## Renormalization-group theory and calculations of tricritical behavior

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The conventional renormalization-group analysis of the tricritical behavior of a metamagnet is completed by a description of the first-order transition below the tricritical temperature, and the conditions for the discontinuity in the magnetization are explicitly verified in an Ising spin model. The singularity structure of the crossover scaling function is derived from relations between the scaling fields for the critical and tricritical fixed points. Numerical calculations illustrating various aspects of the theory are given for a square-lattice Ising model in a four-cell cluster approximation.

## I. INTRODUCTION

The application of scaling ideas and renormalization-group methods to tricritical phase transitions has received considerable attention in the past few years.<sup>1</sup> A particularly interesting aspect of this phenomenon is the occurrence of crossover between different types of critical behavior in the neighborhood of the tricritical point. Early phenomenological scaling theories for this transition were developed by Riedel and Wegner<sup>2</sup> and by Griffiths<sup>3</sup> extending scaling ideas for ordinary critical phase transitions. Following Wilson's development of the renormalization-group approach to critical phenomena, <sup>4</sup> Riedel and Wegner<sup>5</sup> introduced a model for tricritical phase transitions characterized by the occurrence of two related unstable fixed points of the renormalization transformations. This fixed-point structure has become the basis of all subsequent discussions of crossover phenomena.<sup>6</sup> However, while this model describes correctly the second-order phase transition at temperatures T above a tricritical temperature  $T_t$ , it does not account for the first-order phase transition found at temperatures T below  $T_t$ . Recently we have given general conditions for renormalization-group transformations which lead to first-order phase transition, <sup>7</sup> and we have verified them in detail in numerical calculations for an Ising ferromagnet.<sup>8</sup> In this paper we apply these conditions to extend the model of Riedel and Wegner<sup>5</sup> and complete the renormalization-group description of tricritical behavior. Our theory is based also on results found in numerical renormalization-group calculations of a square-lattice Ising model for a metamagnet in a four-cell cluster approximation.  $^{9-11}$  The thermodynamic functions are obtained from the renormalization-group series expansion for the free energy, <sup>11</sup> and results are given for the magnetization, susceptibility, and the crossover scaling function in this model.

In Sec. II we present the renormalization-group

theory for tricritical transitions in the language of scaling fields<sup>5,11,12</sup> following the work of Riedel and Wegner, <sup>5</sup> but without specifying equations for the renormalization-group transformations of the physical parameters of the system. A new fixed point in these transformations is introduced which accounts for the occurrence of the first-order phase transition for temperatures below the tricritical temperature.<sup>7</sup> We then derive the singularity structure of the crossover scaling function associated with the tricritical fixed point from the known singularities of the free energy at the adjacent critical fixed point and from properties at the discontinuity fixed point. In particular we obtain the dominant power-law singularity in the domain of second-order phase transitions deduced by Pfeuty, Jasnow, and Fisher<sup>13</sup> from a scaling hypothesis, but in addition we find also other less singular terms. While the theory is expressed in terms of scaling functions which are regular functions of the physical parameters near the fixed points, for pratical applications we introduce also a new scaling field which vanishes on the critical surface but is singular at the tricritical fixed point. We discuss briefly the role of an additional fixed point associated with the critical antiferromagnetic phase transitions which we found in our renormalization-group calculation of the Ising model of a metamagnet. In particular we give the appropriate conditions in this case which lead to smoothness.<sup>14,15</sup>

In Sec. III we treat some aspects of the renormalization-group transformation for the Ising model of a metamagnet, <sup>16</sup> with nearest-neighbor antiferromagnetic coupling constant  $K_1$  and nextto-nearest-neighbor ferromagnetic coupling constant  $K_2$  in an external magnetic field H. We apply the Niemeijer and van Leeuwen method<sup>9</sup> with basic Kadanoff cells chosen according to a recent suggestion of van Leeuwen. <sup>10</sup> We emphasize in particular the conditions which lead to the occurrence of a first-order phase transition below the tricritical temperature.<sup>7</sup> Finally numerical re-

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sults obtained in a four-cell cluster approximation are presented to illustrate various aspects of tricritical behavior.

## **II. GENERAL THEORY**

We consider a thermodynamic system determined by the temperature T and a second physical variable H which exhibits a tricritical transition<sup>17</sup> at  $T = T_t$  and  $H = H_t$ . For metamagnets, e.g., FeCl<sub>2</sub>, *H* corresponds to the magnetic field, while for  ${}^{3}\text{He}{}^{4}\text{He}$  mixtures, *H* is the difference of chemical potentials of each isotope. Then for  $H \le H_t$ , a second-order phase transition occurs in this system on a critical curve  $T_{\star}(H) > T_{t}$  while for  $H > H_{t}$ the phase transition is first order for  $T_{-}(H) < T_{t}$ , where  $T_{+}(H_{t}) = T_{-}(H_{t}) = T_{t}$ . It has been shown by Riedel and Wegner<sup>5</sup> that the tricritical behavior for  $H \le H_t$  can be described by a model of renormalization-group transformations which contains a tricritical fixed point T at  $T_t$ ,  $H_t$  with eigenvalues  $\lambda_{1t} > \lambda_{2t} > 1$  and a second critical fixed point C located on the critical curve at  $H_c$ ,  $T_c = T_*(H_c)$ , where  $H_c \leq H_t$ , with eigenvalues  $\lambda_{1c} > 1$  and  $\lambda_{2c} \leq 1$ . In order to describe the first-order phase transition associated with tricritical behavior for  $H > H_t$ , we will require in addition the existence of a third fixed point D of these transformations, located at  $H_d$ ,  $T_d = T_{-}(H_d)$ , where  $H_d > H_t$ , with a special relevant eigenvalue  $\lambda_{1d} = L$  and  $\lambda_{2d} < 1$ . Here L is the change of scale of volume under renormalization transformations (or the number of spins in a Kadanoff cell). We have recently shown<sup>7</sup> that these conditions lead to a discontinuity in the order parameter at the critical curve for  $H > H_t$ . Associated with each of these three fixed point  $\tau$ , C, and D we introduce the corresponding scaling fields  $\zeta_{it}$ ,  $\zeta_{ic}$ , and  $\zeta_{id}$ , i = 1, 2, which transform linearly under the renormalization-group transformations<sup>11, 12</sup> according to

$$\zeta_i' = \lambda_i \zeta_i \tag{2.1}$$

and are regular functions of the physical variables T and H. We drop the subscripts c, t, and d here and in subsequent discussions whenever the same equations apply to all three cases. The critical curve  $T_{*}(H)$  for  $H \le H_t$  then corresponds to  $\zeta_{ic} = 0$  while  $T_{-}(H)$  for  $H \ge H_t$  corresponds to  $\zeta_{id} = 0$ .

The complete free energy f of the system can be expressed either as a function of  $\zeta_{id}$  or of  $\zeta_{ic}$ in the domain of first- or second-order phase transitions, respectively, or as a function of  $\zeta_{it}$ in both domains. In each case f satisfies an inhomogeneous scaling equation<sup>11, 18</sup>

$$f(\lambda_1 \zeta_1, \lambda_2 \zeta_2) = L(f(\zeta_1, \zeta_2) - g(\zeta_1, \zeta_2)), \qquad (2.2)$$

where  $g(\zeta_1, \zeta_2)$  is the self-energy per spin of the basic Kadanoff cell and is assumed to be a regular function of  $\zeta_i$ . For simplicity we take no more

irrelevant variables into account than is necessary, but the derivation can readily be extended to include additional variables (see also Ref. 26). To determine  $f(\zeta_1, \zeta_2)$  it is essential to impose physically relevant boundary conditions of the solutions of Eq. (2.2). These boundaries are an important aspect of the model and in fact distinguish tricritical from critical behavior near the fixed point at  $H_t$ ,  $T_t$ . Suppose, for example, that f is assumed to be a regular function of  $\zeta_{ic}$  at  $\zeta_{ic}$ = 0. In that case the curve defined by  $\zeta_{1c} = 0$ ,  $\zeta_{2c}$  $\neq 0$  corresponding to  $T_{+}(H)$  is in fact not a curve of singularities of f, and the fixed point at  $H_t$ ,  $T_t$ gives rise to ordinary critical phase transitions. This is indeed what happens for an Ising model of a ferromagnet which has the same fixed-point structure<sup>8</sup> described above with  $H_c = 0$  and  $T_c = \infty$ (vanishing coupling of the Ising spin). Therefore in order to obtain tricritical behavior near  $H_t$ ,  $T_t$ , the free energy must be singular at  $H_c$ ,  $T_c$ . If  $f_r(\zeta_1, \zeta_2)$  is the regular part<sup>11</sup> of the free energy corresponding to the solution of Eq. (2.2) which is regular at  $\zeta_1 = \zeta_2 = 0$ , the singular part  $f_s$  is defined by  $f_s = f - f_r$  and satisfies the homogeneous scaling equation

$$f_s(\lambda_1\zeta_1, \lambda_2\zeta_2) = L f_s(\zeta_1, \zeta_2) . \tag{2.3}$$

Therefore  $f_s$  can be written in the scaling form

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$$f_s(\zeta_1, \zeta_2) = |\zeta_1|^{2-\alpha} u(x), \qquad (2.4)$$

where  $x = \zeta_2 |\zeta_1|^{-\phi}$  is an invariant under renormalization transformation, and  $\alpha = (2 - \ln L / \ln \lambda_1)$ and  $\phi = \ln \lambda_2 / \ln \lambda_1$ . The scaling function u(x) can be determined<sup>16</sup> in terms of  $g(\zeta_1, \zeta_2)$  and depends in general on the sign of  $\zeta_1$ .

The scaling function associated with one fixed point can be obtained from the corresponding scaling function of an adjacent fixed point (connected by renormalization transformation) because the corresponding scaling fields are related. This leads us to the basic strategy for our approach: We obtain the singularity structure of the crossover scaling function  $u_t(x_t)$  associated with the tricritical fixed point from the known properties of the critical scaling functions  $u_c(x_c)$  associated with the critical fixed point C at  $H_c$ ,  $T_c$  and the properties at the discontinuity fixed point at  $T_d$ ,  $H_d$ . The first step in our procedure is to express the scaling fields  $\zeta_{ic}$  as functions of  $\zeta_{it}$ . According to Eq. (2.1) these are homogeneous scaling functions. Thus in the domain of second-order phase transitions we have for  $\zeta_{ic}$ 

$$\zeta_{ic} = \left| \zeta_{1t} \right|^{\mu_{ic}} v_{ic}(x_t), \qquad (2.5)$$

where  $x_t = \zeta_{2t} |\zeta_{it}|^{-\phi_t}$  and  $\mu_{ic} = \ln \lambda_{ic} / \ln \lambda_{1t}$ ,  $\phi_t = \ln \lambda_{2t} / \ln \lambda_{1t}$ . The condition  $\zeta_{1c} = 0$  for the critical curve  $T = T_+(H)$  for  $H < H_t$  implies  $v_{1c} = 0$  at  $x_t = x_+ > 0$ , which we assume to occur for  $\zeta_{1t} < 0$ . The

equation for the critical curve  $T = T_*(H)$  in terms of  $\zeta_{1t}$  and  $\zeta_{2t} > 0$  is then

$$\zeta_{1t} = - \left| \zeta_{2t} / x_{+} \right|^{1/\phi_{t}} . \tag{2.6}$$

From Eq. (2.5) and the relation  $\mu_{2c} = \phi_c \mu_{1c}$ , where  $\phi_c = \ln \lambda_{2c} / \ln \lambda_{1c}$ , we obtain the scale-invariant variable  $x_c = \xi_{2c} |\xi_{1c}|^{-\phi_c}$  as a function of  $x_t$  only,

$$x_{c} = v_{2c}(x_{t}) \left| v_{1c}(x_{t}) \right|^{-\phi_{c}}.$$
 (2.7)

We now take the second step, which is to substitute Eq. (2.5) into Eq. (2.4) for  $f_s$  as a function of  $\zeta_{ic}$ . This leads to a similar scaling form  $\tilde{f}_s$  as a function of  $\zeta_{it}$ ,

$$\tilde{f}_{s} = |\zeta_{1t}|^{2-\alpha_{t}} \tilde{u}_{t}(x_{t}), \qquad (2.8)$$

where

$$\tilde{u}_t(x) = |v_{1c}(x)|^{2-\alpha} c u_c(x_c)$$
(2.9)

and  $2 - \alpha_t = (2 - \alpha_c)\mu_{1c}$ . However, we must be careful not to identify  $\tilde{f}_s$  as the complete singular part of the free energy when expressed in the variable  $\zeta_{it}$ , because in general a similar contribution is obtained from the regular part  $f_r$  of f at  $H_c$ ,  $T_c$ . However, since this latter contribution is not singular on the critical curve  $\zeta_{1c} = 0$  it will not contribute to the corresponding singularity of the tricritical scaling function  $u_t(x)$ .

Since  $\zeta_{1t}$  and  $\zeta_{ic}$  are regular functions of T and H at  $x_t = x_*$ ,  $v_{1c}(x)$  is also regular and vanishes at  $x_t = x_*$ . We therefore set  $v_{1c}(x) = (x - x_*)\hat{v}_{1c}(x)$  for x near  $x_*$ . The critical scaling function  $u_c(x)$  is regular at x = 0 and we expand  $u_c(x) = \sum u_{nc} x^n$ . Substituting these expressions in Eq. (2.9) we obtain

$$\tilde{u}_t(x) = |x - x_+|^{2-\alpha_c} \sum_{n=0}^{\infty} \omega_{nc}(x) |x - x_+|^{-n\phi_c}, \quad (2.10)$$

where

$$\omega_{nc}(x) = u_{nc} v_{2c}^{n}(x) \left| \hat{v}_{1c}(x) \right|^{2 - \alpha_{c} - n\phi_{c}}$$
(2.11)

is a regular function of x. Since  $\phi_c < 0$ , the dominant singularity  $u_t(x)$  as  $x - x_*$  is  $\tilde{u}_t \sim |x - x_*|^{2-\alpha_c}$  provided  $\hat{v}_{1c}(x_*) \neq 0$ . This result was previously deduced from scaling arguments by Pfeuty, Jasnow, and Fisher, <sup>13</sup> but the singularity structure of  $u_t(x)$  given by Eq. (2.10) is more complex<sup>26</sup> than that conjecture by these authors.

A similar analysis cannot be carried out in the domain of first-order phase transitions, because we do not know the analyticity properties of the scaling function  $u_d(x)$ . In this case the critical curve  $T = T_-(H)$  is obtained by setting  $\xi_{1d} = 0$  corresponding to  $x_t = x_- < 0$ , which gives the condition

$$\zeta_{1t} = -\left|\zeta_{2t}/x_{-}\right|^{1/\phi_{t}}.$$
(2.12)

The eigenvalue  $\lambda_{1d} = L$  at the fixed point *D* implies a discontinuous order parameter at  $\zeta_{1d} = 0$  as was shown in Ref. 7. We shall assume the existence of all higher-order derivatives of  $f_s$ , which implies that

$$u_t(x) = \sum_{n=1}^{\infty} u_{nd} (x - x_{-})^n, \qquad (2.13)$$

where the coefficients  $u_{nd}$  generally differ on opposite sides of the critical curve.

To complete our analysis of the singularities of  $u_t(x)$  we note that in the neighborhood of  $x_t = 0$  corresponding to the limit  $\zeta_{2t} \rightarrow 0$ ,  $\zeta_{1t} \neq 0$ , f is regular in  $\zeta_{2t}$  and therefore  $u_t(x)$  is a regular function at x=0. On the other hand in the limit  $x_t \rightarrow \pm \infty$ , which corresponds to  $\zeta_{1t} \rightarrow 0$ ,  $\zeta_{2t} \neq 0$ , f is regular in  $\zeta_{1t}$ , which implies that

$$u_t(x) = |x|^{\ln L / \ln \lambda_{2t}} \sum_{n=0}^{\infty} b_n |x|^{-n\phi t}.$$
 (2.14)

While the scaling fields  $\zeta_i$  are regular functions of the physical variables T and H this is not the case for the scale invariant variable  $x = \zeta_2 |\zeta_1|^{-\phi}$ . To obtain the dependence of  $x_t$  on T and H in the neighborhood of the tricritical fixed point, we first expand  $\zeta_{it}$  to second order in the variables  $(T - T_t)$ and  $(H - H_t)$ .

$$\xi_{it} = a_i (T - T_t) + b_i (H - H_t) + c_i (T - T_t)^2 + d_i (T - T_t) (H - H_t) + e_i (H - H_i)^2 . \qquad (2.15)$$

Substituting this expansion in the Eqs. (2.6) and (2.12) for the critical curve  $T = T_{\pm}(H)$  we obtain for  $H \leq H_t$ 

$$T_{\pm}(H) = T_t + a(H - H_t) + b(H - H_t)^2 + c_{\pm}(H - H_t)^{1/\circ t},$$
(2.16)

where  $a = -b_1/a_1$ ,  $b = -1/a_1(c_1a^2 + d_1a + e_1)$ , and  $c_{\pm} = -(a_2a + b)^{1/\phi t}/a_1 | x_{\pm}|^{1/\phi t}$ . Hence  $\zeta_{1t}$  is tangential to the critical curve at the tricritical point.

The next step is to introduce scaling fields  $\eta_{\pm}$  for  $\zeta_2 \ge 0$ ,

$$\eta_{\pm} = \zeta_{1t} + \left| \zeta_{2t} / x_{\pm} \right|^{1/\phi_{t}}, \qquad (2.17)$$

which transform like  $\zeta_{1t}$ , but vanish on the critical curve. Then  $x_t$  is given in terms of  $y_{\pm} = \zeta_2 |\eta_{\pm}|^{-\phi_t}$  by

$$x_{t} = y_{\pm} \left| 1 - (\operatorname{sgn} \eta_{\pm}) \right| y_{\pm} / x_{\pm} \left| \frac{1}{\Phi t} \right|^{-\Phi t}.$$
 (2.18)

To first order in  $T - T_{\pm}(H)$  and  $H - H_t$  we have

$$\eta_{\pm} = A(H) \left[ T - T_{\pm}(H) \right], \qquad (2.19)$$

where

$$A(H) = a_1 [1 + (d_1 - 2c_1b_1)(H - H_t)]$$
(2.20)

and

$$\zeta_{2t} = a_2 [T - T_{\pm}(H)] + (b_2 - a_2 b_1 / a_1) (H - H_t). \qquad (2.21)$$

From Eqs. (2.19)-(2.21) we obtain an expansion for  $y_{\pm}$ ,

$$y_{\pm} = p(H - H_t) | T - T_{\pm}(H) |^{-\phi_t} + q | T - T_{\pm}(H) |^{1 - \phi_t}, \qquad (2.22)$$

where

$$b = (a_1b_2 - a_2b_1)a_1^{-(1+\phi_t)}$$
 and  $q = a_2a_1^{-\phi_t}$ . (2.23)

Note that Eqs. (2.18) and (2.22) determine the scale-invariant variable  $x_t$  in terms of the physical parameters T and H, and the directly measurable critical curve  $T_{\pm}(H)$ . The constants p and q depend on the coefficients of the first-order expansion of  $\zeta_{1t}$  and  $\zeta_{2t}$ , Eq. (2.15), but in practice we can choose also  $x_t/p$  as the scale-invariant variable, and then only the unknown coefficient q/p needs to be determined. This can be done, for example, if we first determine  $y_{\pm}$ , Eq. (2.18), for  $T - T_{\pm}(H) \ll H - H_t$ , so that the second term in Eq. (2.18) can be neglected, and then find q/p by determining values of T and H for which  $T - T_{\pm}(H) \simeq H - H_t$  and  $y_{\pm}$  remains unchanged.

For convenience in practical applications we can express also the singular part  $f_s$  of the free energy directly as a function  $\eta_{\pm}$  and  $y_{\pm}$ , <sup>19</sup>

$$f_{s} = |\eta_{+}|^{2-\alpha_{t}} \omega_{*}(y_{*}), \qquad (2.24)$$

where  $\omega_{\star}(y)$  is given in terms of the tricritical scaling function  $u_t(x)$ ,

$$\omega_{\pm}(y) = \left| 1 - (\operatorname{sgn}\eta_{\pm}) \right| y / x_{\pm} \left| \frac{1}{\varphi_{t}} \right|^{2 - \alpha_{t}} u_{t}(x_{t}) . \quad (2.25)$$

The singularities of  $\omega_{\pm}(y)$  as a function of y can readily be obtained from the corresponding singularities of  $u_t(x_t)$ .

The essential features of renormalization-group transformations leading to tricritical behavior have been found in numerical calculations of an Ising model of a metamagnet which we discuss in Sec. III. However, in one respect we have found a different result in our calculations (see also Ref. 16). It is expected for an Ising metamagnet that the fixed point C should be located at  $H_c = 0$ ,  $T_c \neq 0$ , giving rise to the antiferromagnetic critical transition at  $T = T_c$ , H = 0, while for small values of Hthe condition  $\lambda_{ic} < 1$ , i = 2, 3..., implies smoothness, <sup>14</sup> i.e., (i) the critical temperature  $T_*(H)$  is a regular function of H at H = 0,

$$T_{\star}(H) \simeq T_{c'} + \frac{1}{2} \frac{d^2 T_{\star}(0)}{dH^2} H^2 + \cdots;$$
 (2.26)

(ii) the critical exponent of the specific heat is independent of the field H; and (iii) the coefficient of the singular term is a smooth function of H.

We found in the Ising-model calculation that  $H_c \neq 0$ , while an additional fixed point at  $H_{c'} = 0$ ,  $T_{c'} \neq 0$  accounts for the zero-field antiferromagnetic phase transition. This additional fixed point has two eigenvalues  $\lambda_{1c'}$ ,  $\lambda_{2c'}$  greater than<sup>20</sup> 1, which seems to violate the aforementioned conditions for smoothness. However, smoothness can be recovered if there is a relation between the eigenvalues of these two fixed points, as we now shall proceed to show.

Introducing scaling fields  $\zeta_{ic'}$  associated with the fixed point C' at  $H_{c'} = 0$ ,  $T_{c'}$ , we apply Eq. (2.4) for the singular part  $f_s$  of the free energy, where as before the scaling function  $u_{c'}(x_{c'})$  has a powerlaw singularity  $|x_{c'} - x_0|^{2-\alpha_{c'}}$  at  $x_{c} = \zeta_{2c'}|\zeta_{1c'}|^{-\phi_{c'}}$  $= x_0$ . Since H and T are analytic functions of  $\zeta_{ic'}$ at  $\zeta_{1c'} = \zeta_{2c'} = 0$ , Eq. (2.26) is satisfied if  $\phi_{c'} = \frac{1}{2}$ , with  $d^2 T_t(0)/dH^2 = 2/x_0^2$ . If we now introduce the scaling field  $\eta_{c'} = \zeta_{1c'} - (\zeta_{2c'}/x_0)^2$  which vanishes on the critical curve  $T = T_*(H)$  and write

$$f_s = \eta_c^{2-\alpha} c^* \omega(y_{c^*}), \qquad (2.27)$$

where  $y_{c'} = \zeta_{2c'} | \eta_{c'} | {}^{\phi}c'$  we see immediately that smoothness is recovered provided that  $\omega(0) = \omega(\infty) \neq 0$ , which implies that  $\lambda_{1c'} = \lambda_{1c}$ .

It is worthwhile to emphasize there that the degree of instability of a fixed point, i.e., the number of relevant eigenvalues, does not by itself determine the type of critical behavior which occurs. In fact the critical ferromagnetic fixed point, as well as the critical antiferromagnetic and tricritical fixed points, has two eigenvalues greater than 1.<sup>8</sup> What accounts for the essential differences in these three cases is the singularity of the free energy at the adjacent more stable fixed point which has only a single relevant eigenvalue. For critical ferromagnetic behavior, the free energy is actually regular at this fixed point, which leads to the disappearance of the phase transition at finite values of the magnetic field.<sup>8</sup>

## **III. ISING METAMAGNET**

In this section we discuss some theoretical aspects and present numerical calculations of renormalization-group transformations for a squarelattice Ising model of a metamagnet with antiferromagnetic nearest-neighbor coupling constant  $K_1$ , ferromagnetic next-to-nearest-neighbor coupling constant  $K_2$ , and a magnetic field H. The basic Kadanoff cells are chosen according to a recent recipe introduced by van Leeuwen,<sup>9</sup> where each cell consists of a cross of L = 5 next-to-nearestneighbor spin. The importance of this choice is that the corresponding renormalization-group transformations preserve the paramagnetic or antiferromagnetic symmetry of the ground-state spin configuration. These configurations become degenerate on a surface in the coupling-constant space, signaling the onset of a first-order transition.<sup>21</sup> We will show that these properties imply the existence of a scaling field  $\zeta_{1d}$  with eigenvalue  $\lambda_{1d} = L$  which vanishes on this degenerate surface, fulfilling the renormalization-group conditions for the occurrence of a first-order phase transition.7

The ground-state energy or correspondingly the zero-temperature free energy per spin of the Ising model is  $f(K) = \max[f^*(K)]$ , where

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FIG. 1. Schematic diagram of fixed-point structure for tricritical behavior discussed in Sec. III.

$$f^{\pm}(K) = \sum_{\alpha} f^{\pm}_{\alpha} K_{\alpha} . \tag{3.1}$$

The plus and minus superscripts refer to paramagnetic and antiferromagnetic spin order, respectively, and  $f_{\alpha}^{\pm}$  are constants. The condition for degeneracy is then  $\sum_{\alpha} (f_{\alpha}^{+} - f_{\alpha}^{-})K_{\alpha} = 0$ . It can readily be shown that if the renormalization-group transformation preserves the spin order, the scaling equation for the free energy, Eq. (2.2), applies to  $f^{*}(K)$  and  $f^{-}(K)$  separately, with  $g(K) = \sum g_{\alpha}K_{\alpha}$ , provided that periodic boundary conditions are satisfied.<sup>10</sup> Hence the field  $\zeta_{1d} \simeq \sum_{\alpha} (f_{\alpha}^{+} - f_{\alpha}^{-})K_{\alpha}$  scales according to

$$\zeta_{1d}' = L\zeta_{1d} , \qquad (3.2)$$

which corresponds to a renormalization-group condition<sup>7</sup> for a discontinuity in the order parameter conjugate to  $\zeta_{1d}$ .

Our numerical renormalization-group calculations were carried out for a cluster of four cells in a square array with the spins and cells satisfying periodic boundary conditions. In addition to the coupling constants  $K_1$  and  $K_2$  and the magnetic field H which are of interest in this problem, we included also three and four spin coupling constants  $K_3$  and  $K_4$  in order to obtain the complete renormalization-group transformation for this approximation.

A diagram of the fixed points found in the antiferromagnetic domain  $K_1 < 0$  is shown in Fig. 1 in the subspace of temperature  $T \propto |K_1|^{-1}$  and magnetic field H. The fixed point C' for zero magnetic field which gives rise to the critical antiferromagnetic transition has a thermal eigenvalue  $\lambda_{1c'} \simeq 1.79$  and magnetic eigenvalue<sup>20</sup>  $\lambda_{2c'} \simeq 1.44$ . From Onsager's solution we expect  $\lambda_{1c'} = \sqrt{5}$  and the smoothness condition discussed in Sec. II implies  $\lambda_{2c'} = \sqrt{\lambda_{1c'}}$ . The fixed point C has only a

single relevant eigenvalue  $\lambda_{1c} = 2.41$  which should be equal to  $\lambda_{1c}$ , to preserve smoothness. The critical curve  $T_{+}(H)$ , which is defined by the points which map towards the fixed point C, ends in a tricritical fixed point T with two relevant eigenvalues, while below the tricritical temperature the critical curve  $T_{-}(H)$  corresponds to points mapping toward the zero-temperature discontinuity fixed point D with an eigenvalue  $\lambda_{1d} = L = 5$ . We found the relevant eigenvalues of the fixed point T to be  $\lambda_{1t} = 4.44$ ,  $\lambda_{2t} = 1.69$  and correspondingly the tricritical exponents are  $\alpha_t = 0.921$  and  $\phi_t = 0.352$ . Results for the first-order  $\epsilon$  expansion obtained by Chang, Tuthill, and Stanley<sup>27</sup> [see Eq. (14)] give  $\lambda_{1t} = 4.18$  and  $\lambda_{2t} = 2.28$ . Points above the critical curve are mapped toward a fixed point H at infinite magnetic field while points below the critical curve are mapped towards a fixed point A at zero temperature and magnetic field. Both of these fixed points are stable in all directions. At infinite temperature and zero magnetic field corresponding to vanishing spin coupling there is a fixed point 0 which has a single relevant magnetic eigenvalue  $\lambda_H = \frac{15}{16}$  which determines the properties of uncoupled spins in a magnetic field. All points above the critical temperature with zero magnetic field map towards this fixed point. Finally, there exists also a fixed point on the  $K_2$  axis leading to the unusual properties of the Baxter model, as discussed recently by van Leeuwen, <sup>10</sup> which is not shown in this diagram.

In Fig. 2 we show the calculated critical surface in the subspace of the coupling constants  $K_1$  and  $K_2$ and the magnetic field H by a set of curves on this surface with constant H. The almost horizontal line is the line of tricritical points on this surface which separates the domain of first- and second-order phase transitions.<sup>22</sup> For  $K_1/K_2 = -0.5$ results of Monte Carlo calculations for the tricritical temperature have been published<sup>23</sup> which give for the ratio of the tricritical and the Néel temperature  $T_t/T_{c1} = 0.34$  as compared with our corresponding result of 0.22. In the limit  $K_1 \rightarrow 0$  the tricritical curve consisting of points mapping into C' comes together with vertical slopes ending in the Baxter tricritical fixed point on the  $K_2$  axis.

We have calculated the magnetization M as a function of  $K_1 < 0$  for  $K_2/K_1 = -1$  from the series expansion of the free energy, and in Fig. 3 the results are shown for several fixed values of H.<sup>23</sup> The Néel point is located at  $K_{1c'} = -0.157$  and  $H_{c'} = 0$  and the tricritical point is at  $K_t = -0.465$  and  $H_t = 1.84$ . For  $H > H_t$  the magnetization is discontinuous and we obtain the coexistence curve shown by the two dashed lines, while for  $H < H_t$ , M is continuous but the susceptibility  $\chi$  becomes infinite along the critical dashed curve. In Fig. 4



FIG. 2. Critical surface for Ising metamagnet in the subspace of coupling constants  $K_1$  and  $K_2$  and the magnetic field *H*. The vertical curves correspond to constant values of *H* and the horizontal curve is a line of tricritical points.

we show  $\ln \chi$  as a function of  $\ln |K_1 - K(H)|$  for H = 1.8 to illustrate the crossover behavior in the effective critical exponent<sup>5</sup>  $d \ln \chi / d \ln |K_1 - K(H)|$  from its asymptotic tricritical to its critical value near the tricritical point. Finally, Fig. 5 illus-trates the dependence of the cross-over scaling function<sup>24</sup> for the susceptibility on the scaling variable y, Eq. (2.18). For large values of y we find that this function approaches a power-law behavior in accordance with the analysis in Sec. II of the singularities of crossover scaling functions near the critical curve.



FIG. 3. Magnetization M as a function of  $K_1 < 0$  for fixed values of H indicated on figure. The dashed line for  $-0.465 < K_1 < -0.157$  is the line of second-order transitions which splits into two lines corresponding to the discontinuity in M below the tricritical temperature.



FIG. 4. Logarithm of the susceptibility  $\chi$  as a function of  $\ln |K_1 - K(H)|$  for a fixed magnetic field H = 1.8, illustrating the crossover behavior.

In conclusion we note that the numerical results presented here confirm the renormalization-group theory for tricritical behavior and demonstrate the usefulness of this approach to carry out approximate calculations. To get accurate numbers and to test convergence of the results these calculations have to be performed with a larger number of cells, but it is worthwhile to point out that the correct analyticity of the thermodynamic functions is preserved already in our present calculations based on the smallest number of cells (four) which preserve the square-lattice symmetry. In contrast, high-temperature expansions are particu-



FIG. 5. Crossover scaling function for the susceptibility  $\chi$  as a function of the scaling parameter y, Eq. (2.18), for temperatures T above and below the critical temperature T(H).

larly difficult to apply in this case of competing interactions; e.g., the tricritical point cannot be located by present series data, <sup>25</sup> although for the Blume-Capel model successful calculations have been carried out.<sup>28</sup> Finally, we remark that the

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mean-field theory not only gives incorrect critical exponents in two dimensions but fails also to yield the correct dependence of the tricritical point on the relative strength of the competing spin interactions  $K_1$  and  $K_2$ .<sup>22</sup>

- <sup>19</sup>For  $|T_{\star}(H)/T-1| \ll 1$ , this scaling form for  $f_s$  corresponds to the original scaling assumption of Riedel and Wegner, Ref. 2, while the conventional scaling expression, Eq. (2.4), is called extended scaling in Ref. 13. One of us (M.N.) in indebted to A. Aharony for a discussion clarifying the development of tricritical scaling theory and for guidance to the literature.
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- <sup>22</sup>In a mean-field-theory model, the line of tricritical points reaches the asymptotic slope  $K_2/K_1 = -\frac{1}{3}$ , B. Nienhuis (unpublished); this value differs from the result of E. D. G. Cohen, in Fundamental Problems in Statistical Mechanics, edited by E. D. G. Cohen (North-Holland, Amsterdam, 1975), Vol. 3.
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