

## Critical phenomena in semi-infinite systems. II. Mean-field theory

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(Received 20 January 1975)

The critical behavior of a continuous spin system in a semi-infinite sample is studied for all values of the extrapolation length  $\lambda$  using mean-field theory. A new transition, which we have called the extraordinary transition, is found for  $\lambda < 0$  in which the bulk orders at a temperature below the surface ordering temperature. In this paper we have calculated the magnetic susceptibilities  $\chi(z)$  and  $\chi(z, z)$  and the correlation function  $\Gamma(\vec{x}, \vec{x}')$  at all the phase transitions. We have used these results to compute the various  $\gamma$  and  $\eta$  exponents and to study the scaling relations introduced by Binder and Hohenberg.

### I. INTRODUCTION

In a previous paper<sup>1</sup> (hereafter referred to as I), the Wilson-Fisher  $\epsilon$  expansion was used to calculate the critical properties of semi-infinite classical spin systems. Paper I was restricted to the case of positive extrapolation length  $\lambda$ , that is, the spin field  $\vec{S}(\vec{x})$  in the ordered phase would vanish if it were linearly extrapolated a distance  $\lambda$  outside the surface of the system. While preparing to apply the  $\epsilon$  expansion to systems with negative or infinite extrapolation lengths, it became necessary to make a detailed study of the mean-field theory in semi-infinite systems. It quickly became evident that the mean-field theory presented a model in which almost all quantities (susceptibilities, correlation functions, etc.) of interest could be calculated analytically, and that these were of sufficient interest to warrant a separate publication. This paper, the second in a series on critical phenomena in semi-infinite systems, is devoted entirely to the mean-field theory. The third paper<sup>2</sup> (hereafter referred to as III) deals with  $\lambda^{-1} \leq 0$ .

The mean-field theory for semi-infinite magnetic systems has already received considerable attention.<sup>3-10</sup> Mills<sup>3</sup> presented the first detailed analysis of the magnetic phase transition in semi-infinite systems following an earlier experimental and theoretical investigation by Wolfram *et al.*<sup>4</sup> Mills investigated the mean-field theory for Heisenberg ferromagnetic and antiferromagnets in three dimensions and obtained Landau-Ginzburg continuum equations for the spatially dependent magnetization. He obtained the correlation function in the disordered phase and an analytic expression for the magnetization profile in the ordered phase for  $\lambda > 0$ . Concurrent and independent work by Kaganov and Omelyanchouk<sup>5</sup> treated the

mean field in finite samples starting from a Landau-Ginzburg free energy. Random-phase-approximation (RPA) treatments<sup>6,7</sup> of models for itinerant ferromagnetism in semi-infinite systems followed. These were often directed toward the possible role that spin fluctuations might play in catalysis.<sup>6-8</sup> Further work concentrated on the prediction from mean-field theory that the surface orders before the bulk for negative extrapolation length.<sup>9</sup> Important calculations of mean-field critical properties also appear in the papers of Binder and Hohenberg.<sup>10</sup>

Kumar<sup>8</sup> has pointed out that four qualitatively different magnetization profiles in the ordered phase are possible depending on the value of  $\lambda$  and the reduced temperature  $t \sim (T - T_0)/T_0$  where  $T_0$  is the mean-field transition temperature for the bulk system. If  $\lambda^{-1} > 0$ , the mean field on the surface layer is less than the mean field in the bulk, and at  $t=0$  there is a transition to a state in which the average spin curves down at the surface, as depicted in Fig. 1(a). This is the standard bulk driven transition, which we will call the *ordinary transition*. When  $\lambda = \infty$ , the mean field at the surface equals the bulk field and at  $t=0$ , there is a transition to a state with a flat spin profile [Fig. 1(b)]. We will call this the  $\lambda = \infty$  *transition*. If  $\lambda < 0$ , the surface mean field exceeds the bulk field, and there is a transition at  $t = t_s > 0$  to a state in which the spin decays exponentially to zero in the bulk [Fig. 1(c)]; the surface orders before the bulk. We will call this the *surface transition*. Different mean-field critical exponents for the susceptibilities for these three transitions have been defined.<sup>10</sup> Finally, for  $\lambda^{-1} < 0$ , there is a transition from a state of zero bulk magnetization to finite bulk magnetization [Fig. 1(d)] when the bulk correlation length diverges at  $t=0 < t_s$ . This last transition is in fact a phase transition with critical

exponents that can be calculated with the mean field. We call this the *extraordinary transition*. To distinguish the transitions, we will label all exponents with superscripts  $o$ ,  $\infty$ ,  $s$ , and  $e$  referring, respectively, to the ordinary, the  $\lambda = \infty$ , the surface, and the extraordinary transitions.

The starting point for this paper is the Landau-Ginzburg continuum free energy in a semifinite system expressed in terms of the spin  $\vec{S}(\vec{x})$  at point  $\vec{x}$ . The coordinate perpendicular to the surface is  $z$ . The differential equation for  $\vec{S}(\vec{x})$  which results from minimizing the free energy in the presence of an external magnetic field is then solved to obtain the spin  $S(z)$ ,  $\chi(z)$ , the response of a spin in plane  $z$  to a uniform field, and  $\chi(z, z')$ , the response of a spin at  $z$  to a uniform field at the plane  $z'$ , for all values of  $\lambda$  and  $t$ . In addition, the full spin correlation function  $\Gamma(\vec{x}, \vec{x}')$  is obtained in the disordered phase and at the extraordinary transition  $\lambda < 0$ ,  $t = 0$ . In the ordered phases, we will consider only the response of the system to fields parallel to the direction of order. We will not consider transverse response.

The new results of this paper are (i) the calculation of  $\chi(z)$  and  $\chi(z, z')$  in the ordered phases, (ii) the calculation of  $\Gamma(\vec{x}, \vec{x}')$  for  $\lambda = \infty$ , and (iii) the calculation of  $\chi(z, z')$  and  $\Gamma(\vec{x}, \vec{x}')$  at the extraordinary transition. From  $\chi(z, z)$  we calculate  $\gamma_{z,z}$ , the local susceptibility exponent introduced by Binder and Hohenberg.<sup>10</sup> From  $\Gamma(\vec{x}, \vec{x}')$  we are able to compute the  $\eta$  exponents defined in Sec. II and check the Binder-Hohenberg scaling relations.<sup>10</sup>

$$\frac{F}{T} = \int d^d x \left( \frac{1}{2} t' |\vec{S}'(\vec{x})|^2 + \frac{1}{2} K \sum_{\alpha_j} |\nabla_{\alpha} S_j'(\vec{x})|^2 + u |\vec{S}'(\vec{x})|^4 + \frac{1}{2} K \lambda^{-1} |\vec{S}'(\vec{x})|^2 \delta(z) - \vec{B}'(\vec{x}) \cdot \vec{S}'(\vec{x}) - \vec{B}'_1 \cdot \vec{S}'_1(\vec{x}) \delta(z) \right), \quad (2.1)$$

where  $T$  is the temperature,  $t' = (T - T_0)/T$  is the reduced temperature with  $T_0$  equal to the bulk mean-field transition temperature,  $\lambda$  is the extrapolation length,  $\vec{B}'$  and  $\vec{B}'_1$  are, respectively, uniform and surface external magnetic fields divided by  $T$ , and  $K$  and  $u$  are phenomenological constants. As in I,  $\vec{x} = (\vec{\rho}, z)$ , where  $\vec{\rho}$  is the coordinate parallel to the surface and  $z$  is the coordinate perpendicular to the surface.  $z = 0$  is the surface plane. The integral is over the half  $d$ -dimensional space  $z \geq 0$ .  $\vec{S}$  is an  $n$ -component vector so that  $j$  runs from 1 to  $n$  and  $\alpha$  from 1 to  $d$ .  $F/T$  with suitably renormalized spin variables is just the continuum limit of the reduced Hamiltonian used in I and III. In Mills's derivation<sup>3</sup> of Eq. (2.1),  $F$  was obtained from a Heisenberg Hamil-

The analysis presented here is expected to be valid for any semi-infinite system which can be described by the Landau-Ginzburg mean-field theory. In particular, this analysis should be applicable to superconductors where it may be easier to detect the extraordinary transition.

The outline of the rest of the paper is as follows. Section II presents the model and defines all of the relevant exponents for convenient future reference. Section III presents general solutions to the equations for  $S(z)$  and  $\Gamma(\vec{x}, \vec{x}')$  derived in Sec. II. This section is extremely mathematical and may be treated as an appendix by those not interested in calculational details. Section IV treats the disordered state including calculations of  $\chi(z)$ ,  $\chi(z, z')$ , and  $\Gamma(\vec{x}, \vec{x}')$ . Sections V, VI, and VII treat the various ordered phases. Section V is concerned with  $\lambda^{-1} \geq 0$  and  $t < 0$ , Sec. VI with  $\lambda < 0$  and  $0 < t < t_s$ , and Sec. VII with the properties of the extraordinary transition both above and below  $t = 0$ . Section VIII is a summary of the results which are capsulized in the phase diagram of Fig. 2 and in Tables I and II.

## II. PRELIMINARIES

### Model

Throughout this paper, we will use the continuum phenomenological free energy which generates the field equation originally derived by Mills,<sup>3</sup>

tonian on a discrete lattice with nearest-neighbor exchange  $J(1 + \Delta_s)$  on the surface layer and  $J$  between all other spins. In this case,  $K = J/T$  and  $\lambda^{-1} = 1 - \Delta_s/\Delta_c$ , where  $\Delta_c = 2(d - 1)$  ( $\Delta_c = 4$  in three dimensions) is the critical value of  $\Delta_s$  for which  $\lambda^{-1}$  changes sign.

It may be of interest to note that if the coupling between the surface layer and its neighboring layer is allowed to be  $J(1 + \Delta_1)$ , then Eq. (2.1) is unchanged but  $\lambda$  is now given by

$$\lambda^{-1} = 1 - \frac{2\Delta_1 + 2(d-1)\Delta_s}{1 + \Delta_1};$$

consequently,  $\lambda$  changes sign when  $\Delta_1 + 2(d - 1)\Delta_s = 1$ . This may be easily shown by following Mills's argument<sup>3</sup> with the extra coupling term.

The derivation of the continuum free energy assumes the variations in  $\vec{S}(\vec{x})$  are slow on the scale of a lattice constant  $a$ . *A priori*, this does not put any restrictions on  $\lambda$ ; *a posteriori*, however, we will see in Sec. IV that  $|\lambda|$  must be much larger than a lattice constant. We should note the assumption that  $a|\nabla\vec{S}(\vec{x})|/|\vec{S}(\vec{x})|\ll 1$  implies that the surface region must in fact penetrate several layers into the sample and not be sharply restricted to the plane  $z=0$ .

There are at least two methods for studying Eq. (2.1). One method is to diagonalize the quadratic part of the free energy by finding its normal modes. This technique is used in I and III and is useful in proceeding to the  $\epsilon$  expansion. The other is to study the equation for  $\vec{S}(\vec{x})$  obtained by minimizing  $F$ . With the latter technique it is easier to obtain information about the system below any ordering temperature, and is the one we will pursue in this paper. To simplify the equations which minimize  $F$ , we will rescale  $\vec{S}$ ,  $t$ ,  $\vec{B}$ , and  $\vec{B}_1$  via  $\vec{S}=(4u/K)^{1/2}\vec{S}'$ ,  $t=t'/K$ ,  $\vec{B}=(1/K)(4u/K)^{1/2}\vec{B}'$ , and  $\vec{B}_1=(1/K)(4u/K)^{1/2}\vec{B}'_1$ . Then, minimization of  $F$  with respect to  $\vec{S}(\vec{x})$  yields

$$t\vec{S}(\vec{x}) - \nabla^2\vec{S}(\vec{x}) + |\vec{S}(\vec{x})|^2\vec{S}(\vec{x}) = \vec{B}(\vec{x}), \quad (2.2a)$$

$$\left(\frac{\partial\vec{S}(\vec{x})}{\partial z} - \frac{1}{\lambda}\vec{S}(\vec{x})\right)_{z=0} = \vec{B}_1, \quad (2.2b)$$

$$\vec{S}(\vec{x})|_{z=\infty} = \vec{S}(\infty), \quad (2.2c)$$

where  $\vec{S}(\infty)$  is the value of the spin in an infinite system. The system is translationally invariant parallel to the surface so that states which minimize  $F$  will depend only on the coordinate  $z$ . We will thus seek solutions to Eqs. (2.2) of the form

$$\vec{S}(\vec{x}) = \hat{e}S(z), \quad (2.3)$$

where  $\hat{e}$  is a unit vector along  $\vec{B}$  and/or  $\vec{B}_1$  if either is nonzero (for simplicity, we assume  $\vec{B}$  and  $\vec{B}_1$  are parallel.) Substituting Eq. (2.3) into Eq. (2.2) and allowing  $\vec{B}(\vec{x}) = \vec{B}$  to be uniform, we obtain

$$\frac{d^2S(z)}{dz^2} - tS(z) - S^3(z) = -B, \quad (2.4a)$$

$$\left(\frac{dS(z)}{dz} - \lambda^{-1}S(z)\right)_{z=0} = -B_1 \quad (2.4b)$$

$$S(z)|_{z=\infty} = S(\infty). \quad (2.4c)$$

Solutions to the homogeneous part of Eqs. (2.4) ( $B$  and  $B_1=0$ ) will give  $S(z)$  in ordered states with no external fields. These solutions for specific cases will be discussed in Secs. IV-VI. Given the solutions to the homogeneous equations, we can find solutions for  $S(z)$  to first order in  $B$  and  $B_1$  from which we can obtain the susceptibilities

$$\chi(z) = \frac{\partial S(z)}{\partial B}, \quad (2.5a)$$

$$\chi(z, 0) = \frac{\partial S(z)}{\partial B_1}. \quad (2.5b)$$

These are the continuum generalizations of the susceptibilities  $\chi_n$  and  $\chi_{n,1}$  introduced by Binder and Hohenberg.<sup>10</sup> (Our surface is at  $z=0$  rather than at the discrete variable  $n=1$ .) In the disordered phases, Eqs. (2.5) give the isotropic susceptibility. In ordered phases, Eqs. (2.5) only give the susceptibility for fields parallel to  $\vec{S}$ . In this paper, we will not calculate perpendicular susceptibilities or correlation functions in ordered phases.

In order to obtain the spin-spin correlation function  $\Gamma(\vec{x}, \vec{x}')$ , we use

$$\Gamma(\vec{x}, \vec{x}') = \frac{\delta S(\vec{x})}{\delta B(\vec{x}')} \quad (2.6)$$

Then, varying Eq. (2.2), we find

$$\nabla_x^2 \Gamma(\vec{x}, \vec{x}') - t \Gamma(\vec{x}, \vec{x}') - 3S^2(\vec{x}) \Gamma(\vec{x}, \vec{x}') = -\delta(\vec{x} - \vec{x}'), \quad (2.7a)$$

$$\left(\frac{\partial}{\partial z} \Gamma(\vec{x}, \vec{x}') - \lambda^{-1} \Gamma(\vec{x}, \vec{x}')\right)_{z=0} = 0. \quad (2.7b)$$

$\Gamma(\vec{x}, \vec{x}')$ , of course, contains the susceptibilities  $\chi(z)$  and  $\chi(z, z')$  as special cases. In particular,

$$\chi(z) = \int d^d \vec{x}' \Gamma(\vec{x}, \vec{x}'), \quad (2.8a)$$

$$\chi(z, z') = \int d^{d-1} \vec{p}' \Gamma(\vec{x}, \vec{x}') \quad (2.8b)$$

Equation (2.8b) allows us to determine the susceptibility  $\chi(z, z')$ , which is the response of the spin on the plane  $z$  to a uniform external field applied at the plane  $z'$ .

In subsequent sections, we will calculate  $S(z)$ ,  $\chi(z)$ , and  $\chi(z, z')$  for all values of  $\lambda$  and  $t$ . In addition, we will calculate  $\Gamma(\vec{x}, \vec{x}')$  in the disordered phase and at the extraordinary transition ( $\lambda < 0$ ,  $t=0$ ). Though our solutions will be valid for all values of  $\lambda$  and  $t$ , our primary interest will be in the behavior of these functions near the four phase transitions discussed in the introduction. In particular, we will be interested in the critical exponents characterizing these transitions, which we label in the manner described in Sec. I. Thus each transition has a divergent correlation length

$$\xi^i \sim (t - t_i)^{-\nu^i}, \quad i = (o, \infty, s, e), \quad (2.9)$$

where  $t_i$  is the reduced transition temperature for transition  $i$ . Within the mean field,  $t_o = t_\infty = t_e = 0$  and  $t_s = |\lambda|^{-2}$ , as we will see in Sec. II. Exponents describing the temperature dependence of spin and

susceptibilities are defined as follows:

$$S(z) = (t_i - t)^{\beta_z^i}, \tag{2.10}$$

$$\chi(z) = \begin{cases} (t - t_i)^{-\gamma_z^i}, & t > t_i \\ (t_i - t)^{-\gamma_{zz}^i}, & t < t_i \end{cases} \tag{2.11}$$

and

$$\chi(z, z) = \begin{cases} (t - t_i)^{-\gamma_{zz}^i}, & t > t_i \\ (t_i - t)^{-\gamma_{zz}^i}, & t < t_i \end{cases} \tag{2.12}$$

These exponents are just the continuum analogs of the exponents  $\beta_n$ ,  $\gamma_n$ , and  $\gamma_{n,n}$  introduced by Binder and Hohenberg.<sup>10</sup> ( $n$  is a discrete lattice variable with the surface located at  $n=1$ .) We have allowed for the possibility of having different values for the susceptibility exponents above and below the transition. In addition, Eq. (2.10) is valid for  $t_e - t$  both positive and negative for the extraordinary transition. As indicated, it is in principle possible to have different exponents for each value of  $z$ . We will see, however, that there are only two independent values of the exponents depending on whether  $z \gg \xi$  or  $z \ll \xi$  with crossover occurring at  $z \approx \xi$ . We label these two exponents with the subscript 1 for  $z \ll \xi$  (following Binder and Hohenberg<sup>10</sup>) and  $\infty$  for  $z \gg \xi$ . For the ordinary and  $\lambda = \infty$  transitions, the exponents for  $z \gg \xi$  must be the bulk exponents. For the surface and extraordinary transitions, the exponents for  $z \gg \xi$  may either be undefined or different from normal exponents. We therefore retain the  $\infty$  subscript even though it is superfluous in some cases.

The exponents for  $\Gamma(\vec{x}, \vec{x}')$  at  $t = t_i$  are defined as follows:

$$\Gamma(\vec{x}, 0) \sim \frac{A_i(\theta)}{|\vec{x}|^{d-2+\eta_1^i}}, \quad |\vec{x}|, z \gg 1 \tag{2.13}$$

$$A_i(\theta) = (\cos \theta)^{\mu^i}, \tag{2.14}$$

$$\Gamma(\vec{p}, 0) \sim \frac{1}{|\vec{p}|^{d-2+\eta_1^i}}, \quad |\vec{p}| \gg 1 \tag{2.15}$$

$$\Gamma(\vec{x}, \vec{x}') - \Gamma_\infty(\vec{x}, \vec{x}') \sim \frac{1}{(z + z')^{d-2+\eta_1^i}}, \tag{2.16}$$

$z, z' \gg |\vec{x} - \vec{x}'|$

$$\Gamma_\infty(\vec{x}, \vec{x}') \sim \frac{1}{|\vec{x} - \vec{x}'|^{d-2+\eta_1^\infty}}, \quad z, z' \gg |\vec{x} - \vec{x}'| \tag{2.17}$$

where  $\Gamma_\infty(\vec{x}, \vec{x}')$  refers to the correlation function when  $z, z'$  are much greater than  $|\vec{x} - \vec{x}'|$ . We have introduced two new exponents,  $\mu^i$  and  $\eta_1^i$  describing, respectively, the angular dependence of the surface bulk correlation function and the approach

to  $\Gamma_\infty$  as  $z$  and  $z'$  go into the bulk.  $\eta_1^s, \mu^s, \eta_1^s,$  and  $\eta_\infty^s$  are undefined.  $\eta_\infty^o$  must equal  $\eta_\infty^s$  and both must be equal to the bulk exponent  $\eta$ .  $\eta_\infty^o$  may, however, differ from  $\eta$ .

### III. GENERAL SOLUTIONS

In this section, we will present general solutions to Eqs. (2.4) and (2.7) which will be applied to particular ranges of the values of the parameters  $\lambda$  and  $t$  in subsequent sections. For  $t > t_i$ ,  $S(z)$  to first order in  $B$  and  $B_1$  can be obtained directly from Eq. (2.4) by ignoring the  $S^3(z)$  term. This solution will be presented in Sec. IV. When  $t < t_i$ ,  $S(z)$  has a nonvanishing value  $S_0(z)$  even when  $B$  and  $B_1$  are zero, and one solves for  $S(z)$  by reducing Eq. (2.4) to quadratures.<sup>5</sup> Multiplying Eq. (2.4a) by  $dS/dz$  and integrating over  $z$ , we obtain

$$\frac{1}{2} \left( \frac{dS(z)}{dz} \right)^2 - \frac{1}{2} t S^2(z) - \frac{1}{4} S^4(z) = -BS(z) + C, \tag{3.1}$$

where

$$C = BS(\infty) - \frac{1}{2} t S^2(\infty) - \frac{1}{4} S^4(\infty), \tag{3.2}$$

since  $dS/dz$  tends to zero as  $z$  becomes infinite.  $S(\infty)$  is the bulk ( $z = \infty$ ) spin. We now solve Eq. (3.1) perturbatively to first order in  $B$ ,

$$S(z) = S_0(z) + S_1(z), \tag{3.3}$$

where

$$\frac{1}{2} \left( \frac{dS_0(z)}{dz} \right)^2 - \frac{1}{2} t S_0^2(z) - \frac{1}{4} S_0^4(z) = -\frac{1}{4} t S_0^2(\infty), \tag{3.4}$$

and

$$\begin{aligned} \frac{dS_1}{dz} \frac{dS_0}{dz} - t S_0(z) S_1(z) - S_0^3(z) S_1(z) \\ = -B[S_0(z) - S_0(\infty)], \end{aligned} \tag{3.5}$$

where to evaluate  $C$  we have used

$$S_0(\infty) = 0, \quad S_1(\infty) = B/t, \quad t > 0 \tag{3.6a}$$

$$S_0(\infty) = \sqrt{-t}, \quad S_1(\infty) = B/-2t, \quad t < 0. \tag{3.6b}$$

The boundary condition at  $z=0$  (2.4b), is linear; so we have

$$\left( \frac{dS_0}{dz} - \lambda^{-1} S_0 \right) = 0, \tag{3.7a}$$

$$\left( \frac{dS_1}{dz} - \lambda^{-1} S_1 \right) = -B_1. \tag{3.7b}$$

Equation (3.4) is solved implicitly for  $S(z)$

$$\frac{1}{\sqrt{2}}(z + \phi) = \int^{S_0(z)} \frac{dS}{[S^4 + 2tS^2 - tS_0^2(\infty)]^{1/2}}, \tag{3.8}$$

where  $\phi$  is an integration constant determined by

the boundary condition at the surface.

Equation (3.5) is linear and is also easily solved. First observe that the coefficient of  $S_1(z)$  is equal to  $-d^2S_0/dz^2$ . Thus, Eq. (3.5) reduces to

$$S_0'(z)S_1'(z) - S_0''(z)S_1(z) = -B[S_0(z) - S_0(\infty)], \quad (3.9)$$

with a prime indicating differentiation with respect to  $z$ . Next, note that

$$\frac{d}{dz} \left( \frac{S_1}{S_0'} \right) = \frac{S_1'S_0' - S_0''S_1}{(S_0')^2} = - \frac{S_0 - S_0(\infty)}{(S_0')^2} B. \quad (3.10)$$

Integrating, we obtain

$$S_1(z) = S_0'(z) \left( \frac{S_1(0)}{S_0'(0)} - B \int_0^z \frac{S_0(z') - S_0(\infty)}{[S_0'(z')]^2} dz' \right). \quad (3.11)$$

The boundary condition Eq. (3.7b) for  $S_1(0)$  becomes

$$\left( \frac{S_0''(0)}{S_0'(0)} - \frac{1}{\lambda} \right) S_1(0) = -B_1 - B \frac{S_0(\infty) - S_0(0)}{S_0'(0)}. \quad (3.12)$$

Using the boundary condition Eq. (3.7a) and Eq. (2.4a) with  $B=0$  to eliminate  $S_0''$ , we find

$$S_1(0) = \lambda^{-1} [t - \lambda^{-2} + S_0''(0)]^{-1} \times \left[ B_1 + \lambda \left( \frac{S_0(\infty)}{S_0'(0)} - 1 \right) B \right]. \quad (3.13)$$

Equations (3.11) and (3.13) give the general solution for  $S_1(z)$  to first order in  $B$  and  $B_1$ . We will use them in subsequent sections to calculate  $\chi(z)$  and  $\chi(z, 0)$ .

We now turn to the calculation of the correlation function and  $\chi(z, z')$ . Equations (2.7a) and (2.7b) are linear and can be solved generally. Since the system has translational invariance parallel to the surface, we may write

$$\Gamma(\vec{x}, \vec{x}') = \int_{\vec{p}} e^{i\vec{p} \cdot (\vec{p} - \vec{p}')} \Gamma(z, z'; \vec{p}), \quad (3.14)$$

where

$$\int_{\vec{p}} = \int_{-\infty}^{\infty} \prod_{j=1}^{d-1} \frac{dp_j}{2\pi}.$$

Note that it follows from Eq. (2.8b) that

$$\Gamma(z, z'; \vec{p}=0) = \chi(z, z').$$

Equations (2.7a) and (2.7b) become

$$\frac{\partial^2}{\partial z^2} \Gamma(z, z'; \vec{p}) - [p^2 + t + 3S_0''(z)] \Gamma(z, z'; \vec{p}) = -\delta(z - z'), \quad (3.15a)$$

$$\left( \frac{\partial}{\partial z} \Gamma(z, z'; \vec{p}) - \lambda^{-1} \Gamma(z, z'; \vec{p}) \right)_{z=0} = 0. \quad (3.15b)$$

These equations can be solved by standard techniques.<sup>11</sup> If  $W_1(z, \vec{p})$  and  $W_2(z, \vec{p})$  are two linearly independent solutions to the equation

$$\frac{d^2}{dz^2} W(z, \vec{p}) - [p^2 + t + 3S_0''(z)] W(z, \vec{p}) = 0, \quad (3.16)$$

where

$$W_1(z, \vec{p}) \rightarrow e^{-[p^2 + t + 3S_0''(\infty)]^{1/2} z} \text{ as } z \rightarrow \infty,$$

then

$$\Gamma(z, z'; \vec{p}) = \begin{cases} W_1(z, \vec{p}) U(z', \vec{p}), & z > z' \\ U(z, \vec{p}) W_1(z', \vec{p}), & z < z' \end{cases} \quad (3.17)$$

where

$$U(z, \vec{p}) = C_1 W_1(z, \vec{p}) + C_2 W_2(z, \vec{p}), \quad (3.18)$$

with  $C_1$  and  $C_2$  chosen to satisfy

$$\left( \frac{dU}{dz} - \frac{1}{\lambda} U \right)_{z=0} = 0, \quad (3.19)$$

and

$$\left( \frac{dW_1(z, \vec{p})}{dz} U(z', \vec{p}) - W_1(z', \vec{p}) \frac{dU(z, \vec{p})}{dz} \right)_{z=z'} = 1. \quad (3.20)$$

These equations yield

$$C_2 = [W_2'(z', \vec{p}) W_1(z', \vec{p}) - W_1'(z', \vec{p}) W_2(z', \vec{p})]^{-1}, \quad (3.21)$$

$$C_1 = -C_2 \frac{W_2'(0, \vec{p}) - \lambda^{-1} W_2(0, \vec{p})}{W_1'(0, \vec{p}) - \lambda^{-1} W_1(0, \vec{p})}. \quad (3.22)$$

$C_2$  is the inverse of the Wronskian and is, therefore, independent of  $z'$ . We will use these equations to determine  $\Gamma(\vec{x}, \vec{x}')$  in the disordered phase and at  $t=0$  for  $\lambda^{-1} < 0$  and  $\chi(z, z')$  in all of the ordered phases.

#### IV. DISORDERED PHASE

##### A. Susceptibilities

In the disordered phase,  $S_0(z)$  is zero. We may, therefore, linearize Eq. (2.4) to obtain  $\chi(z)$  and  $\chi(z, 0)$ . We find

$$S_1(z) = \frac{B}{t} \left( 1 - \frac{1}{\lambda \sqrt{t} + 1} e^{-\sqrt{t} z} \right) + \frac{\lambda}{\lambda \sqrt{t} + 1} e^{-\sqrt{t} z} B_1, \quad (4.1)$$

and

$$\chi(z) = \frac{1}{t} \left( 1 - \frac{1}{1 + \lambda/\xi} e^{-z/\xi} \right), \quad (4.2a)$$

$$\chi(z, 0) = \frac{\lambda}{1 + \lambda/\xi} e^{-z/\xi}, \quad (4.2b)$$

where we have introduced the bulk correlation length  $\xi = t^{-1/2}$  for  $t > 0$ . These equations are valid

regardless of the sign of  $\lambda$  provided the system is in the disordered phase.

We now investigate Eqs. (4.2) in detail. First note that when  $\lambda > 0$  or infinite,  $\chi(z)$  diverges only at  $t=0$ , and  $\chi(z, 0)$  has no divergences. If  $\lambda < 0$ , both  $\chi(z)$  and  $\chi(z, 0)$  diverge at  $\xi = |\lambda|$ , i.e., at  $t = |\lambda|^{-2}$ . As we shall see in Secs. V and VI the divergence at  $t=0$  signals a transition in which spins order throughout the sample, while the divergence at  $t = |\lambda|^{-2}$  signals a transition in which spin ordering is restricted to the surface. Thus,  $t_s = |\lambda|^{-2}$  and  $t_o = t_\infty = 0$ . Since  $t_s$  is greater than  $t_o$ , if  $\lambda < 0$  the surface will always order before the bulk.<sup>3-5</sup> Both surface and bulk fluctuations contribute equally to  $\chi(z)$ , whereas surface fluctuations are dominant in  $\chi(z, 0)$ . Thus, for  $\lambda < 0$ ,  $\chi(z)$  appears as the sum of two independent parts which diverge at different temperatures.

We now calculate  $\Gamma(z, z'; \vec{p})$  from Eqs. (3.15a) and (3.15b) in order to find the various  $\gamma$  exponents. Since  $S_0(z) = 0$ , Eq. (3.16) can readily be solved

$$W_1(z, \vec{p}) = e^{-(p^2+t)^{1/2}z}, \quad (4.3a)$$

$$U(z, \vec{p}) = D \sinh[(p^2+t)^{1/2}z + \theta(\vec{p})], \quad (4.3b)$$

where

$$e^{-2\theta(\vec{p})} = \frac{1 - \lambda(p^2+t)^{1/2}}{1 + \lambda(p^2+t)^{1/2}}, \quad (4.4)$$

and  $D = (p^2+t)^{-1/2}e^{-\theta}$ . Using the above and Eq. (3.14), we find

$$\Gamma(z, z'; \vec{p}) = \frac{1}{2(p^2+t)^{1/2}} (e^{-(p^2+t)^{1/2}|z-z'|} - e^{-2\theta(\vec{p})} e^{-(p^2+t)^{1/2}(z+z')}), \quad (4.5)$$

and from  $\chi(z, z') = \Gamma(z, z'; 0)$ ,

$$\chi(z, z') = \frac{\xi}{2} \left( e^{-|z-z'|/\xi} - \frac{1 - \lambda/\xi}{1 + \lambda/\xi} e^{-(z+z')/\xi} \right). \quad (4.6)$$

The reader can check that Eq. (4.6) reduced to Eq. (4.2b) when  $z' = 0$ .

We now list the exponents which can be obtained by evaluating the appropriate limiting forms of Eqs. (4.2a) and (4.6):

(i)  $\lambda > 0$ ,  $\xi \gg \lambda, z$ ,

$$\chi(z) \sim \frac{\lambda+z}{\sqrt{t}}, \quad \gamma_1^0 = \frac{1}{2} \quad (4.7a)$$

$$\chi(z, z) \sim \frac{2\lambda}{1 + \lambda\sqrt{t}}, \quad \gamma_{1,1}^0 = -\frac{1}{2}; \quad (4.7b)$$

(ii)  $\lambda > 0$ ,  $z \gg \xi$ ,

$$\chi(z) = \frac{1}{t}, \quad \gamma_\infty^0 = 1 \quad (4.8a)$$

$$\chi(z, z) = \frac{1}{2\sqrt{t}}, \quad \gamma_{\infty, \infty}^0 = \frac{1}{2}; \quad (4.8b)$$

(iii)  $\lambda = \infty$

$$\chi(z) = \frac{1}{t}, \quad \gamma_1^\infty = \gamma_\infty^\infty = 1 \quad (4.9a)$$

$$\chi(z, z) = \frac{1}{2\sqrt{t}} (1 + e^{-2z/\xi}), \quad \gamma_{1,1}^\infty = \gamma_{\infty, \infty}^\infty = \frac{1}{2}; \quad (4.9b)$$

(iv)  $\lambda < 0$ ,  $t \sim |\lambda|^{-2}$ ,

$$\chi(z) \sim \frac{2}{t - |\lambda|^{-2}} e^{-z/|\lambda|}, \quad \gamma_1^s = 1; \quad \gamma_\infty^s = \text{undefined} \quad (4.10a)$$

$$\chi(z, z) \sim \frac{2|\lambda|^{-1}}{t - |\lambda|^{-2}} e^{-2z/|\lambda|}, \quad \gamma_{1,1}^s = 1; \quad \gamma_{\infty, \infty}^s = \text{undefined}. \quad (4.10b)$$

Note that when  $z \gg \xi$ ,  $\chi(z)$  and  $\chi(z, z)$  are independent of  $\lambda$  for  $\lambda^{-1} \geq 0$ .

Crossovers between regions (i), (ii), and (iii) occur when  $\xi$  is of order  $\lambda$  or  $z$ . For example, if  $\xi \gg \lambda$ , then  $\chi(z)$  behaves as  $t^{-\gamma_1^0}$  for  $z \ll \xi$  and as  $t^{-\gamma_\infty^0}$  for  $z \gg \xi$ . All of the above exponents are in agreement with those calculated by Binder and Hohenberg<sup>10</sup> for a discrete lattice.

We see that for  $\lambda < 0$ ,  $|\lambda|$  is the penetration depth for the surface effects. The assumption upon which the use of the continuum model is based therefore requires  $|\lambda| \gg 1$ . This is the *a posteriori* requirement mentioned in Sec. II.

## B. Correlation functions $\lambda^{-1} \geq 0$

$\Gamma(\vec{x}, \vec{x}')$  is obtained by Fourier transforming Eq. (4.5) with respect to  $\vec{p}$  and is given by

$$\Gamma(\vec{x}, \vec{x}') = G_d(\vec{x} - \vec{x}', t) - H_d(x - \nu \vec{x}', \lambda, t), \quad (4.11)$$

where  $\nu \vec{x} = (\vec{p}, -z)$ , and

$$G_d(\vec{x}, t) = \int_{\vec{q}} \frac{1}{q^2 + t} e^{i\vec{q} \cdot \vec{x}}, \quad (4.12)$$

$$H_d(\vec{x}, \lambda, t) = \int_{\vec{q}} \frac{1}{q^2 + t} e^{i\vec{q} \cdot \vec{x}} e^{2i\phi(k)}, \quad (4.13)$$

with  $\vec{q} = (\vec{p}, k)$ ,  $\int_{\vec{p}} = \int_{-\infty}^{\infty} dk/2\pi$ , and  $\tan \phi = k\lambda$ . The equivalence of Eq. (4.11) and the Fourier transform of Eq. (4.5) can easily be verified by contour integration with the observation that

$$e^{2i\phi(k)} = (1 + ik\lambda)/(1 - ik\lambda) \quad (4.14)$$

is analytic in the upper-half-plane provided  $\lambda^{-1} \geq 0$ .

When  $k\lambda \ll 1$  or  $\lambda = \infty$ , Eq. (4.14) may be written so that the evaluation of  $H_d(\vec{x}, \lambda, t)$  is very simple,

$$H_d(\vec{x} - \nu \vec{x}', \lambda, t) = \begin{cases} G_d(\vec{x} - \nu \vec{x}' + 2\lambda \hat{e}_\perp, t) \left[ 1 + O\left(\frac{\lambda^3}{|\vec{x} - \nu \vec{x}'|^3}\right) \right] & \text{if } |\vec{x} - \nu \vec{x}'| \gg \lambda, \\ -G_d(\vec{x} - \nu \vec{x}', t) \left[ 1 + O\left(\frac{|\vec{x} - \nu \vec{x}'|}{\lambda}\right) \right] & \text{if } |\vec{x} - \nu \vec{x}'| \ll \lambda, \end{cases} \quad (4.16)$$

where  $\hat{e}_\perp$  is the unit vector perpendicular to the surface,

$$G_d(\vec{x}, t) = \frac{\Gamma(\frac{1}{2}d - 1)}{4\pi^{d/2} |\vec{x}|^{d-2}} g_d(|\vec{x}|/\xi), \quad (4.17)$$

$\Gamma(x)$  is the  $\Gamma$  function, and

$$g_d(u) = \frac{1}{\Gamma(\frac{1}{2}d - 1)} \left(\frac{u}{2}\right)^{d/2-1} K_{d/2-1}(u), \quad (4.18)$$

where  $K_{d/2-1}$  is the Bessel function of imaginary argument.

It should be noted that the corrections to the leading terms in Eq. (4.16) are of higher order than the leading terms obtained from Eq. (4.11) in the various limits of interest. This is important since Eq. (4.11) is the difference of two functions. Using the fact that  $g_d(u) = 1$  at  $u = 0$ , we can obtain  $\Gamma^*(\vec{x}, \vec{x}')$  the correlation function at  $t = 0$ :

(i)  $\lambda^{-1} > 0$ ,

$$\Gamma^*(\vec{x}, \vec{x}') = \frac{\Gamma(\frac{1}{2}d - 1)}{4\pi^{d/2}} \times \left( \frac{1}{|\vec{x} - \vec{x}'|^{d-2}} - \frac{1}{|\vec{x} - \nu \vec{x}' + 2\lambda \hat{e}_\perp|^{d-2}} \right); \quad (4.19)$$

(ii)  $\lambda = \infty$ ,

$$\Gamma^*(\vec{x}, \vec{x}') = \frac{\Gamma(\frac{1}{2}d - 1)}{4\pi^{d/2}} \times \left( \frac{1}{|\vec{x} - \vec{x}'|^{d-2}} + \frac{1}{|\vec{x} - \nu \vec{x}'|^{d-2}} \right). \quad (4.20)$$

Evaluating  $\Gamma^*(\vec{x}, \vec{x}')$  in the limits of Eqs. (2.13)–

$$e^{2i\phi(k)} = \begin{cases} e^{2ik\lambda} + O(k\lambda)^3, & k\lambda \ll 1 \\ -1, & \lambda = \infty. \end{cases} \quad (4.15)$$

Then, it is shown in Appendix A that

(2.17), we obtain

$$\begin{aligned} \eta_\infty^0 &= \eta_I^0 = 0, \\ \eta_\perp^0 &= 1, \quad \eta_\parallel^0 = 2, \quad \mu^0 = 1, \end{aligned} \quad (4.21)$$

and

$$\eta_\infty^\infty = \eta_I^\infty = \eta_\perp^\infty = \eta_\parallel^\infty = \mu^\infty = 0. \quad (4.22)$$

It is interesting to note that  $\gamma_1^i$  and  $\gamma_{1,1}^i$  for  $i = 0, \infty$  as calculated in Sec. IV A obey the Binder-Hohenberg<sup>10</sup> scaling relations

$$\gamma_1^i = \nu(2 - \eta_\perp^i), \quad (4.23a)$$

$$\gamma_{1,1}^i = \nu(1 - \eta_\parallel^i), \quad (4.23b)$$

where  $\eta_\perp^i$  and  $\eta_\parallel^i$  are given above. These equations are expected to be valid beyond the mean-field approximation and have already been used in I to evaluate  $\gamma_1^0$  and  $\gamma_{1,1}^0$  to first order in  $\epsilon = 4 - d$ . They will be used in III to evaluate  $\gamma_1^\infty$  and  $\gamma_{1,1}^\infty$  from  $\eta_\perp^\infty$  and  $\eta_\parallel^\infty$  calculated to first order in  $\epsilon$ .  $\gamma_\infty^i$  and  $\gamma_{\infty,\infty}^i$  obey scaling relations similar to Eq. (4.23),

$$\gamma_\infty^i = \nu(2 - \eta_\infty^i), \quad (4.24a)$$

$$\gamma_{\infty,\infty}^i = \nu(1 - \eta_\infty^i). \quad (4.24b)$$

Equation (4.24a) is the standard bulk scaling relation. Equation (4.24b) follows directly from Eq. (2.8b) and the scaling form for  $\Gamma(\vec{x}, \vec{x}', t)$  implied by Eqs. (4.11), (4.16), and (4.17).

### C. Correlation function $\lambda^{-1} < 0$

If  $\lambda < 0$ ,  $e^{2i\phi(k)}$  in Eq. (4.14) has a pole in the upper half  $k$  plane, and we have

$$\int_{-\infty}^{\infty} \frac{dk}{2\pi} \frac{1}{q^2 + t} e^{ikz} e^{2i\phi(k)} = \frac{1}{2(p^2 + t)^{1/2}} e^{-(p^2 + t)^{1/2}|z|} e^{-2\theta(\vec{p})} + \frac{2}{\lambda} \frac{1}{p^2 + t - |\lambda|^{-2}} e^{-z/|\lambda|}. \quad (4.25)$$

Hence, from Eq. (4.11), we have

$$\Gamma(\vec{x}, \vec{x}') = \Gamma_\sigma(\vec{x}, \vec{x}') + \Gamma_\Sigma(\vec{x}, \vec{x}'), \quad (4.26)$$

where  $\Gamma_\sigma(\vec{x}, \vec{x}')$  is given by Eq. (4.11) with  $\lambda < 0$  and

$$\Gamma_\Sigma(\vec{x}, \vec{x}') = \frac{2}{|\lambda|} e^{-(z+z')/|\lambda|} \int_{\vec{p}} \frac{1}{p^2 + t - |\lambda|^{-2}} e^{i\vec{p} \cdot (\vec{p} - \vec{p}')} \quad (4.27)$$

The subscript  $\sigma$  refers to the bulk field  $\sigma$  used in I, and  $\Sigma$  refers to a new surface field which appears when  $\lambda < 0$  and which will be discussed more fully in III. The evaluation of  $\Gamma_\Sigma(\vec{x}, \vec{x}')$  follows directly from Eq. (4.17),

$$\Gamma_\Sigma(\vec{x}, \vec{x}') = \frac{2}{|\lambda|} \frac{\Gamma[(d-3)/2]}{(2\pi)^{(d-1)/2}} \frac{1}{|\vec{p} - \vec{p}'|^{d-3} g_{d-1}} \left( \frac{|\vec{p} - \vec{p}'|}{\xi_s} \right) e^{-(z+z')/|\lambda|}, \quad (4.28)$$

where  $\xi_s = (t - |\lambda|^{-2})^{-1/2}$  is the surface correlation length. Thus,  $\nu_s = \frac{1}{2}$ . Equations (4.26) and (4.28) imply that when  $\lambda < 0$  and  $t > |\lambda|^{-2}$ , there are two correlation lengths diverging at different temperatures: the bulk correlation length  $\xi$  diverging at  $t = t_0 = 0$  and the surface correlation. If  $t_0$  and  $t_s$  are approximately equal, for  $t \approx t_s + \frac{1}{2}(t_s - t_0) = \frac{3}{2}t_s$  the fluctuations in  $\Gamma_\sigma$  and  $\Gamma_\Sigma$  may be comparable.

At  $t = t_s$ ,  $\Gamma_\sigma$  can be neglected, and we can obtain all of the surface exponents from  $\Gamma_\Sigma$ . The exponents  $\eta_\perp^s$ ,  $\eta_\parallel^s$ ,  $\eta_s^s$ , and  $\mu^s$  are undefined since  $\Gamma_\Sigma$  decays exponentially rather than algebraically into the bulk.  $\eta_\parallel^s$  follows from Eq. (4.28),

$$\eta_\parallel^s = -1. \quad (4.29)$$

$\gamma_{1,1}^s$  satisfies the Binder-Hohenberg relations Eqs. (4.23b) with the above value of  $\eta_\parallel^s$ .  $\gamma_1^s$  obeys the same scaling relation as  $\gamma_{1,1}^s$ , as can be seen from

$$\begin{aligned} \chi(0) &= \int d^{d-1} \rho' \int dz' \Gamma_\Sigma(0, \vec{x}') \\ &\sim \xi_s^{1-\eta_\parallel^s} \sim (t - t_s)^{-\nu_s(1-\eta_\parallel^s)}. \end{aligned} \quad (4.30)$$

Hence,

$$\gamma_1^s = \nu_s(1 - \eta_\parallel^s). \quad (4.31)$$

This relation should also be true beyond the mean-field approximation.

$$v. \lambda^{-1} \geq 0, t \leq 0$$

In this section, we consider spin and susceptibilities for  $t < 0$  and  $\lambda^{-1} \geq 0$ .  $S_0(z)$  follows from Eq. (3.8)<sup>3-5</sup>

$$S_0(z) = \sqrt{-t} \tanh(z/\xi' + \phi_1), \quad (5.1)$$

where  $\xi' = (2/-t)^{1/2}$  is the bulk correlation length, and

$$\sinh 2\phi_1 = 2\lambda/\xi'. \quad (5.2)$$

This function is plotted in Fig. 1(a). Note that it bends down at  $z = 0$  reflecting the reduced mean field at the surface. Noting that  $\phi_1 \sim \lambda/\xi$  for  $\lambda/\xi \ll 1$  and  $\tanh$  is approximately one if  $z/\xi$  or  $\lambda/\xi \gg 1$ , the

interesting limits of Eq. (5.1) are easily evaluated.

$$\begin{aligned} S_0(z) &\sim \sqrt{-t} \frac{z + \lambda}{\xi'} \\ &= \frac{1}{\sqrt{2}} (z + \lambda)(-t), \quad z, \lambda \ll \xi' \end{aligned} \quad (5.3)$$

$$S_0(z) \sim \sqrt{-t} \quad z \gg \xi' \text{ or } \lambda \gg \xi'. \quad (5.4)$$

Equation (5.4) says that the profile of  $S_0(z)$  for  $\lambda = \infty$  is completely flat as shown in Fig. 1(b). This is because at  $\lambda = \infty$ , the surface exchanged is sufficiently greater than the bulk exchange that the surface mean field equals the bulk mean field. The  $\beta$  exponents follow directly from Eqs. (5.3) and (5.4),

$$\beta_1^0 = 1, \quad \beta_\infty^0 = \frac{1}{2}; \quad (5.5)$$

$$\beta_1^\infty = \beta_\infty^\infty = \frac{1}{2}. \quad (5.6)$$

Using Eq. (5.1) for  $S_0(z)$  and Eq. (3.11) for  $S_1(z)$ , we find

$$\begin{aligned} S_1(z) &= \frac{1}{\cosh^2 u_1} \\ &\times \left( \cosh^2 \phi_1 S_1(0) + B \xi'^2 \int_{\phi_1}^{u_1} e^{-y} \cosh^3 y \, dy \right), \end{aligned} \quad (5.7a)$$

$$\begin{aligned} S_1(0) &= \lambda(1 + 2\sinh^2 \phi_1)^{-1} \\ &\times \left( B_1 + \lambda \frac{e^{-\phi_1}}{\sinh \phi_1} B \right), \end{aligned} \quad (5.7b)$$

where  $u_1 = z/\xi' + \phi_1$ . The integral in Eq. (5.7a) can easily be evaluated, but for our purposes it is not necessary.  $\chi(z, z')$  is calculated in Appendix B following the procedure outlined in Sec. III and is given by

$$\begin{aligned} \chi(z, z') &= \frac{1}{\cosh^2 u_1} \frac{1}{\cosh^2 u_1'} \\ &\times \left( \frac{\lambda \cosh^4 \phi_1}{\cosh 2\phi_1} + \xi [V_2^0(u_1) - V_2^0(\phi_1)] \right), \end{aligned} \quad (5.8)$$

where



$$V_2^o(\tilde{u}_1) = \frac{3}{8}\tilde{u}_1 + \frac{1}{4}\sinh 2\tilde{u}_1 + \frac{1}{32}\sinh 4\tilde{u}_1, \quad (5.9)$$

with

$$u_1' = \frac{z'}{\xi'} + \phi_1, \quad \tilde{u}_1 = \frac{\tilde{z}}{\xi'} + \phi_1,$$

and

$$\tilde{z} = \frac{1}{2}(z + z' - |z - z'|).$$

The relevant limits of  $\chi(z)$  and  $\chi(z, z)$  can be calculated from Eqs. (5.7) and (5.8):

(i)  $\lambda > 0, \xi \gg \lambda, z,$

$$\chi(z) \sim (\lambda + z) \left(\frac{2}{-t}\right)^{1/2}, \quad \gamma_{1,1}'^o = \frac{1}{2} \quad (5.10)$$

$$\chi(0, 0) \sim \frac{\lambda}{1 + \frac{1}{2}\lambda^2(-t)}, \quad \gamma_{1,1}'^o = 0; \quad (5.11)$$

(ii)  $\lambda > 0, z \gg \xi,$

$$\chi(z) \sim \frac{1}{2(-t)}, \quad \gamma_{\infty}'^o = 1 \quad (5.12)$$

$$\chi(z, z) \sim \frac{1}{4}(2/-t)^{1/2}, \quad \gamma_{\infty, \infty}'^o = \frac{1}{2}; \quad (5.13)$$

(iii)  $\lambda = \infty$

$$\chi(z) = \frac{1}{2(-t)}, \quad \gamma_{1,1}'^{\infty} = \gamma_{\infty}'^{\infty} = 1 \quad (5.14)$$

$$\chi(z, z) = \frac{1}{2(-2t)^{1/2}}(1 + e^{-2z/\xi}), \quad \gamma_{1,1}'^{\infty} = \gamma_{\infty, \infty}'^{\infty} = \frac{1}{2}. \quad (5.15)$$

The solutions for  $\lambda = \infty$  are exact and can be obtained from the solutions in the disordered phase with the replacement of  $t$  by  $-2t$ .

By comparing (4.7b) with (5.11), we see that for the ordinary transition  $\gamma_{1,1}'^o$  is not equal to  $\gamma_{1,1}'^{\infty}$ . Thus although  $\chi(0, 0)$  approaches  $\lambda$  as  $t$  goes to zero from both above and below, the rate of approach is different.  $d\chi(0, 0)/dt$  diverges as  $t \rightarrow 0^+$  and is finite as  $t \rightarrow 0^-$ . Scaling, however, is not violated. To see this, let

$$\chi_{\pm}(0, 0) = \lambda F_{\pm}(\lambda/\xi), \quad (5.16)$$

where the “+” and “-” subscripts refer, respectively, to  $t > 0$  and  $t < 0$ . Both  $F_+$  and  $F_-$  tend to 1 as  $t \rightarrow 0$ .  $F_-$  is even in  $\lambda/\xi$ , whereas  $F_+$  contains both even and odd terms in  $\lambda/\xi$ , as can be seen from Eqs. (4.6) and (5.8). Thus around  $t=0$ ,  $F_-$  is an analytic function of  $(-t)$ , whereas  $F_+$  is an analytic function of  $\sqrt{t}$ .

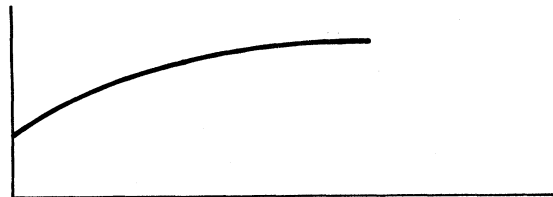
VI. SURFACE TRANSITION,  $t < |\lambda|^{-2}$

If  $\lambda < 0$  and  $0 < t < |\lambda|^{-2}$ , there is an ordered phase in which the spin is zero at  $z = \infty$ .  $S_0(z)$  can be obtained from Eq. (3.8) with this boundary condition

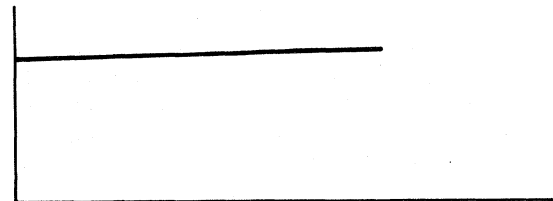
$$S_0(z) = (2t)^{1/2} 1/\sinh(z/\xi + \phi_2), \quad (6.1)$$

where

$$\tanh \phi_2 = |\lambda|/\xi, \quad (6.2)$$



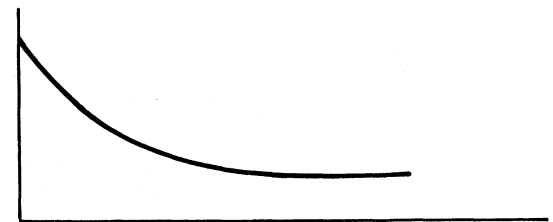
(a)



(b)



(c)



(d)

FIG. 1. (a) Spin profile for  $\lambda^{-1} > 0, t < 0$ . The transition from the isotropic state to this state is the ordinary transition. (b) Spin profile for  $\lambda^{-1} = 0, t = 0$ . The transition from the isotropic state to this state is the  $\lambda = \infty$  transition. (c) Spin profile for  $\lambda^{-1} < 0, 0 < t < t_s$ . The transition from the isotropic state to this state is the surface transition. (d) Spin profile for  $\lambda^{-1} < 0, t < 0$ . The transition from profile 1(c) to this state is the extraordinary transition.

and  $\xi = (1/t)^{1/2}$  is the bulk correlation length for  $t > 0$ . Equation (6.1) is plotted in Fig. 1(c).  $S_0(z)$  is zero at  $z = \infty$  for all  $t > 0$ . Hence  $\beta_\infty^s$  is undefined;  $\beta_1^s$  is determined by the behavior of  $S_0(0)$  near  $t = |\lambda|^{-2}$ .

$$S_0(0) = \frac{(2t)^{1/2}}{\sinh\phi_2} = (2)^{1/2}(|\lambda|^{-2} - t)^{1/2}, \quad (6.3)$$

$$\beta_1^s = \frac{1}{2}.$$

Using Eqs. (6.1) and (3.11), we have

$$S_1(z) = -\frac{\cosh u_2}{\sinh^2 u_2} \left( \frac{\sinh^2 \phi_2}{\cosh \phi_2} S_1(0) - B\xi^2 \int_{\phi_2}^{u_2} \frac{\sinh^3 y}{\cosh^2 y} dy \right), \quad (6.4)$$

where  $u_2 = z/\xi + \phi_2$  and

$$S_1(0) = (1/\lambda)(|\lambda|^{-2} - t)^{-1}(B_1 - \lambda B). \quad (6.5)$$

$\chi(z, z')$  is calculated in Appendix B;

$$\chi(z, z') = \frac{\cosh u_2 \cosh u_2'}{\sinh^2 u_2 \sinh^2 u_2'} \times \left\{ |\lambda| \sinh^4 \phi_2 + \xi [V_2^s(\tilde{u}_2) - V_2^s(\phi_2)] \right\}, \quad (6.6)$$

where  $u_2' = z'/\xi + \phi_2$ ,  $\tilde{u}_2 = \bar{z}/\xi + \phi_2$ , and

$$V_2^s(\tilde{u}_2) = -\frac{3}{2}\tilde{u}_2 + \frac{1}{4}\sinh 2\tilde{u}_2 + \tanh \tilde{u}_2. \quad (6.7)$$

Again, we obtain the  $\gamma$  exponents by evaluating the relevant limits of  $\chi(z)$  and  $\chi(z, z)$ . Both  $\chi(z)$  and  $\chi(z, z)$  are zero at  $z = \infty$  for  $t \sim |\lambda|^{-2}$ .  $\gamma_\infty^s$  and  $\gamma_{\infty, \infty}^s$  are therefore undefined. The surface exponents follow from

$$\chi(0) = -\frac{1}{|\lambda|^{-2} - t}, \quad \gamma_1^s = 1 \quad (6.8)$$

$$\chi(0, 0) = \frac{1}{\lambda} \frac{1}{|\lambda|^{-2} - t}, \quad \gamma_{1,1}^s = 1. \quad (6.9)$$

These exponents agree with those derived for  $t \gtrsim |\lambda|^{-2}$  in Sec. IV A; consequently, the scaling relations discussed at the end of Sec. IV B are satisfied when the critical temperature is approached from both above and below.

## VII. EXTRAORDINARY TRANSITION

If  $\lambda < 0$  and  $t < 0$ ,  $S_0(z)$  is enhanced near the surface but has a finite value at  $z = \infty$ ,

$$S_0(z) = \sqrt{-t} \coth(z/\xi' + \phi_3), \quad (7.1)$$

where  $\xi' = (2/-t)^{1/2}$  and

$$\sinh 2\phi_3 = 2|\lambda|/\xi'. \quad (7.2)$$

As required by the  $z = \infty$  boundary condition, we have

$$S_0(\infty) = \sqrt{-t}, \quad \beta_\infty^e = \frac{1}{2}. \quad (7.3)$$

The spin profile at  $t=0$  decays algebraically to zero at  $\lambda = \infty$ . The  $t=0$  limit of both Eqs. (6.1) and (7.1) is

$$S_0(z, 0) = \sqrt{2}/z + |\lambda|. \quad (7.4)$$

More generally, we expect

$$S_0(z, t) = |t|^{\beta_\infty^e} J\left(\frac{z + |\lambda|}{\xi}\right), \quad (7.5)$$

where  $J$  is a function which ensures that  $S_0(z, t) = (-t)^{\beta_\infty^e}$  at  $z = \infty$  and that  $S_0(z, t=0)$  is finite

$$J(x) \rightarrow \begin{cases} 1 & \text{as } x \rightarrow \infty \\ x^{-\beta_\infty^e/\nu^e} & \text{as } x \rightarrow 0. \end{cases} \quad (7.6)$$

Thus, we expect

$$S_0(z, 0) \sim (z + |\lambda|)^{-\beta_\infty^e/\nu^e}, \quad (7.7)$$

even when the mean field is not valid.

A surface  $\beta$  exponent can be obtained from  $S_0(0, t) - S_0(0, 0) \sim |t|^{\beta_1^e}$ . Using Eqs. (6.1), (7.1), and (7.4) we obtain

$$S_0(0, t) - S_0(0, 0) = -(|\lambda|/\sqrt{2})t, \quad (7.8)$$

$$\beta_1^e = \beta_{1^e}^e = 1.$$

From Eqs. (7.1) and (3.11), we have

$$S_1(z) = \frac{1}{\sinh^2 u_3} \left( \sinh^2 \phi_3 S_1(0) + B\xi'^2 \int_{\phi_3}^{u_3} e^{-y} \sinh^3 y dy \right), \quad (7.9)$$

where  $u_3 = z/\xi' + \phi_3$  and

$$S_1(0) = +\lambda^{-1} \left( \frac{t}{\sinh^2 \phi_3} - \lambda^{-2} \right)^{-1} \times [B_1 + \lambda(\tanh \phi_3 - 1)B]. \quad (7.10)$$

From Eqs. (6.4) and (7.9), we find  $\chi(\infty)$  as  $t$  approaches zero from above and below,

$$\chi(\infty, t=0^+) = 1/t, \quad \gamma_\infty^e = 1; \quad (7.11)$$

$$\chi(\infty, t=0^-) = 1/-2t, \quad \gamma_\infty^e = 1.$$

If  $z$  is fixed,  $\chi(z)$  approaches the same limit as  $t$  tends to zero from above and below,

$$\chi(z, 0) = \frac{1}{4} \left( (|\lambda| + z)^2 - 5 \frac{|\lambda|^4}{(|\lambda| + z)^2} \right). \quad (7.12)$$

Note that  $\chi(z, 0)$  is finite for all  $z < \infty$ . Applying a scaling argument similar to the one used for  $S_0(z)$  [Eq.(7.7)], we expect that, in general,

$$\chi(z) \sim z \gamma_\infty^e / \nu^e \quad (7.13)$$

as  $z \rightarrow \infty$ .  $\gamma_1^e$  will be negative or zero since  $\chi(z)$  is finite at  $z=0$ . From Eqs. (6.8), (7.10), and (7.12) we have

$$\begin{aligned} \chi(z, t=0^+) &= -|\lambda|^2 - t|\lambda|^4, \quad \gamma_1^e = 0 \\ \chi(z, t=0^-) &= -|\lambda|^2 + (-t/2)^{1/2}|\lambda|^3, \quad \gamma_1^{e'} = \frac{1}{2}. \end{aligned} \tag{7.14}$$

The response  $\bar{\chi}$  of the total spin of a sample to a uniform magnetic field is often experimentally more accessible than either  $\chi(z)$  or  $\chi(z, 0)$ . If  $\bar{\chi}$  is measured in a sample with  $\lambda < 0$ , two divergences should appear as the temperature is lowered. The first will appear at  $t_s$  with  $\bar{\chi} \sim (t - t_s)^{-\gamma_1^e A \xi}$ , where  $A$  is the surface area of the sample and  $\xi$  is the bulk correlation length which is finite at  $t_s$ . The second divergence appears at  $t=0$ , with  $\bar{\chi} \sim t^{-\gamma_{\infty}^e} V$ , where  $V$  is the volume of the sample  $\chi(z, z')$  for  $\lambda < 0, t < 0$  is calculated using the results of Appendix B.

$$\begin{aligned} \chi(z, z') &= \frac{1}{\sinh^2 u_3} \frac{1}{\sinh^2 u'_3} \\ &\times \left( |\lambda| \frac{\sinh^4 \phi_3}{\sinh 2\phi_3} + \xi [V_2^e(\bar{u}_3) - V_2^e(\phi_3)] \right), \end{aligned} \tag{7.15}$$

where  $u_3 = z'/\xi' + \phi_3, \bar{u}_3 = \bar{z}/\xi' + \phi_3$ , and

$$V_2^e(x) = \frac{3}{8}x - \frac{1}{4} \sinh 2x + \frac{1}{32} \sinh 4x. \tag{7.16}$$

The infinite  $z$  limit of  $\chi(z, z)$  follows from Eqs. (7.15) and (6.6),

$$\begin{aligned} \chi(\infty, \infty; t=0^+) &\sim \frac{1}{2}(1/t)^{1/2}, \quad \gamma_{\infty, \infty}^e = \frac{1}{2} \\ \chi(\infty, \infty; t=0^-) &\sim \frac{1}{4}(2/t)^{1/2}, \quad \gamma_{\infty, \infty}^{e'} = \frac{1}{2}. \end{aligned} \tag{7.17}$$

$$\Gamma(\bar{\mathbf{x}}, \bar{\mathbf{x}}') - \Gamma_{\infty}(\bar{\mathbf{x}}, \bar{\mathbf{x}}') \sim \begin{cases} \frac{1}{(z+z')^{d-2}}, & d < 4, \quad \eta_I^e = \min(0, 4-d) \\ \frac{1}{(z+z')^2}, & d > 4. \end{cases} \tag{7.24}$$

At  $d=4, \eta_I^e=0$  but the leading term Eq. (7.24) has a logarithmic term, as shown in Eq. (C18).

The surface exponent  $\gamma_1^{e'}$  satisfies the scaling relation Eq. (4.23a), but  $\gamma_1^e$ , and  $\gamma_{1,1}^e = \gamma_{1,1}^{e'}$  do not satisfy the scaling relations.

VIII. SUMMARY

We may summarize our results by starting with the phase diagram shown in Fig. 2 where we have plotted the surface coupling enhancement  $\Delta_s$  against the reduced temperature  $t$ . We recall that the extrapolation length  $\lambda$  is related to  $\Delta_s$  by  $\lambda^{-1} = 1 - \Delta_s/\Delta_c$ , where  $\Delta_c = 2(d-1)$  is the critical surface enhancement.

Both Eqs. (6.6) and (7.15) give

$$\begin{aligned} \chi(z, z'; t=0) &= \frac{1}{5} \left( \frac{(\bar{z} + |\lambda|)^5}{(z + |\lambda|)^2(z' + |\lambda|)^2} \right. \\ &\quad \left. + \frac{4|\lambda|^5}{(z + |\lambda|)^2(z' + |\lambda|)^2} \right). \end{aligned} \tag{7.18}$$

In general, we should have

$$\chi(z, z'; t=0) \sim z \gamma_{\infty, \infty}^{e'} \nu \tag{7.19}$$

as  $z \rightarrow \infty$ . The surface exponents follow from

$$\begin{aligned} \chi(0, 0, t=0^+) &= \frac{|\lambda|}{1-t|\lambda|^2}, \quad \gamma_{1,1}^e = 0 \\ \chi(0, 0, t=0^-) &= \frac{|\lambda|}{1-4t|\lambda|^2}, \quad \gamma_{1,1}^{e'} = 0. \end{aligned} \tag{7.20}$$

Finally, we have derived an analytic expression for  $\Gamma(z, z'; \bar{\mathbf{p}})$  for  $\lambda < 0$  and  $t=0$ . From this we have obtained the interesting asymptotic limits of  $\Gamma(\bar{\mathbf{x}}, \bar{\mathbf{x}}')$ . These calculations, which are quite complicated, are discussed in Appendix C.

The asymptotic limits of  $\Gamma(\bar{\mathbf{x}}, \bar{\mathbf{x}}')$  when compared with Eqs. (2.13)–(2.17) yield

$$\Gamma(\bar{\mathbf{x}}, 0) \sim \frac{(\cos \theta)^3}{|\bar{\mathbf{x}}|^{d+1}}, \quad \eta_{\perp}^e = 3, \quad \mu_e = 3 \tag{7.21}$$

$$\Gamma(\bar{\mathbf{e}}, 0) \sim \frac{1}{|\bar{\mathbf{e}}|^{d+4}}, \quad \eta_{\parallel}^e = 6 \tag{7.22}$$

$$\Gamma_{\infty}(\bar{\mathbf{x}}, \bar{\mathbf{x}}') \sim \frac{1}{|\bar{\mathbf{x}} - \bar{\mathbf{x}}'|^{d-2}}, \quad \eta_{\infty}^e = 0 \tag{7.23}$$

In Fig. 2 there are three lines which define the boundaries of the four phase transition discussed in this paper: (i) the line  $t=1/\lambda^2, \lambda < 0$ , which meets the axis at  $t=0$  with an infinite slope at  $\Delta_s = \Delta_c$ , is the surface transition line; (ii) the line  $t=0$  for  $\Delta_s > \Delta_c$  corresponds to the extraordinary transition for which the bulk orders after the surface; (iii) the line  $t=0$  for  $\Delta_s < \Delta_c$  corresponds to the ordinary transition which is the transition found in the infinite system. The surface effects in this case simply change the shape of the magnetization near the surface.

When  $\Delta_s = \Delta_c$  the three lines meet and  $\lambda = \infty$ . This point corresponds to the transition we have labeled the  $\lambda = \infty$  transition. In this case the coupling in the

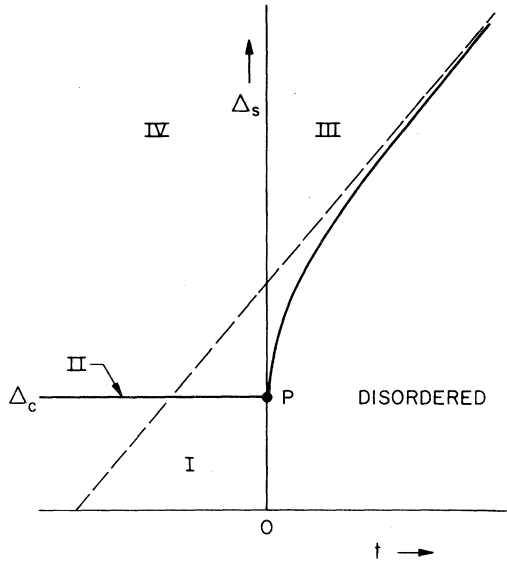


FIG. 2. Phase diagram as a function of  $\Delta_s$  and  $t$ . The region  $t > \max(0, t_s)$  is the disordered phase. Region I has the spin profile shown in Fig. 1(a), region II (the line  $\Delta_s = \Delta_c$ ) that of Fig. 1(b), region III that of Fig. 1(c), and region IV that of Fig. 1(d). The ordinary transition corresponds to crossing the line  $t=0$  for  $\Delta_s < \Delta_c$ , the  $\lambda = \infty$  transition to passing through  $t=0$  at the point  $P$  ( $\Delta_s = \Delta_c$ ,  $t=0$ ), the surface transition to crossing the line  $t=t_s$  for  $\Delta_s > \Delta_c$ , and the extraordinary transition to crossing the line  $t=0$  for  $\Delta_s > \Delta_c$ . The dotted line represents the transition temperature of a  $(d-1)$ -dimensional system with exchange  $J_s = J(1 + \Delta_s)$ . The curve  $t_s=0$  approaches this line for large  $\Delta_s$ .

surface layer is sufficiently enhanced so that the magnetization profile is flat. The nature of this transition will be discussed in more detail in Ref. 2.

The values of the mean-field critical exponents are given in Tables I and II. The scaling relations given in Eqs. (4.23a), (4.23b), and (4.31) are satisfied for ordinary,  $\lambda = \infty$ , and surface transitions with one exception;  $\gamma_{1,1}^{\circ}$  does not satisfy Eq. (4.23b). The scaling relations are not satisfied for the extraordinary transition with one exception;  $\gamma_{1,1}^{\circ}$  satisfies Eq. (4.23a). The cases in which the scaling relations fail all correspond to exponents which are not positive; consequently, scaling may still hold.

We should note that in Ref. 2 we show that at the surface transition a new order parameter appears whose correlation function is denoted by  $\Gamma_{\Sigma}$  [see Eq. (4.28)]. It is shown in Ref. 2 that the surface and bulk order parameters decouple and that the surface behaves like a  $(d-1)$ -dimensional bulk system. This is already evident in Eq. (4.28), where  $\Gamma_{\Sigma}$  is just a function of  $z$  and  $|\lambda|$  times a

TABLE I. Critical exponents for the transitions discussed in the text.

	$o$	$\infty$	$s$	$e$
$\eta_{\infty}$	0	0	$\dots^a$	0
$\eta_{\parallel}$	2	0	-1	6
$\eta_{\perp}$	1	0	$\dots$	3
$\eta_I$	0	0	$\dots$	0
$\mu$	1	0	$\dots$	3
$\beta_{\infty}$	$\frac{1}{2}$	$\frac{1}{2}$	$\dots$	$\frac{1}{2}$
$\beta_1$	1	$\frac{1}{2}$	$\frac{1}{2}$	$1^b$

<sup>a</sup> Three dots means the exponent is undefined.

<sup>b</sup>  $\beta_1^{\circ}$  is defined for  $t=0^+$  and  $t=0^-$  and has the same value in both cases.

$(d-1)$ -dimensional bulk correlation function. The critical exponents for the surface transition thus may be calculated from those of a  $(d-1)$ -dimensional bulk system.

It is clear from Tables I and II that the exponents for all the transitions far from the surface, i.e., when  $z \gg \xi$ , are the same as the bulk exponents. This result is not unexpected, and we conjecture that it is true even when mean-field theory no longer applies.

In Ref. 1, the exponent  $\tilde{\eta}$  was defined for the ordinary transition. It was possible to write  $\eta_{\parallel}^{\circ}$ ,  $\eta_{\perp}^{\circ}$ , and  $\mu^{\circ}$  to order  $\epsilon=4-d$  in terms of  $\tilde{\eta}$ . In this paper we have defined  $\eta_I$  which turns out to equal  $2\tilde{\eta}$  for the ordinary transition. A similar result will be shown to hold for the  $\lambda = \infty$  transition in Ref. 2.

Next, note that for the three transitions for which the exponents  $\mu$  and  $\eta$  are defined we have the relation  $\mu + \eta_{\perp} = \eta_{\parallel}$ . This relation remains true to order  $\epsilon$  for both the ordinary<sup>1</sup> and  $\infty$ -transitions.<sup>2</sup>

TABLE II.  $\gamma$  exponents for the transition discussed in the text.

	$o$		$\infty$		$s$		$e$	
	$+^a$	$-^a$	$+$	$-$	$+$	$-$	$+$	$-$
$\gamma_1$	$\frac{1}{2}$	$\frac{1}{2}$	1	1	1	1	0	$-\frac{1}{2}$
$\gamma_{1,1}$	$-\frac{1}{2}$	0	$\frac{1}{2}$	$\frac{1}{2}$	1	1	0	0
$\gamma_{\infty}$	1	1	1	1	$\dots^b$	$\dots$	1	1
$\gamma_{\infty, \infty}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\dots$	$\dots$	$\frac{1}{2}$	$\frac{1}{2}$

<sup>a</sup> The plus and minus denote, respectively, the limit as the transition temperature is approached from above and below.

<sup>b</sup> Three dots means the exponent is undefined.

The origin of this result may be found in Eqs. (2.13) and (2.14), where we consider the case  $|\vec{x}|, z \gg 1, \vec{x}' = 0$ . If we subsequently fix  $z$  and let  $|\vec{\rho}|$  become much larger than  $z$ , we obtain a form like that given in Eq. (2.15) with  $\eta_{||} = \mu + \eta_{\perp}$ . This does not constitute a proof of this relation but is suggestive of the fact that the form in Eq. (2.13) and (2.14) for  $\Gamma(\vec{x}, 0)$  is a correct limiting form for all  $\theta \neq \frac{1}{2}\pi$ . In fact, if  $\cos\theta$  is defined by  $(z + |\lambda|)/|\vec{x}| = \cos\theta$ , rather than by  $z/|\vec{x}| = \cos\theta$ , then Eqs. (2.13) and (2.14) include Eq. (2.15) when  $z = 0$ , provided  $\eta_{||} = \mu + \eta_{\perp}$ .

Finally, we note that the exponents for the ordinary and infinite transitions are expected to be exact for  $d > 4$ , while the exponents for the surface transition are expected to be exact for  $d > 5$ . These results are implied by the renormalization group calculations of Refs. 1 and 2 and may also be obtained from a straightforward application of the Ginzburg criterion. To obtain the limit of validity of mean-field theory for the extraordinary transition is more difficult. If it is assumed that the surface and bulk order parameters remain decou-

pled down to four dimensions; then applying the Ginzburg criterion far from the surface would lead one to conclude that the exponents which are derived for  $z \gg \xi$  are correct for  $d > 4$ . However, below five dimensions a Ginzburg-like argument is more difficult to make because the surface is no longer described by mean-field theory. We have not investigated this case in detail.

ACKNOWLEDGMENTS

One of the authors (M.H.R.) wishes to express his gratitude for the hospitality of the Aspen Center for Physics where part of the research reported here was performed and the the University of Maryland Baltimore County for a faculty summer research grant.

APPENDIX A

In this appendix we evaluate  $H_d(\vec{x}, \lambda, t)$  defined in Eq. (4.13). The  $p$  integration may be done by first performing the angular integration and then

using Eq. (6.566.2) of Ref. 12,

$$H_d(\vec{x}, \lambda, t) = \left(\frac{1}{2\pi\rho}\right)^{(d-3)/2} \int_{-\infty}^{\infty} \frac{dk}{(2\pi)^2} e^{ikz} \frac{1 + ik\lambda}{1 - ik\lambda} (k^2 + t)^{(d-3)/4} K_{(d-3)/2}[(k^2 + t)^{1/2}\rho], \tag{A1}$$

where  $K$  is a Bessel function of imaginary argument.

Since we are always interested in  $\rho \gg 1$ , and since  $K$  decays exponentially, only small values of  $k$  are important in the integrand. Thus if  $\lambda^{-1} > 0$ , we may set

$$\frac{1 + ik\lambda}{1 - ik\lambda} = e^{2ik\lambda} [1 + O(k^3\lambda^3)];$$

then Eq. (A1) becomes

$$H_d(\vec{x}, \lambda, t) = \left[1 + O\left(\lambda^3 \frac{\partial^3}{\partial z^3}\right)\right] \left(\frac{1}{2\pi\rho}\right)^{(d-3)/2} \int_{-\infty}^{\infty} \frac{dk}{(2\pi)^2} e^{i\lambda(kz + 2\lambda)} (k^2 + t)^{(d-3)/4} K_{(d-3)/2}[(k^2 + t)^{1/2}\rho].$$

The integral is given by Eq. (6.726.4) of Ref. 12 and yields Eqs. (4.16) and (4.17) for  $|\vec{x} - \nu\vec{x}'| = [\rho^2 + (z + z')^2]^{1/2} \gg \lambda$ .

We next evaluate the  $1/\lambda$  correction to the  $\lambda = \infty$  limit of  $H_d$ :

$$C = H_d(\vec{x}, \lambda, t) - H_d(\vec{x}, \infty, t) = \left(\frac{1}{2\pi\rho}\right)^{(d-3)/2} \int_{-\infty}^{\infty} \frac{dk}{(2\pi)^2} \left( e^{ikz} \frac{2}{1 - ik\lambda} (k^2 + t)^{(d-3)/4} K_{(d-3)/2}(\sqrt{k^2 + t}\rho) \right), \tag{A2}$$

where  $H_d(\vec{x}, \infty, t)$  is given by Eqs. (4.16)–(4.18).

To evaluate the  $1/\lambda$  term in Eq. (A2), we use the identity

$$\frac{1}{1 - ik\lambda} = \int_0^{\infty} ds e^{-s(1 - ik\lambda)},$$

and perform the  $k$  integration using Eq. (6.726.4) in Ref. 12. After a change of variables,  $s\lambda + z = u$ , we get

$$C = \left(\frac{t}{2\pi}\right)^{(d-2)/2} \frac{1}{\lambda} \int_z^{\infty} du e^{-1/\lambda(u-z)} w^{-(d-2)/2} K_{(d-2)/2}(w), \tag{A3}$$

where  $w = (t)^{1/2}(\rho^2 + u^2)^{1/2}$ . Since we are only interested in the  $1/\lambda$  term in  $C$ , we may set the exponential term in the integral equal to 1. Next we estimate the integral by writing

$$w^{-(d-2)/2} K_{(d-2)/2}(w) = -\frac{1}{u} \frac{d}{du} w^{-(d-4)/2} K_{(d-4)/2}(w),$$

and integrating Eq. (A3) by parts,

$$C = \left(\frac{t}{2\pi}\right)^{(d-2)/2} \frac{1}{z\lambda} \left( [(t)^{1/2}(\rho^2 + z^2)^{1/2}]^{-(d-4)/2} K_{(d-4)/2} [(t)^{1/2}(\rho^2 + z^2)^{1/2}] - \int_z^\infty du \frac{1}{u^2} w^{-(d-4)/2} K_{(d-4)/2}(w) \right). \tag{A4}$$

Repeated integration by parts generates an asymptotic alternating series. Thus the first term of the series is an upper bound on the series. Rewriting the first term in Eq. (A4) as

$$G_d(\vec{x}, t) \frac{|\vec{x}|}{\lambda} \frac{|\vec{x}|}{z} \frac{2}{d-4} \frac{g_{d-1}(\sqrt{t}|\vec{x}|)}{g_d(\sqrt{t}|\vec{x}|)}, \tag{A5}$$

where  $G_d$  is defined in Eq. (4.17) and  $g_d$  in Eq. (4.18), we obtain the correction quoted in Eq. (4.16).

If  $z \approx 0$  this result is no longer useful. We may evaluate Eq. (A3) to leading in  $1/\lambda$  when  $z=0$  by using Eq. (6.596.3) of Ref. 12. We find

$$C = \left(\frac{1}{2\pi}\right)^{(d-3)/2} \rho^{1/(d-2)} \frac{\rho}{\lambda} (\sqrt{t}\rho)^{(d-3)/2} K_{(d-3)/2}(\rho\sqrt{t}),$$

which again is of the form given in Eq. (4.16).

Finally, we note that there is no singularity in Eq. (A5) at  $d=4$ . The term  $1/(d-4)$  is cancelled by the  $\Gamma$  functions in the  $g$ 's.

APPENDIX B

In this appendix we will obtain the solutions for  $\chi(z, z')$  quoted in the text in Secs. V-VII of the text. We begin with Eq. (3.16).

$$\frac{d}{dz^2} W(z, \vec{p}) - [p^2 + t + 3S_0^2(z)] W(z, \vec{p}) = 0. \tag{B1}$$

$S_0(z)$  is a function of  $u_i = z/\xi + \phi_i$  for  $i=0, s$ , and  $e$ . Therefore, suppressing the index  $i$  referring to the transition and writing

$$W(z, \vec{p}) = g(u) V(u, \vec{p}), \tag{B2}$$

where  $g$  is a solution to

$$g'' - \xi^2 [t + 3S_0^2(u)] g = 0, \tag{B3}$$

which tends to  $\exp\{-\xi[t + 3S_0^2(\infty)]^{1/2} u\}$  as  $u \rightarrow \infty$ , we have

$$V'' + 2(g'/g) V' - \xi^2 p^2 V = 0. \tag{B4}$$

When  $p=0$ , Eq. (B4) is easily solved.

$$V'' + 2(g'/g) V' = 0. \tag{B5}$$

One solution is  $V_1=1$ . A second solution is  $V_2(u) = \int^u g^{-2}(u') du'$ . Thus we have

$$W_1(z, \vec{0}) = g(u), \tag{B6}$$

and

$$W_2(z, \vec{0}) = g(u) \int^u du' g^{-2}(u'). \tag{B7}$$

$u = z/\xi + \phi$ . Using these results in Eqs. (3.21) and (3.22), we find

$$C_2 = \xi \tag{B8}$$

and

$$C_1 = -\xi [V_2(\phi) + h(\phi)], \tag{B9}$$

where

$$h(\phi) = [g(\phi)g'(\phi) - (1/\lambda)g^2(\phi)]^{-1} \tag{B10}$$

Finally, from Eqs. (3.17), (3.18), and the above Eqs., we have for  $z > z'$ ,

$$\chi(z, z') = g(u)g(u') \times \xi [V_2(u') - V_2(\phi) - h(\phi)]. \tag{B11}$$

This is the general equation for  $\chi(z, z')$  for all the ordered states.

The  $g$ 's are easily determined for the three forms of  $S_0(z)$ .

$$(i) g_o(u) = \cosh^{-2} u, \quad \lambda > 0, \quad t < 0 \tag{B12}$$

$$(ii) g_s(u) = \frac{\cosh u}{\sinh^2 u}, \quad \lambda < 0, \quad 0 < t < |\lambda|^{-2} \tag{B13}$$

$$(iii) g_e(u) = \sinh^4 u, \quad \lambda < 0, \quad t < 0. \tag{B14}$$

Equation (B12)-(B14) when inserted into Eq. (B11) with the appropriate  $V_2$  and  $h$  as calculated from Eqs. (B7) and (B10), give Eqs. (5.8), (6.6), and (7.19) in the text.

APPENDIX C

In this appendix we present the calculation of  $\Gamma(z, z'; \vec{p})$  defined in Eqs. (3.15)–(3.22) and  $\Gamma(\vec{x}, \vec{x}')$  for  $\lambda < 0$  and  $t = 0$ .

At  $t = 0$  Eq. (3.16) becomes

$$W''(z, \vec{p}) - (p^2 + 6/y^2)W(z, \vec{p}) = 0, \tag{C1}$$

where  $y = z + |\lambda|$  and Eq. (7.4) has been used for  $S_0(z, 0)$ . This is a form of Bessel's equation [Ref. 12, Eq. (8.491.8)] with independent solutions

$$W_1(z, \vec{p}) = (2py/\pi)^{1/2} K_{5/2}(py), \tag{C2}$$

$$W_2(z, \vec{p}) = (\pi py/2)^{1/2} I_{5/2}(py). \tag{C3}$$

$W_1$  satisfies the boundary condition following Eq. (3.16). Using Eq. (3.21), we calculate

$$C_2 = 1/p, \tag{C4}$$

and from Eq. (3.22),

$$C_1 = \frac{\pi}{2p} \frac{UI_{3/2}(U) - I_{5/2}(U)}{UK_{3/2}(U) - K_{5/2}(U)}, \tag{C5}$$

where  $U = p|\lambda|$ . In the long-wavelength limit  $U \ll 1$ ,

$$C_1 = \frac{4}{45} (1/p) U^5 [1 + O(U^2)]. \tag{C6}$$

Finally,  $\Gamma(z, z'; \vec{p})$  is given by Eqs. (3.17), (3.18), and (C2)–(C5).

We now turn to the calculation of  $\Gamma(\vec{x}, \vec{x}')$  defined by

$$\Gamma(\vec{x}, \vec{x}') = \int_{\vec{p}} \Gamma(z, z'; \vec{p}) e^{i\vec{p} \cdot \vec{r}},$$

where  $\vec{x} = (z, \vec{p})$  and  $\vec{x}' = (z', \vec{p}')$ . Since  $\Gamma(z, z'; \vec{p})$  is a function of  $|\vec{p}|$  only, the  $(d - 1)$ -dimensional angular integral is easily evaluated. It will be convenient to break  $\Gamma(\vec{x}, \vec{x}')$  into two pieces.

$$\Gamma(\vec{x}, \vec{x}') = \Gamma_{11}(\vec{x}, \vec{x}') + \Gamma_{12}(\vec{x}, \vec{x}'), \tag{C7}$$

where

$$\Gamma_{11}(\vec{x}, \vec{x}') = \frac{1}{(2\pi)^{(d+1)/2}} \frac{1}{\rho^{(d-3)/2}} \frac{16}{45} (yy')^{1/2} |\lambda|^5 \int_0^\infty dp p^{(d+9)/2} [K_{5/2}(py) K_{5/2}(py') J_{(d-3)/2}(p\rho)], \tag{C8}$$

$$\Gamma_{12}(\vec{x}, \vec{x}') = \frac{1}{(2\pi)^{(d-1)/2}} \frac{1}{\rho^{(d-3)/2}} (yy')^{1/2} \int_0^\infty dp p^{(d-1)/2} [K_{5/2}(py) I_{5/2}(py') J_{(d-3)/2}(p\rho)], \tag{C9}$$

$y = z + |\lambda|$ , and  $y' = z' + |\lambda|$ . We have written Eq. (C9) under the condition  $z > z'$ ; since  $\Gamma(\vec{x}, \vec{x}')$  is symmetric in  $\vec{x}$  and  $\vec{x}'$ , there is no loss of generality. Finally, in Eq. (C8) we have used the long-wavelength limit of  $C_1$  given in Eq. (C6).

The integral in Eq. (C9) is given by Eq. (6.578.11) of Ref. 12 in terms of a Legendre function of the second kind. We find

$$\Gamma_{12}(\vec{x}, \vec{x}') = \frac{1}{(2\pi)^{d/2}} \frac{1}{(yy')^{(d-2)/2}} \frac{1}{(U^2 - 1)^{(d-2)/4}} e^{-[(d-2)/2]i\pi} Q_2^{(d-2)/2}(U), \tag{C10}$$

where  $U = (1/2yy')(y^2 + y'^2 + \rho^2)$ . For  $d \neq 4$ , Eq. (C10) may be rewritten using Eq. [3.32(15)] of Ref. 13 as

$$\Gamma_{12}(\vec{x}, \vec{x}') = \frac{\Gamma(\frac{1}{2}d - 1)}{4\pi^{d/2}} \left[ \frac{1}{|\vec{x} - \vec{x}'|^{d-2}} F\left(\frac{|\vec{x} - \vec{x}'|^2}{yy'}\right) - \frac{1}{|\vec{x} - \nu\vec{x}' + 2|\lambda|\hat{e}_\perp|^{d-2}} F\left(-\frac{|\vec{x} - \nu\vec{x}' + 2|\lambda|\hat{e}_\perp|^2}{yy'}\right) \right], \tag{C11}$$

where

$$F(u) = 1 - \frac{3}{d-4}u + \frac{3}{(d-4)(d-6)}u^2. \tag{C12}$$

The evaluation of  $\Gamma_{11}$  is more complicated and tedious. We start with Eq. (6.623.2) of Ref. (12).

$$I(\rho, w) = \int_0^\infty dp p^{(d-1)/2} J_{(d-3)/2}(p\rho) e^{-wp} = 2^{(d-1)/2} \Gamma(\frac{1}{2}d) \frac{1}{\sqrt{\pi}} \rho^{(d-3)/2} \frac{w}{(\rho^2 + w^2)^{d/2}}. \tag{C13}$$

The integral in Eq. (C8) is rewritten by using Eq. (8.468) of Ref. (12) to express

$$p^5 K_{5/2}(py) K_{5/2}(py') = \frac{\pi}{2} \left(\frac{1}{yy'}\right)^{1/2} \left(\frac{9}{y^2 y'^2} - \frac{9}{y^2 y'^2} w \frac{\partial}{\partial w} + \frac{3}{y^2 y'^2} w^2 \frac{\partial^2}{\partial w^2} + \frac{3}{yy'} \frac{\partial^2}{\partial w^2} + \frac{3}{yy'} w \frac{\partial^3}{\partial w^3} + \frac{\partial^4}{\partial w^4}\right) e^{-pw},$$

where  $w$  is set equal to  $y + y'$  after the differentiation is carried out. Eq. (C8) may now be evaluated by first interchanging the order of the differentiation with respect to  $w$  and the integration with respect to  $p$  and then using Eq. (C13). After some algebraic manipulation, we find

$$\Gamma_{11}(\vec{x}, \vec{x}') = \frac{\Gamma(\frac{1}{2}d+4)}{\pi^{d/2}} \frac{16|\lambda|^5}{45} \frac{w}{(\rho^2+w^2)^{(d+4)/2}} \times \left( \frac{3w^4}{y^2y'^2} - \frac{15w^2}{yy'} + 3(d+4) \frac{w^4}{yy'(\rho^2+w^2)} + 15 - 10(d+4) \frac{w^2}{\rho^2+w^2} + (d+4)(d+6) \frac{w^4}{(\rho^2+w^2)^2} \right), \tag{C14}$$

where  $w = y + y' = z + z' + 2|\lambda|$ , and  $\rho^2 + w^2 = |\vec{x} - \nu\vec{x}' + 2|\lambda|\hat{e}_\perp|^2$ .

Equations (C11), (C12), and (C14) complete the evaluation of  $\Gamma(\vec{x}, \vec{x}')$  for  $d \neq 4$ . For  $d=4$ ,  $\Gamma_{11}$  may be evaluated from Eq. (C14) by simply setting  $d=4$ . However, to evaluate  $\Gamma_{12}$ , we must carefully take the limit  $d \rightarrow 4$  of Eqs. (C11) and (C12), or we may use Eq. (C10) and evaluate  $Q_{\frac{1}{2}}(u)$  directly. Either way, we find

$$\Gamma_{12}(\vec{x}, \vec{x}') = \frac{1}{4\pi^2} \left( \frac{3}{yy'} + \frac{1}{|\vec{x} - \vec{x}'|^2} - \frac{1}{|\vec{x} - \nu\vec{x}' + 2|\lambda|\hat{e}_\perp|} - \frac{3}{4} \frac{y^2 + y'^2 + \rho^2}{y^2y'^2} \ln \frac{|\vec{x} - \nu\vec{x}' + 2|\lambda|\hat{e}_\perp|^2}{|\vec{x} - \vec{x}'|^2} \right), \tag{C15}$$

and

$$\Gamma_{11}(\vec{x}, \vec{x}') = \frac{1}{4\pi^2} \frac{32|\lambda|^5}{15} \frac{(y+y')}{|\vec{x} - \nu\vec{x}' + 2|\lambda|\hat{e}_\perp|^3} \left[ 15 - 80 \frac{(y+y')^2}{|\vec{x} - \nu\vec{x}' + 2|\lambda|\hat{e}_\perp|^2} + 80 \frac{(y+y')^4}{|\vec{x} - \nu\vec{x}' + 2|\lambda|\hat{e}_\perp|^4} - \frac{3(y+y')^2}{yy'} \left( 5 - 8 \frac{(y+y')^2}{|\vec{x} - \nu\vec{x}' + 2|\lambda|\hat{e}_\perp|^2} \right) + \frac{3(y+y')^4}{y^2y'^2} \right]. \tag{C16}$$

We are now in a position to compute the various asymptotic limits of interest.

(i)  $z, z' \rightarrow \infty, |\vec{x} - \vec{x}'|$  fixed: This limit is easily evaluated; we find for  $d \neq 4$

$$\Gamma_{12}(\vec{x}, \vec{x}') \rightarrow \frac{\Gamma(\frac{1}{2}d-1)}{4\pi^{d/2}} \left( \frac{1}{|\vec{x} - \vec{x}'|^{d-2}} - \frac{1}{(z+z')^2} \frac{1}{|\vec{x} - \vec{x}'|^{d-4}} \frac{12}{d-4} \right), \quad d > 4 \tag{C17}$$

$$\Gamma_{12}(\vec{x}, \vec{x}') \rightarrow \frac{\Gamma(\frac{1}{2}d-1)}{4\pi^{d/2}} \left( \frac{1}{|\vec{x} - \vec{x}'|^{d-2}} - \frac{1}{(z+z')^{d-2}} \frac{d(d+2)}{(d-4)(d-6)} \right), \quad d < 4,$$

and  $\Gamma_{11}(\vec{x}, \vec{x}') \rightarrow O(1/(z+z')^{d+4})$ . The first term in Eq. (C17) is  $\Gamma_\infty(\vec{x}, \vec{x}')$ , which equals the bulk correlation function. The second term leads to the results quoted in Eq. (7.24). When  $d=4$ ,

$$\Gamma_{12}(\vec{x}, \vec{x}') - \Gamma_\infty(\vec{x}, \vec{x}') \rightarrow -\frac{1}{4\pi^2} \frac{6}{(z+z')^2} \times \ln \frac{(z+z')^2}{|\vec{x} - \vec{x}'|^2}. \tag{C18}$$

(ii)  $|\vec{x}| \rightarrow \infty, \vec{x}' = 0$  and  $z/|\vec{x}| = \cos\theta$  fixed and non-zero: The calculation of this limit is tedious and we quote the result only. We find that the lead-

ing term of  $\Gamma_{11}(\vec{x}, \vec{0})$  equals  $\Gamma_{12}(\vec{x}, \vec{0})$  and

$$\Gamma(\vec{x}, \vec{0}) \rightarrow \frac{1}{4\pi^{d/2}} \Gamma\left(\frac{d+4}{2}\right) \frac{32}{15} \frac{|\lambda|^3(\cos\theta)^3}{|\vec{x}|^{d+1}}, \tag{C19}$$

which holds for all  $d$ . This result leads to the exponents given in Eq. (7.21).

(iii)  $|\vec{\rho}| \rightarrow \infty, z = z' = 0$ : In this limit we find that the leading terms in  $\Gamma_{11}$  and  $\Gamma_{12}$  satisfy  $\Gamma_{11} = 8\Gamma_{12}$ , and

$$\Gamma(\vec{\rho}, 0) \rightarrow \frac{\Gamma(\frac{1}{4}d+4)}{4\pi^{d/2}} \frac{48}{5} \frac{|\lambda|^6}{|\vec{\rho}|^{d+4}}, \tag{C20}$$

which is the result quoted in Eq. (7.22).

\*Supported in part by a grant from the National Science Foundation.

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