be short ranged, ferromagnetic, and translationally invariant, and it may then be diagonalized to  $g_{\vec{q}}$  by Fourier transformation. It is assumed that  $g_0=0$  and  $g_{\vec{q}} > 0$  for all  $\vec{q} \neq 0$ , which may be arranged by subtracting a diagonal term from  $J_{ij}$  and adding it into  $\phi$  so that the Hamiltonian is unchanged. The principal assumption for  $\phi$  is that it is well behaved and analytic so that all singularities may be attributed to critical phenomena.

For  $n \rightarrow \infty$ ,  $Z_n$  may be evaluated by making a double integral representation of  $e^{-\mathcal{H}}$  after which the  $S_{i\alpha}$  integrals become Gaussian and the representation integrals may be carried out by the method of steepest descents. This is described for more general Hamiltonians in Ref. 9. Here, however, the model will be solved by proving upper and lower bounds on the free energy which become equal as  $n \rightarrow \infty$ . This approach is rather more convenient to use in practice for first-order transitions, and it can be made rigorous, with the final result independent of whether  $N \rightarrow \infty$  before or after  $n \rightarrow \infty$  or  $n, N \rightarrow \infty$  together. It also leads to a rather simpler self-consistency condition. The analog of the "sticking" problem of the steepest-descents approach is

avoided by working in a finite magnetic field and only allowing it to become zero after the limit  $N \rightarrow \infty$  has been taken.

#### A. Upper bound on the free energy

To obtain bounds on the free energy, define

$$\mathcal{H}_0 = \sum_{i,j} (J_{ij} + \kappa^2 \delta_{ij}) \vec{S}_i \cdot \vec{S}_j + \sum_i \vec{H} \cdot \vec{S}_i, \quad (2.3)$$

so that, from Eqs. (2.1) and (2.3),

$$\mathcal{H} - \mathcal{H}_0 = n \sum_i \left( \phi(\Delta, n^{-1}\vec{S}_i^2) - \frac{\kappa^2}{n} \vec{S}_i^2 \right). \quad (2.4)$$

Then if the free energy per site per degree of freedom is

$$F = - (1/Nn) \ln Z_n, \quad (2.5)$$

the thermodynamic variation principle<sup>12</sup> gives

$$F \leq F_0 + (1/nN) \langle \mathcal{H} - \mathcal{H}_0 \rangle_0, \quad (2.6)$$

where  $nNF_0$  is the free energy for  $\mathcal{H}_0$  and  $\langle \mathcal{H} - \mathcal{H}_0 \rangle_0$  is the thermodynamic average of  $\mathcal{H} - \mathcal{H}_0$  taken with weight  $e^{-\mathcal{H}_0}$ . Since  $\mathcal{H}_0$  in Eq. (2.3) is quadratic, the integrals for the partition function are Gaussian and  $F_0$  may be evaluated exactly to give, in the limit  $N \rightarrow \infty$ ,

$$\lim_{N \rightarrow \infty} F_0 = \frac{1}{16\pi^3} \int d\vec{q} \ln(g_{\vec{q}} + \kappa^2) - \frac{H^2}{4\kappa^2} - \ln \pi^{1/2}, \quad (2.7)$$

using  $g_0=0$ . To determine  $\langle \mathcal{H} - \mathcal{H}_0 \rangle_0$ , it is simplest to use a double integral representation of  $\phi$ :

$$\langle \phi(\Delta, n^{-1}\vec{S}_p^2) \rangle_0 = \frac{1}{2\pi i} \int_{-\infty}^{\infty} dt \times \int_{-i\infty}^{i\infty} d\lambda \phi(\Delta, t) e^{\lambda t} \langle e^{-\lambda n^{-1}\vec{S}_p^2} \rangle_0. \quad (2.8)$$

This equation may be proved by first completing the  $\lambda$  integration to obtain  $\delta(t - n^{-1}\vec{S}_p^2)$ , after which the  $t$  integral is trivial. The integrals which come into the statistical average in Eq. (2.8) are products over  $\alpha$  of  $n$  identical terms so

$$\langle e^{-\lambda n^{-1}\vec{S}_p^2} \rangle_0 = \left( \int_{-\infty}^{\infty} dS \nu_0(S) e^{-\lambda n^{-1}S^2} \right)^n, \quad (2.9)$$

where  $\nu_0(S)$  is the single-spin distribution function for the one-component Gaussian model. By translational invariance  $\nu_0(S)$  is independent of  $p$ , and it is also of order unity, with a well-defined limit as  $N \rightarrow \infty$ . Then the limits  $N \rightarrow \infty$  and  $n \rightarrow \infty$  may be taken in either order in Eq. (2.9) to give

$$\lim_{\substack{n \rightarrow \infty \\ N \rightarrow \infty}} \langle e^{-\lambda n^{-1}\vec{S}_p^2} \rangle_0 = \exp \left( -\lambda \int_{-\infty}^{\infty} dS_p \nu_0(S) S^2 \right) = \exp[-\lambda F'_0(\kappa^2)]. \quad (2.10)$$

The right-hand sides of these equations involve alternative ways of writing the mean value of  $S_i^2$ . If Eq. (2.10) is substituted into Eq. (2.8), the  $\lambda$  and  $t$  integrals may be carried out and, using Eq. (2.4), the inequality (2.6) becomes

$$\lim_{\substack{n \rightarrow \infty \\ N \rightarrow \infty}} F \cong F_H,$$

where

$$F_H = F_0 + \phi(\Delta, F'_0(\kappa^2)) - \kappa^2 F'_0(\kappa^2). \quad (2.11)$$

The strongest form of inequality is obtained by minimizing  $F_H$  with respect to  $\kappa^2$  to give

$$F \cong F_H(\kappa_0^2), \quad (2.12)$$

where  $\kappa_0$  satisfies

$$\frac{\partial \phi(\Delta, F'_0)}{\partial F'_0} = \kappa_0^2. \quad (2.13)$$

which gives a minimum provided

$$\left( \frac{\partial^2 \phi(\Delta, \tau)}{\partial \tau^2} \right)_{\tau = F'_0(\kappa_0^2)} > \frac{1}{F''_0(\kappa_0^2)}. \quad (2.14)$$

This is a stability condition on  $\phi$ , which is assumed to be satisfied. A more explicit version of (2.14) will be given in Sec. III. Equation (2.11) for  $F_H$  is a generalization of the Hartree approximation, with the self-consistent field  $\kappa_0^2$  given by Eq. (2.13).

#### B. Lower bound on the free energy

If the roles of  $\mathcal{H}_0$  and  $\mathcal{H}$  are interchanged in the thermodynamic variation principle, it becomes

$$F_0 \cong F + (1/nN) \langle \mathcal{H}_0 - \mathcal{H} \rangle, \quad (2.15)$$

where, now, the average of  $\mathcal{H}_0 - \mathcal{H}$  is taken in the distribution  $e^{-\mathcal{H}}$ . From Eq. (2.4), the integrals over the  $\vec{S}_p$  may be carried out in  $n$ -dimensional polar coordinates leaving only the integral over  $\tau = |\vec{S}_p|^2$  to be carried out. Then, using translational invariance, Eq. (2.15) may be written

$$F \cong F_0(\kappa^2) + \int_0^\infty d\tau w(\tau) [\phi(\Delta, \tau) - \kappa^2 \tau]. \quad (2.16)$$

Here  $w(\tau)$  is a single-site distribution function and it is a property of the exact distribution  $e^{-\mathcal{H}}$ . The right-hand side of Eq. (2.16) may be maximized with respect to variation of  $\kappa$  by choosing  $\kappa$  to be the solution of

$$F'_0(\kappa^2) = \int_0^\infty d\tau w(\tau) \tau, \quad (2.17)$$

since, from Eq. (2.7),  $F''_0(\kappa^2) < 0$ . This gives the strongest form of inequality. With  $\kappa$  given by Eq. (2.17), the right-hand side of (2.16) is a functional of  $w(\tau)$  only. Then if  $w(\tau)$  is replaced by the function  $w_0(\tau)$  which minimizes the right-hand side of (2.16), the inequality still holds. The extremal

form of  $w(\tau)$  is  $\delta(\tau - \tau_0)$  and, with this, Eq. (2.17) becomes

$$F'_0(\kappa^2) = \tau_0. \quad (2.18)$$

The minimization is now to be carried out by using Eq. (2.18) to eliminate  $\kappa$  from (2.16) and minimizing with respect to variation of  $\tau_0$ . Since Eq. (2.18) gives a one-to-one correspondence between  $\kappa$  and  $\tau_0$ , this is completely equivalent to using Eq. (2.18) to eliminate  $\tau_0$  from (2.16) and minimizing with respect to  $\kappa$ . The right-hand side of (2.16) then becomes equal to  $F_H$  as in Eq. (2.11) and thus

$$F \cong F_H(\kappa_0). \quad (2.19)$$

This is true for any  $n$  and  $N$  but when combined with (2.12) it shows that

$$\lim_{\substack{n \rightarrow \infty \\ N \rightarrow \infty}} F = F_H(\kappa_0). \quad (2.20)$$

It will be seen in Sec. III that, in the first-order region,  $\partial^2 \phi(\Delta, \tau) / \partial \tau^2 < 0$ , and it is important that this is not excluded by (2.14), since  $F''_0(\kappa^2) < 0$ . In order to achieve this condition it was necessary to maximize (2.16) with respect to  $\kappa^2$  before minimizing with respect to  $w(\tau)$ . Reversing the order requires that  $\phi(\Delta, \tau)$  have an absolute minimum in the region of interest and therefore gives a weaker inequality which also could have been obtained more directly by replacing  $\mathcal{H} - \mathcal{H}_0$  by its minimum value in the integral (2.2) for  $Z_n$ . The method of steepest descents gives a condition similar to Eq. (2.13) but with  $\kappa^2$  dependent upon  $i$  so that there are  $N$  equations. The derivation given here shows directly that the optimum solution of these equations is uniform.

#### C. Magnetization and correlation functions

The basic equation to be solved is Eq. (2.13), and the free energy is then given by Eqs. (2.7) and (2.11). In the ordered phase, it will be seen that the role of  $\kappa$  is taken over by the magnetization per site per degree of freedom

$$m = - \frac{\partial F_H}{\partial H}. \quad (2.21)$$

Using Eqs. (2.7), (2.12), and (2.13),  $m$  becomes

$$m = H/2\kappa^2. \quad (2.22)$$

If  $\kappa_0$  is determined from Eq. (2.13) and substituted into Eq. (2.22), the equation of state is obtained. In the ordered phase ( $m \neq 0$ ),  $\kappa^2 \sim H/2m$  for small  $H$  and therefore, when  $H \rightarrow 0$ ,  $m$  reflects the existence of  $\kappa$ . In Eq. (2.22),  $m$  is formally identical to that of the Gaussian model, but it will be seen that, at a normal critical point,  $\kappa$  is constrained by Eq. (2.13) leading to a change in its critical behavior.

To obtain the spin- and square-spin correlation functions, imagine there are fields  $\sum_i^N \lambda_i \vec{S}_i^2$  and

$\sum_i^N \vec{H}_i \cdot \vec{S}_i$  applied to the system. Then, in finding the free energy,  $\kappa$  has to be replaced by a site-dependent function  $\kappa_i$  and  $F_0$  becomes

$$NF_0 = \frac{1}{2} \text{Tr} \ln(\hat{J} + \hat{\kappa}^2 + \hat{\lambda}) - \frac{1}{4} \underline{H}' (\hat{J} + \hat{\kappa}^2 + \hat{\lambda})^{-1} \underline{H}, \quad (2.23)$$

where  $\hat{J}$ ,  $\hat{\kappa}^2$ , and  $\hat{\lambda}$  are matrices with elements  $J_{ij}$ ,  $\kappa_i^2 \delta_{ij}$ , and  $\lambda_i \delta_{ij}$ , respectively, and  $\underline{H}$  is a column vector with elements  $H + H_i$ . The spin-correlation function in zero magnetic field is then

$$G_{ij} = n^{-1} (\langle \vec{S}_i \cdot \vec{S}_j \rangle - \langle \vec{S}_i \rangle \cdot \langle \vec{S}_j \rangle) \\ = - \left( \frac{\partial^2 NF_H}{\partial H_i \partial H_j} \right)_{\lambda_p, H_p=0} \quad (2.24)$$

$$= - \left( \frac{\partial^2 NF_0}{\partial H_i \partial H_j} \right)_{\lambda_p, H_p=0}, \quad (2.25)$$

using Eqs. (2.11), (2.13), and (2.20). Then with (2.23),

$$G_{ij} = \frac{1}{2} \left( \frac{1}{\hat{J} + \kappa_0^2} \right)_{ij}, \quad (2.26)$$

which may be diagonalized by Fourier transformation to

$$G_{\vec{q}} = \frac{1}{2} (g_{\vec{q}} + \kappa_0^2)^{-1}. \quad (2.27)$$

Similarly the square-spin correlation function is

$$C_{ij} = n^{-1} (\langle \vec{S}_i^2 \vec{S}_j^2 \rangle - \langle \vec{S}_i^2 \rangle \langle \vec{S}_j^2 \rangle), \quad (2.28)$$

$$= - \left( \frac{\partial^2 NF_H}{\partial \lambda_i \partial \lambda_j} \right)_{\lambda_p, H_p=0}, \quad (2.29)$$

and it is related to the density-density correlation function in helium mixtures,<sup>1</sup> which has been obtained from light-scattering experiments.<sup>6</sup> It is of order unity, whereas  $\langle \vec{S}_i^2 \vec{S}_j^2 \rangle / n$  and  $\langle \vec{S}_i^2 \rangle \langle \vec{S}_j^2 \rangle / n$  are of order  $n$ .

Substituting Eqs. (2.11) and (2.23) into Eq. (2.29),

$$C_{ij} = C_{ij}^0 + \sum_p^N C_{ip}^0 \frac{\partial \kappa_p^2}{\partial \lambda_j}, \quad (2.30)$$

where

$$C_{ij}^0 = 2G_{ij}^2 + 2m^2 G_{ij} \quad (2.31)$$

is the square-spin correlation function of the Gaussian model. On differentiating the site-dependent version of Eq. (2.13) and using Eq. (2.29), it is found that

$$\frac{\partial \kappa_p^2}{\partial \lambda_j} = -\phi'' C_{pj}, \quad (2.32)$$

with

$$\phi'' = \frac{\partial^2 \phi(\Delta, F_0')}{\partial (F_0')^2}. \quad (2.33)$$

Equations (2.30) and (2.32) may be solved by Fourier transformation to give

$$C_{\vec{q}} = C_{\vec{q}}^0 / (1 + \phi'' C_{\vec{q}}^0), \quad (2.34)$$

where  $C_{\vec{q}}^0$  and  $C_{\vec{q}}$  are the Fourier transforms of  $C_{ij}^0$  and  $C_{ij}$ , respectively. The interest in  $C_{\vec{q}}$  is that it is the correlation function for nonordering fluctuations which become critical at a tricritical point. This will be shown explicitly after the solution of the self-consistency condition has been obtained in Sec. III.

#### D. Corrections of order $n^{-1}$

The discussion so far has regarded the model as one which is exactly solvable as  $n \rightarrow \infty$ , but it may equally well be taken to be one in which  $n$  is large, and the free energy is evaluated as a series in  $n^{-1}$ . If we expand Eq. (2.4) in powers of  $(\vec{S}^2/n - \langle \vec{S}^2 \rangle/n)$ , using Eq. (2.13),<sup>1</sup> then, in lowest order, the change in  $\mathcal{F} - \mathcal{F}_0$  is

$$\delta(\mathcal{F} - \mathcal{F}_0) = \frac{1}{2} n \phi'' \sum_i^N (\vec{S}_i^2/n - \langle \vec{S}_i^2 \rangle/n)^2, \quad (2.35)$$

where  $\phi''$  is defined in Eq. (2.33), and the change in the mean value of  $\mathcal{F} - \mathcal{F}_0$  is

$$\langle \delta(\mathcal{F} - \mathcal{F}_0) \rangle = \phi'' \sum_i^N C_{ii}, \quad (2.36)$$

using Eq. (2.28). The correction to the free energy is obtained by introducing a coupling constant  $\lambda$ , multiplying  $\phi$ , and integrating over it in the usual way. Using Eq. (2.34) for  $C$ , we obtain

$$F = F_H + \frac{1}{16\pi^3 n} \int d\vec{q} \ln(1 + \phi'' C_{\vec{q}}^0), \quad (2.37)$$

which gives the free energy to order  $n^{-1}$ . This is the generalization of the form used by Ferrel and Scalapino<sup>13</sup> to obtain order  $n^{-1}$  corrections to critical exponents near to an ordinary critical point. We shall consider the consequences near to a tricritical point in Sec. III.

### III. SOLUTION OF THE SELF-CONSISTENCY CONDITION

The self-consistency condition is given in Eq. (2.13). It involves  $F_0'(\kappa^2)$  which may be evaluated in terms of  $m$  and  $\kappa$  from Eqs. (2.7) and (2.22):

$$F_0'(\kappa^2) = (16\pi^3)^{-1} \int d\vec{q} (g_{\vec{q}} + \kappa^2)^{-1} + m^2. \quad (3.1)$$

To bring out the  $\kappa$  dependence, this equation will be rewritten

$$F_0'(\kappa^2) = W - \gamma(\kappa) + m^2, \quad (3.2)$$

where  $W$  is the value of the integral in Eq. (3.1) for  $\kappa = 0$ , and is a Watson integral for the lattice in question. For short-range forces,  $g_{\vec{q}} \sim q^2$  for small  $q$  and it is easy to see that

$$\gamma(\kappa) \approx \gamma_d \kappa^{d-2} \quad (3.3)$$

for small  $\kappa$  and  $2 < d < 4$ .

Equation (2.22) shows that when  $H \rightarrow 0$ , either  $m \rightarrow 0$  or  $\kappa \rightarrow 0$  or both. Across a  $\lambda$  line, the transition from  $\kappa \neq 0$  to  $m \neq 0$  takes place continuously and it must be the line  $m=0$ ,  $\kappa=0$ , which according to Eqs. (2.13), (3.2) and (3.3) is

$$\frac{\partial \phi(\Delta, W)}{\partial W} = 0. \quad (3.4)$$

Since both  $\phi$  and  $W$  depend upon  $T$ , this is the equation of a line  $T = T_c(\Delta)$  in the  $(\Delta, T)$  plane. Equation (2.13) is an equation of constraint<sup>14</sup> on the Gaussian free energy  $F_0$ , and hence the critical exponents are those of the spherical model.<sup>15</sup> This requires that  $\phi(\Delta, \tau)$  is analytic at  $\tau = W$  so that Eq. (2.13) may be expanded for small  $m$  and  $\kappa$ , using Eq. (3.2), to obtain, in second order,

$$\kappa_0^2 = \phi'_0 + \phi''_0 [m^2 - \gamma(\kappa_0)] + \frac{1}{2} \phi'''_0 [m^2 - \gamma(\kappa_0)]^2, \quad (3.5)$$

where

$$\phi_0^{(n)} \equiv \frac{\partial^n \phi(\Delta, W)}{\partial W^n}. \quad (3.6)$$

From Eq. (3.3), it is clear that for  $m=0$  and  $d < 4$ , the first two terms on the right-hand side of Eq. (3.5) dominate, and if  $\phi'_0$  is proportional to  $T - T_c$ , then  $\kappa \sim (T - T_c)^{1/d-2}$ , as in the spherical model.<sup>15</sup> The other exponents may be obtained in a similar way.

However, Eq. (3.4) is only a necessary condition for a continuous transition. If, for  $\phi'_0=0$ , the solution ( $\kappa_0=0$ ,  $m=0$ ) of Eq. (3.5) does not give the lowest free energy, the transition takes place away from the  $\lambda$  line, and hence it cannot be continuous. The condition for this to occur depends upon the number of space dimensions, and it is convenient first to study the most important case  $d=3$ , for which it will be shown there are additional solutions when  $\phi'' < 0$ , and that there is a tricritical point where the line  $\phi''_0=0$  intersects the  $\lambda$  line. The situation for  $d \neq 3$  will then be considered separately. In this discussion, it is assumed that there are no solutions of Eq. (2.13) for large  $|m^2 - \gamma(\kappa)|$  and that  $\phi'''_0 > 0$ . Then it is sufficient to use the expansion of Eq. (2.13) up to the order given in Eq. (3.5). This is exact if  $\phi$  is at most sixth order in the  $S_i$ , as frequently assumed in the discussion of tricritical points.<sup>2,4</sup> In the general case, it is possible to obtain a wide variety of phase diagrams, which we do not wish to consider here.

#### A. Three dimensions

##### 1. Tricritical point and coexistence curve for $H=0$

In three dimensions,  $\gamma(\kappa) = \gamma_3 \kappa$  for small  $\kappa$ . When  $\phi''_0 > 0$ , Eq. (3.5) has no solution with  $\kappa=0$  for  $\phi'_0 > 0$  or with  $m=0$  for  $\phi'_0 < 0$ , and a continuous transition across the  $\lambda$  line  $\phi'_0=0$  is the only possibility. On the other hand, when  $\phi''_0 < 0$ , there are two solu-

tions

$$\kappa_0 = \frac{-\gamma_3 \phi''_0 + [\gamma_3^2 (\phi''_0)^2 + 4\phi'_0(1 - \gamma_3^2 \phi''_0/2)]^{1/2}}{2(1 - \gamma_3^2 \phi''_0/2)}, \quad (3.7)$$

$$m=0,$$

and

$$\kappa_0=0, \quad (3.8)$$

$$m_0^2 = \frac{-\phi'_0 + [(\phi''_0)^2 - 2\phi''_0 \phi'_0]^{1/2}}{\phi'''_0},$$

provided  $|(\phi''_0)^2/\phi'_0|$  is large enough for real roots. For the  $\kappa_0 \neq 0$  solution to exist with  $\phi'_0 > 0$  and arbitrary  $\phi''_0$ , it is necessary that

$$\gamma_3^2 \phi'''_0 < 2, \quad (3.9)$$

and it is easily verified that this is also the condition for stability of the model at small  $\kappa$ , according to (2.14), and it is assumed to be satisfied. Then there is a first-order transition along the line in the  $(\Delta, T)$  plane for which the solutions (3.8) and (3.9) give equal free energies.

Along the  $\lambda$  line, the solution (3.7) gives

$$\delta F = \frac{1}{8} \gamma_3^4 (\phi''_0)^3 (1 - \gamma_3^2 \phi''_0/2)^{-2}, \quad (3.10)$$

for  $m=0$ , whereas, with Eq. (3.8),

$$\delta F = 2(\phi''_0)^3 / 3(\phi'''_0)^2, \quad (3.11)$$

for  $\kappa_0=0$ . Here  $\delta F$  is the difference between the free energy  $F_H$  and its value for  $\kappa=0$ ,  $m=0$ . If  $\gamma_3 \phi'''_0 < 1$ , Eq. (3.11) gives the lower free energy and the first-order transition has taken place above the  $\lambda$  line, otherwise it occurs below. As  $\phi''_0 \rightarrow 0$ , the two free energies become equal and hence the coexistence curve meets the  $\lambda$  line at the point  $\phi''_0 = 0$ . It is then a tricritical point and its position in the  $(\Delta, T)$  plane will be denoted by  $(\Delta_t, T_t)$ . For some purposes, it is useful to regard  $(\phi'_0, \phi''_0)$  as the coordinates of a point in the  $(\Delta, T)$  plane near to the tricritical point, where both quantities are small.

In general, in order to have the freedom to equate the free energies, it is necessary that neither  $\phi'_0$  nor  $\phi''_0$  be negligible in the solutions (3.7) and (3.8), which means that the coexistence curve must have the form

$$\phi'_0 = \alpha(\phi''_0)^2, \quad (3.12)$$

for small  $|\phi'_0|$  and  $|\phi''_0|$ . The two free energies are of order  $(\phi''_0)^3$  and  $\alpha$  may be determined by equating them. The result will not be written down since only the general form of Eq. (3.12) will be important for the subsequent discussion.

##### 2. Concentration susceptibility and tricritical exponents

The analog of the concentration  $x$  of  ${}^3\text{He}$ - ${}^4\text{He}$  mixtures is the variable thermodynamically conjugate to  $\Delta$ , that is  $x = -(\partial F_H / \partial \Delta)_T$ . Since  $F_H$  is stationary

with respect to variation of  $\kappa$ , it follows that

$$x = -\frac{\partial\phi(\Delta, F'_0)}{\partial\Delta}. \quad (3.13)$$

The concentration susceptibility is given by

$$\left(\frac{\partial x}{\partial\Delta}\right)_T = -\frac{\partial^2\phi(\Delta, F'_0)}{\partial\Delta^2} - \frac{\partial^2\phi(\Delta, F'_0)}{\partial\Delta\partial F'_0} \left(\frac{\partial F'_0}{\partial\Delta}\right)_T, \quad (3.14)$$

where, using Eqs. (2.13), (2.33) and (3.2) for  $m=0$ ,

$$\left(\frac{\partial F'_0}{\partial\Delta}\right)_T = \frac{-\gamma'(\kappa_0)\partial^2\phi/\partial\Delta\partial F'_0}{2\kappa_0 + \gamma'(\kappa_0)\phi''}. \quad (3.15)$$

Along the  $\lambda$  line,  $(\partial x/\partial\Delta)_T$  is a nonordering susceptibility and it is finite since  $\kappa_0$  vanishes but  $\gamma'(\kappa_0)$  and  $\phi''$  do not. At the tricritical point ( $\kappa_0=0$ ,  $\phi''=0$ ),  $(\partial F'_0/\partial\Delta)_T$  diverges and hence so does  $(\partial x/\partial\Delta)_T$ . The critical exponents depend upon the path of approach. For  $\Delta$  constant and equal to  $\Delta_t$ , Eqs. (2.33), (3.2), and (3.3) show that the denominator on the right-hand side of Eq. (3.15) is  $2\kappa_0(1 - \frac{1}{2}\gamma_3^2 \times \phi_0''') + \gamma_3\phi_0''$  which is positive because of the stability condition (3.9). Then, since both  $\phi_0'$  and  $\phi_0''$  are proportional to  $T - T_t$  near to the tricritical point, Eq. (3.5) gives  $\kappa_0 \sim (T - T_t)^{1/2}$  and hence from Eqs. (3.14) and (3.15),  $(\partial x/\partial\Delta)_T \sim (T - T_t)^{-1/2}$ . These are Gaussian exponents and the same results may be obtained from renormalization-group arguments<sup>2,4</sup> or high-temperature series expansions<sup>8</sup> of the BEG model. On the other hand, along the coexistence curve, Eqs. (3.5) and (3.12) show that  $\kappa \sim (T - T_t)$  and hence  $(\partial x/\partial\Delta)_T \sim (T - T_t)^{-1}$ . Also, for  $x$  a constant and equal to its tricritical value  $x_t$ ,  $\Delta$  varies and expansion of Eq. (3.13) near to the tricritical point, using Eqs. (3.2) and (3.3), gives

$$\frac{\partial^2\phi_0}{\partial\Delta^2}(\Delta - \Delta_t) - \frac{\partial\phi_0'}{\partial\Delta}\gamma(\kappa) = 0. \quad (3.16)$$

Now if Eq. (3.5) is expanded to first order in  $\Delta - \Delta_t$  and Eq. (3.16) is used to express  $\Delta - \Delta_t$  in terms of  $\kappa_0$ , it follows that  $\kappa \sim T - T_t$  since  $\gamma(\kappa) = \gamma_3\kappa$ , and again  $(dx/dT)_T \sim (T - T_t)^{-1}$ . Another way of looking at these results is to see that the tricritical exponents are Gaussian because when  $\phi_0'' \sim T - T_t$ ,  $\phi_0' \sim T - T_t$ , the constraint (3.5) does not renormalize the exponents as it does at other points of the  $\lambda$  line. But, when Eq. (3.12) is satisfied, or  $x = \text{const.}$ , the constraint (3.5) is significant and the exponents are renormalized. The exponents for the susceptibility divergence at the tricritical point are in agreement with experiments on liquid-helium mixtures.<sup>5,6</sup> Of course it is a property of the model that the unrenormalized exponents are Gaussian along the  $\lambda$  line as well as at the tricritical point. Later it will be shown how Eqs. (3.14) and (3.15) may be obtained from the wave-vector-dependent susceptibility and the corresponding results for  $m \neq 0$  will be given.

### 3. Slope of the phase boundary

Suppose that the phase boundary in the  $(\Delta, T)$  plane is  $T = T_0(\Delta)$ . Along the coexistence curve,  $T_0(\Delta)$  is obtained by solving Eqs. (3.12) and

$$T'_0(\Delta_t) = \left(\frac{\partial\phi_0'}{\partial\Delta} / \frac{\partial\phi_0'}{\partial T}\right)_{\substack{\Delta=\Delta_t \\ T=T_t}}, \quad (3.17)$$

since  $\phi_0'' = 0$  at  $(\Delta_t, T_t)$ . But this is exactly the result for the  $\lambda$  line  $\phi_0' = 0$  and hence the slope of the phase boundary in the  $(\Delta, T)$  plane is continuous at the tricritical point. However this is not true of the phase boundary in the  $(x, T)$  plane, where the first-order region has two values of  $x$  for every  $T$ , one for each of the two coexisting phases. The phase boundary for  $m \neq 0$  makes a large angle with the  $\lambda$  line, but the other branch has only a small discontinuity in slope. This discontinuity does not appear in mean-field theories,<sup>1</sup> but it is seen in experiments<sup>5,7</sup> on helium mixtures and  $\text{FeCl}_2$ , as well as in series solutions<sup>8</sup> of the BEG model. It has been speculated that in some way it is associated with critical fluctuations, but in the model under consideration it is a consequence of the variation of  $\kappa_0$  along the coexistence curve. Suppose the  $m=0$  phase boundary is  $x = x_0(T)$  in the  $(x, T)$  plane. Then from Eqs. (3.2) and (3.13),

$$x'_0(T_t) = -\left(\frac{\partial^2\phi_0}{\partial\Delta^2} / T'_0(\Delta_t)\right) - \frac{\partial\phi_0'}{\partial\Delta} \left[ \frac{dW}{dT} - \gamma'(\kappa) \left(\frac{d\kappa}{dT}\right)_{\text{PB}} \right]. \quad (3.18)$$

Here  $(d\kappa/dT)_{\text{PB}}$  is the derivative of  $\kappa$  with respect to  $T$  taken along the phase boundary. The derivatives of  $\phi_0$ ,  $W$ , and  $\gamma(\kappa)$  are assumed to be continuous in defining the model and  $T'_0(\Delta_t)$  has just been shown to be continuous. However  $(d\kappa/dT)_{\text{PB}}$  is discontinuous at the tricritical point, since  $\kappa$  is constant and equal to zero along the  $\lambda$  line but  $\kappa \sim T - T_t$  along the coexistence curve. In three dimensions  $\gamma'(\kappa) = \gamma_3$ ; so the discontinuity in  $x'_0(T_t)$  does not vanish. The value of the discontinuity depends upon  $\phi_0'''$ ; so there is not much point in evaluating it for this model to compare with experiment.

### 4. Correlation functions

The correlation function with the interesting structure is  $C_q$  of Eqs. (2.28) and (2.34), since it refers to fluctuations in a nonordering density which become critical at the tricritical point. In order to evaluate the integrals, it will be assumed that  $\mathcal{J}_q = q^2$ . The exchange constant and numerical factors have been absorbed into  $q$  by choice of units. If  $\vec{r}$  is the separation of two lattice sites, the Fourier transform of  $G_q$  in Eq. (2.27) is

$$G(\vec{r}) = e^{-\kappa_0 r} / 8\pi r. \quad (3.19)$$

Substituting this expression into Eq. (2.31) and Fourier transforming gives

$$C_{\bar{q}}^0 = \frac{\arctan(q/2\kappa_0)}{8\pi q} + \frac{m^2}{q^2 + \kappa_0^2}. \quad (3.20)$$

If Eq. (3.20) is substituted into Eq. (2.34), the resultant expression for  $C_{\bar{q}}$  is valid in the ordered and the disordered phases and it satisfies tricritical scaling with Gaussian exponents.<sup>16</sup> This expression for  $C_{\bar{q}}$  in the disordered phase ( $m=0$ ) was obtained by Amit and de Dominicis<sup>2</sup> who used it to discuss crossover from critical to tricritical behavior and to evaluate the crossover exponent. In the ordered phase  $\kappa_0=0$  and

$$C_{\bar{q}} = \frac{m^2 + q/16}{q^2 + \phi''(m^2 + q/16)}. \quad (3.21)$$

In particular, along the coexistence curve near the tricritical point, both  $m^2$  and  $\phi''$  are proportional to  $T - T_t$  and  $C_{\bar{q}}$  has the form

$$C_{\bar{q}} = \frac{a(T - T_t) + q/16}{q^2 + ab(T - T_t)^2 + b(T - T_t)q/16}. \quad (3.22)$$

This may be compared with the calculation of Furman and Blume,<sup>17</sup> who evaluated  $C_{\bar{q}}$  using mean-field theory. Their result does not have the term of order  $q$  in the numerator and denominator of Eq. (3.22). However, the coefficient of this term is small, and existing light-scattering experiments<sup>6</sup> are well fitted without it.

At  $T = T_t$ ,  $C_{\bar{q}} = (16q)^{-1} \rightarrow \infty$  as  $q \rightarrow 0$ , reflecting the divergence of  $C_{\bar{q}}$  for  $T \rightarrow T_{t+}$ . In contrast, mean-field theory<sup>17</sup> gives a term of order  $q^2$  in the numerator of  $C_{\bar{q}}$  in place of the linear term, and at  $T = T_t$ ,  $C_{\bar{q}}$  remains finite as  $q \rightarrow 0$ . This is related to the fact that mean-field theory fails to give a divergence in the nonordering susceptibility as the tricritical point is approached from above.

It is also of interest to consider the limit  $\bar{q} \rightarrow 0$ , since  $C_{\bar{q}=0}$  is related to the concentration susceptibility  $(\partial x / \partial \Delta)_T$ . This may be seen formally by differentiating  $F = -(nN)^{-1} \ln Z_n$ , using Eqs. (2.2) and (2.1),

$$\begin{aligned} \left(\frac{\partial x}{\partial \Delta}\right)_T &= -\frac{1}{N} \frac{\partial}{\partial \Delta} \left\langle \sum_i^N \frac{\partial \phi(\Delta, n^{-1} \bar{S}_i^2)}{\partial \Delta} \right\rangle \\ &= -\frac{1}{N} \left\langle \sum_i^N \frac{\partial^2 \phi(\Delta, n^{-1} \bar{S}_i^2)}{\partial \Delta^2} \right\rangle \\ &\quad + \frac{n}{N} \left[ \left\langle \left( \sum_i^N \frac{\partial \phi(\Delta, n^{-1} \bar{S}_i^2)}{\partial \Delta} \right)^2 \right\rangle \right. \\ &\quad \left. - \left\langle \sum_i^N \frac{\partial \phi(\Delta, n^{-1} \bar{S}_i^2)}{\partial \Delta} \right\rangle^2 \right]. \end{aligned} \quad (3.23)$$

To order unity,  $n^{-1} \bar{S}_i^2$  may be replaced by  $F'_0(\kappa^2)$  in the first term on the right-hand side of Eq.

(3.23), but it is necessary to expand the second term to first order in  $(n^{-1} \bar{S}_i^2 - F'_0)$  as in Sec. IID, to obtain

$$\begin{aligned} \left(\frac{\partial x}{\partial \Delta}\right)_T &= -\frac{\partial^2 \phi(\Delta, F'_0)}{\partial \Delta^2} + \frac{\partial^2 \phi(\Delta, F'_0)}{\partial \Delta \partial F'_0} \frac{1}{N} \sum_{i,j}^N C_{ij} \\ &= -\frac{\partial^2 \phi(\Delta, F'_0)}{\partial \Delta^2} + \frac{\partial^2 \phi(\Delta, F'_0)}{\partial \Delta \partial F'_0} C_{\bar{q}=0}. \end{aligned} \quad (3.24)$$

Now from Eqs. (2.34) and (3.20),

$$C_{\bar{q}=0} = \frac{(8\pi)^{-1} 2m^2 / \kappa_0}{2\kappa_0 + \phi''[(8\pi)^{-1} + 2m^2 / \kappa_0]}. \quad (3.25)$$

When  $m=0$ , Eqs. (3.24) and (3.25) give the same expression for  $(\partial x / \partial \Delta)_T$  as Eqs. (3.14) and (3.15), since  $\gamma'(\kappa_0) = (8\pi)^{-1}$  for  $d=3$ , when  $g_q = q^2$ . On the other hand, in the ordered phase where  $\kappa_0=0$ ,

$$C_{\bar{q}=0} = (\phi'')^{-1}, \quad (3.26)$$

and, from Eqs. (3.24),

$$\left(\frac{\partial x}{\partial \Delta}\right)_T = -\frac{\partial^2 \phi}{\partial \Delta^2} + \frac{\partial^2 \phi}{\partial \Delta \partial F'_0} / \phi''. \quad (3.27)$$

Along the coexistence curve this diverges as  $(T - T_t)^{-1}$  near the tricritical point since  $\phi'' = \phi'_0 + \phi'_0 m^2$  which is proportional to  $T - T_t$ .

### 5. Order $n^{-1}$

The correction of order  $n^{-1}$  to  $F$  was evaluated in Sec. IID and was given in Eq. (2.37). Along the  $\lambda$  line, there is an ordinary critical point and the critical exponents have an order  $n^{-1}$  correction, as evaluated by Ferrel and Scalapino.<sup>13</sup> For  $\Delta = \Delta_t$ ,  $\phi'' \approx \phi'_0 - \gamma_3 \kappa \phi_0'''$  and it becomes negative above the tricritical point, but the stability condition (3.9) ensures that the argument of the logarithm in Eq. (2.37) remains positive. Since  $\phi'_0 = O(T - T_t)$ , the logarithmic correction evaluated by Ferrel and Scalapino<sup>13</sup> disappears and the tricritical exponents are Gaussian to order  $n^{-1}$ . This shows, in particular, that when a tricritical point comes about by variation of a nonordering field such as  $\Delta$ , unusual forms of exchange integrals do not give rise to non-Gaussian tricritical exponents to order  $n^{-1}$ .

### 6. Logarithmic singularities

Wegner and Riedel<sup>3</sup> pointed out that there may be logarithmic corrections to the Gaussian exponents at a tricritical point for  $d=3$  just as there are at an ordinary critical point for  $d=4$ . In particular they appeared in the magnetization as  $T \rightarrow T_{t-}$ . According to their argument, the singularities should be there for  $n \rightarrow \infty$ . In the present model, when  $d=4$ ,  $\gamma(\kappa)$  in Eq. (3.3) acquires a factor of  $\log \kappa$  which gives rise to the usual logarithmic singularities. For  $d=3$ ,  $\gamma(\kappa)$  is given correctly by Eq. (3.3) for small  $\kappa$ , and  $m$  may be obtained from Eq. (3.8).

There are no logarithmic singularities. The source of this disagreement with the conclusions of Wegner and Riedel is not understood at present.

### B. Other than three dimensions

#### 1. $d > 3$

For this case, many of the above results are unchanged and, in particular, there is still a tricritical point. The main qualitative changes are in the determination of the coexistence curve and the existence of a discontinuity in the phase boundary at the tricritical point.

Using Eqs. (3.2) to expand Eq. (2.11) in powers of  $m$  for  $\kappa=0$ ,

$$\delta F = \phi'_0 m^2 + \frac{1}{2} \phi''_0 m^4 + \frac{1}{6} \phi'''_0 m^6. \quad (3.28)$$

This expression has a minimum at  $m = m_0$  with  $\delta F$  equal to its value at  $m=0$  if Eq. (3.28) can be written as a constant  $+ Am^2(m^2 - m_0^2)^2$ , that is if

$$\phi'_0 = 3(\phi''_0)^2 / 8\phi'''_0. \quad (3.29)$$

This is the point at which an ordered phase can first be contemplated. The phase transition does not take place there because there is a solution with  $\kappa_0 \neq 0$  which has a still-lower free energy. However, for  $d > 3$ , the transition is close by. If  $\phi'_0$  and  $\phi''_0$  satisfy Eq. (3.12) with  $\alpha$  just less than  $3/8\phi'''_0$ , the minimum of  $\delta F$  in Eq. (3.28) is of order  $(\phi''_0)^3$ . On the other hand, the solution of Eq. (3.5) is still  $\kappa \sim \phi''_0$  and then Eq. (2.11) gives  $\delta F$  of order  $(\phi''_0)^d$  which is much smaller than  $(\phi''_0)^3$  close to the tricritical point. Thus,  $\alpha - \frac{3}{8}\phi'''_0$  is small, and expanding Eq. (3.28) shows that it is of order  $(\phi''_0)^{d-3}$ .

The absence of a discontinuity in slope of the phase boundary in the  $(x, T)$  plane may be seen from Eq. (3.18). There is still a discontinuity in  $(d\kappa/dT)_{PB}$ , but it is multiplied by  $\gamma'(\kappa)$  which is proportional to  $\kappa^{d-3}$  and vanishes as  $\kappa \rightarrow 0$ .

#### 2. $d < 3$

The nature of the phase diagram changes qualitatively when  $d$  is decreased below 3. This may be seen from Eq. (3.5) since, at the point  $\phi'_0 = 0 = \phi''_0$ , there is a solution  $\kappa_0 = (\frac{1}{2}\gamma_d^2 \phi'''_0)^{1/(6-2d)}$ , with a lower free energy than at  $\kappa_0 = 0$ . It follows that, along the  $\lambda$  line ( $\phi'_0 = 0$ ), there is a discontinuous change from  $\kappa_0 = 0$  to  $\kappa_0 \neq 0$  at some value of  $\phi''_0 > 0$ , and the  $\lambda$  line ends at that point—a critical end point. [In general, higher derivatives of  $\phi_0$  should be included in this discussion but Eq. (3.5) is exact for the usual sixth-order model.<sup>2,4</sup>] It is interesting to consider the implications of this result for the expansion of tricritical exponents in powers of  $3-d$  obtained by Stephen and McCauley,<sup>18</sup> who obtain well-defined non-Gaussian tricritical exponents in the limit  $n \rightarrow \infty$ . Presumably a more detailed calcu-

lation might reveal that the tricritical fixed point is not stable for large  $n$  and  $d < 3$  and show at which value of  $n$  (if any) it becomes absolutely stable. [For long-range forces,  $\gamma(\kappa)$  has a different behavior for small  $\kappa$  and it is possible to have a tricritical point with non-Gaussian exponents.]

### IV. CONCLUSIONS

We have described an exactly solvable model which enables us to calculate tricritical properties analytically and to obtain explicitly many of the features of tricritical points such as crossover from non-Gaussian to Gaussian exponents, divergences of correlation functions and the discontinuity in slope of the phase boundary in the  $(x, T)$  plane. Clearly, it would be desirable to have an approximate method with these features that could be applied to models which have finite  $n$  and are directly related to discrete-spin models as described in the Appendix. Such a method is suggested by the discussion of Secs. II A and II B. The Hartree approximation is a lower bound on  $F$  for all  $n$  and the variational upper bound could have been evaluated for finite  $n$ . Clearly, for finite  $n$ , both would have the same properties as the  $n \rightarrow \infty$  limit, and therefore would be qualitatively much superior to mean-field theory. With the form of  $\phi$  given in the appendix, the behavior of the BEG model may be obtained in this way. This will be described in a separate publication.

The thermodynamic variational principle which gives the upper bound in Sec. II A was first used for the spin- $\frac{1}{2}$  Ising model by Mühlischlegel and Zitzartz,<sup>19</sup> who showed that it is equivalent to quite elaborate summations of diagrams in perturbation theory applied to the original discrete-spin problem. The discussion of Secs. II and III gives a new perspective on this method by showing that it is exact as  $n \rightarrow \infty$  and that it does not realize its full potential until it is applied to models with higher spin.

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### APPENDIX

The BEG partition function<sup>1</sup> may be written in the form

$$Z = \sum_{\{\sigma_i\}} e^{\beta(\underline{\sigma}' \hat{K} \underline{\sigma} - \Delta \underline{\sigma}' \underline{g} - \underline{h}' \Delta)}, \quad (A1)$$

where  $\hat{K}$  is a matrix with elements  $K_{ij}$  equal to the exchange coupling,  $\underline{\sigma}$  is a column vector with elements  $\sigma_i$  for lattice sites  $i$ , and  $\underline{h}$  is a column vec-



tor with all elements equal to the magnetic field  $h$ . The  $\sigma_i$  are summed over values  $\pm 1$  and 0. Ferromagnetic coupling is assumed so  $\hat{K}$  is positive definite. The crystal-field splitting is  $\Delta$  and biquadratic exchange has been omitted for the moment. Now make a Gaussian integral representation of the exchange term:

$$Z = |\det \pi \hat{K}|^{1/2} \int_{-\infty}^{\infty} \prod_i dx_i e^{-(1/\beta) \underline{x}^{-1} \hat{K}^{-1} \underline{x}} \times \sum_{(\sigma_i)} e^{2 \underline{x}' \underline{\sigma} - \beta (\Delta \underline{\sigma}' \underline{\sigma} + \underline{h}' \underline{\sigma})}. \quad (\text{A2})$$

To show that this is equal to  $Z$  in Eq. (A1), make a displacement  $\underline{x} = \underline{x}' + \beta \hat{K} \underline{\sigma}$  which removes the linear terms in the exponent in Eq. (A2) and adds  $(\beta \underline{\sigma}' \hat{K} \underline{\sigma})$ . Then the integral over the  $x_i$  may be completed to give Eq. (A1). In Eq. (A2), the exponent is a sum of site-diagonal terms; so the sums over the  $\sigma_i$  may be carried out to give

$$Z = |\det \pi \beta \hat{K}|^{-1/2} \int_{-\infty}^{\infty} \prod_i dx_i \times \exp \left( -\frac{1}{\beta} \underline{x}' K^{-1} \underline{x} + \sum_i \ln [1 + 2e^{-\beta \Delta} \cosh(2x_i - \beta h)] \right). \quad (\text{A3})$$

Now change variables to  $S_i = x_i - \beta h/2$  and obtain Eq. (2.2) with  $n=1$  and

$$\phi(\Delta, S_i^2) = -\ln(1 + 2e^{-\beta \Delta} \cosh 2S_i) + (1/2N) \ln(\det \beta \pi \hat{K}), \quad (\text{A4})$$

$$H = h / \sum_j K_{ij}, \quad (\text{A5})$$

$$J_{ij} = (1/\beta) (\hat{K}^{-1})_{ij}.$$

The inclusion of a biquadratic exchange term requires an additional integral representation analogous to Eq. (A2) and leads to a continuous-spin model with two order parameters.

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