Critical phenomena in semi-infinite systems. I. ϵ expansion for positive extrapolation length

T. C. Lubensky*

Department of Physics and Laboratory for Research, in the Structure of Matter, University of Pennsylvania, Philadelphia, Pennsylvania 19174

Morton H. Rubin

Department of Physics, University of Maryland, Baltimore County, Baltimore, Maryland 21228

(Received 5 August 1974)

The Wilson-Fisher ϵ expansion is used to calculate critical exponents to first order in $\epsilon = 4 - d$ for n-dimensional classical spins on a semi-infinite lattice with surface exchange such that the extrapolation length is positive. It is found that to first order in ϵ, all surface exponents can be calculated from bulk exponents and a single surface exponent, $\tilde{\eta} = (1/2)\epsilon(n+2)/(n+8)$, describing the rate at which bulk correlation functions are approached when all coordinates are far from the surface. The exponents $\eta_\perp$ and $\eta_\parallel$ introduced by Binder and Hohenberg are, respectively, $1 - \tilde{\eta}$ and $2(1-\tilde{\eta})$. A form for the fixed-point spin correlation valid for all dimensions containing only the exponents η and $\tilde{\eta}$ is proposed. With this form, all critical exponents for a semi-infinite system can be obtained from η, ν, and $\tilde{\eta}$ if scaling is assumed.

I. INTRODUCTION

There has recently been a great deal of interest in the effects of surfaces on magnetic phase transitions.[1–20] Most of the theoretical tools developed to study phase transitions in bulk systems have been applied to system with surfaces, including mean-field theories,[1–5] high-temperature expansions,[4–7] low-temperature expansions,[8,9] Monte Carlo analyses,[5,10] scaling analyses,[4,5,11–13] and exact solutions in the cases of the two-dimensional Ising model[14–16] and a spherical model.[17,18] To date, only one definitive experiment[19] on surface ordering has been presented, but there is hope that other experiments will be performed shortly.

In a recent letter,[20] the authors reported the application of the highly successful Wilson renormalization procedure[21–24] to the calculation of critical exponents in semi-infinite Ising systems. In this and a following paper,[25] the ϵ expansion[22,24] is applied to a semi-infinite lattice of n-component classical spins. The system is allowed to have a different exchange between spins on the surface layer than between other pairs of neighboring spins. In the mean field, this model allows for the possibility of the surface ordering before the bulk if the exchange on the surface is greater than some critical value.[1,3] At this value of the surface exchange, the extrapolation length λ becomes infinite; below it is positive, and above it is negative. This paper, which is the first in a series of three, deals only with positive extrapolation length. The second paper treats the mean-field theory of phase transitions in semi-infinite systems with emphasis on the particularly rich behavior when $\lambda^{-1} \leq 0$. Finally, the third paper will consider the ϵ expansion for $\lambda^{-1} \leq 0$.

The renormalization-group transformation used to obtain the ϵ expansion consists of a removal of high-wave-number degrees of freedom followed by a scale transformation. The scale transformation involves a spin or wave-function renormalization in addition to the change of length scale. In semi-infinite systems, the spin renormalization is nonlocal, i.e., the spins at successive iterations of the renormalization transformation are related by an integral over a nonlocal kernel. With this nonlocal spin renormalization, the relevant parameters in the Hamiltonian are renormalized exactly as in bulk systems. Hence, all information about the surface in semi-infinite systems is contained in the spin renormalization. This means that all surface critical exponents can be obtained by scaling from bulk exponents and any exponents contained in the spin correlation function $\Gamma^*(\vec{x}, \vec{x}')$ at the critical point. In this paper we calculate $\Gamma^*(\vec{x}, \vec{x}')$ to first order in $\epsilon = 4 - d$. We find one new surface exponent, which we call $\tilde{\eta}$, which describes the rate of approach to the asymptotic correlation function characteristic of infinite systems as the coordinates $\vec{x}$ and $\vec{x}'$ go into the bulk. The exponents $\eta_\perp$ and $\eta_\parallel$ introduced by Binder and Hohenberg[4] are simply related to $\tilde{\eta}$ to first order in ϵ: $\eta_\perp = 1 - \tilde{\eta}$ and $\eta_\parallel = 2 - 2\tilde{\eta}$. $\tilde{\eta}$ also gives the asymptotic angular dependence of Γ when $\vec{x}$ is fixed near the surface and $\vec{x}'$ goes into the bulk. The existence of a single surface exponent is consistent with scaling theories[4,5,11–13] which we show imply that $\eta_\parallel = 2\eta_\perp - \eta$, where η is the bulk exponent. In Sec. IV, we suggest a form for $\Gamma^*(\vec{x}, \vec{x}')$ which will yield this relation for arbitrary η.

This paper is divided into four sections of which the introduction is the first. In Sec. II we develop the model Hamiltonian and introduce the extrapolation length. In Sec. III we outline the renormalization procedure with emphasis on the special feature of the semi-infinite lattice: the nonlocal spin renormalization. In Sec. IV we calculate the exponents $\bar{\eta}$, $\eta_\perp$, and $\eta_\parallel$, and using scaling relations, we calculate a variety of surface exponents.

II. MODEL

Our calculations will be based on a continuous spin model on a semi-infinite d-dimensional simple cubic lattice with lattice sites $\vec{x}=(\vec{\rho}, z)$, where $z>0$ is the coordinate perpendicular to the surface and $\vec{\rho}$ is the $(d-1)$-dimensional coordinate parallel to the surface. The surface is located at $z=0$. For simplicity, we take the lattice spacing to be unity. Following Wilson,[22,24] we associate with each n-dimensional spin $\vec{s}(\vec{x})=[s_j(\vec{x})]$, $j=1,2,\ldots,n$, a statistical weighting function

$$P(\vec{s}(\vec{x}))=e^{-|\vec{s}(\vec{x})|^2/2-\tilde{u}|\vec{s}(\vec{x})|^4}, \tag{2.1}$$

with $\tilde{u}>0$. The Hamiltonian we consider is the standard Heisenberg Hamiltonian with nearest-neighbor exchange

$$H=-\tfrac{1}{2}J\sum_{\vec{x},\vec{\delta}}\vec{s}(\vec{x})\cdot\vec{s}(\vec{x}+\vec{\delta}) -\tfrac{1}{2}J\Delta_s\sum_{\vec{x},\vec{\delta}_\parallel}\vec{s}(\vec{x})\cdot\vec{s}(\vec{x}+\vec{\delta}_\parallel)\delta_{z0}, \tag{2.2}$$

where δ_{z0} is the Kronecker delta, $\vec{\delta}=(\vec{\delta}_\parallel, \delta_\perp)$ is a nearest-neighbor vector (of unit length), J is the exchange in the bulk, and $J(1+\Delta_s)$ is the exchange on the surface. $\vec{\delta}$ takes on both positive and negative values except on the surface layer where $\delta_\perp$ is either $+1$ or zero. Δ_s can be positive or negative and measures the degree of enhancement or depression of the exchange in the surface layer.

The partition function for this system is

$$\tilde{z}=\mathrm{Tr}\prod_{\vec{x}}P(\vec{s}(\vec{x}))\,e^{-H/T}\equiv \mathrm{Tr}\,e^{-\tilde{\mathcal{H}}(\vec{s}(\vec{x}))}, \tag{2.3}$$

where T is the temperature and Tr denotes an integration over all spin variables $s_j(\vec{x})$. $\tilde{\mathcal{H}}$ is the reduced Hamiltonian

$$\tilde{\mathcal{H}}=\sum_{\vec{x}}[\tfrac{1}{2}|\vec{s}(\vec{x})|^2+\tilde{u}|\vec{s}(\vec{x})|^4]+\frac{H}{T}, \tag{2.4}$$

which is conveniently divided into a Gaussian or quadratic part

$$\tilde{\mathcal{H}}_0=\frac{1}{2}\sum_{\vec{x}}|\vec{s}(\vec{x})|^2-\tfrac{1}{2}K\sum_{\vec{x}\vec{\delta}}\vec{s}(\vec{x})\cdot\vec{s}(\vec{x}+\vec{\delta}) -\tfrac{1}{2}K\Delta_s\sum_{\vec{x}\vec{\delta}_\parallel}\vec{s}(\vec{x})\cdot\vec{s}(\vec{x}+\vec{\delta}_\parallel)\delta_{z0}, \tag{2.5}$$

where $K=J/T$, and an interaction term

$$\tilde{\mathcal{H}}_1=\tilde{u}\sum_{\vec{x}}|\vec{s}(\vec{x})|^4. \tag{2.6}$$

In order to cast the above Hamiltonian into a form susceptible to treatment by the ϵ expansion, it is necessary to transform from coordinate spin variable to momentumlike spin variables. This is achieved by performing a Fourier transformation to variables which diagonalize $\tilde{\mathcal{H}}_0$. In Appendix A, we show that the functions

$$\psi_{\vec{q}}(\vec{x})=\sqrt{2}\,e^{i\vec{p}\cdot\vec{\rho}}\sin(kz+\varphi), \tag{2.7}$$

where $\vec{q}=(\vec{p}, k)$ and

$$\tan\varphi=\sin k\Big/\Big(\cos k-\Delta_s\sum_{\vec{\delta}_\parallel}\cos\vec{p}\cdot\vec{\delta}_\parallel\Big) \tag{2.8}$$

form an orthonormal basis when $2(d-1)\Delta_s<1$ which diagonalizes $\tilde{\mathcal{H}}_0$. In particular, if we expand $\vec{s}(\vec{x})$ in terms of $\psi_{\vec{q}}(\vec{x})$,

$$\vec{s}(\vec{x})=\frac{1}{\sqrt{K}}\int_{\vec{q}}\vec{\sigma}(\vec{q})\psi_{\vec{q}}(\vec{x}), \tag{2.9}$$

where

$$\int_{\vec{q}}=\int_{-\pi}^{\pi}\frac{d^dq}{(2\pi)^d},$$

then

$$\tilde{\mathcal{H}}_0=\frac{1}{2}\int_{\vec{q}}\vec{\sigma}(\vec{q})\cdot\vec{\sigma}(-\nu\vec{q})\Big(r_0+\sum_{\vec{\delta}}(1-\cos\vec{q}\cdot\vec{\delta})\Big), \tag{2.10}$$

where $\nu\vec{q}=(\vec{\rho}, -k)$, $r_0=2d[(T-T_0)/T_0]$, and $T_0=2dJ$ is the mean-field transition temperature. Since $\vec{s}(\vec{x})$ is real, we must have $\vec{\sigma}^*(\vec{q})=\vec{\sigma}(-\nu\vec{q})$, and since the integral over k in Eq. (2.9) is symmetric, we may take $\vec{\sigma}(\vec{q})=-\vec{\sigma}(\nu\vec{q})$.

When $2(d-1)\Delta_s$ is greater than unity, there is an additional surface "bound state" in the Gaussian Hamiltonian. This can lead to ordering of the surface before the bulk and will be discussed in the following paper. Note that in the long wavelength limit, the phase φ reduces to

$$\tan\varphi\sim\varphi=k\lambda, \tag{2.11}$$

where

$$\lambda=[1-2(d-1)\Delta_s]^{-1} \tag{2.12}$$

is the extrapolation length introduced by Mills[1] when $d=3$. The appearance of the bound state in the Gaussian Hamiltonian occurs when the extrapolation length goes from $+\infty$ to $-\infty$. In this paper we will restrict ourselves to $\lambda>0$. When the surface exchange equals the bulk exchange, $\lambda=1$; i.e., the extrapolation length is equal to the lattice spacing.

We now express $\tilde{\mathcal{H}}_1$ in terms of $\vec{\sigma}(\vec{q})$,

$$\tilde{\mathcal{H}}_1=u_0\int[\vec{\sigma}(\vec{q}_1)\cdot\vec{\sigma}(\vec{q}_2)\,\vec{\sigma}(\vec{q}_3)\cdot\vec{\sigma}(\vec{q}_4) \times\delta^d(\vec{q}_1,\vec{q}_2,\vec{q}_3,\vec{q}_4)]+R(\vec{q}_1,\vec{q}_2,\vec{q}_3,\vec{q}_4), \tag{2.13}$$

where $u_0 = \tilde{u}/K^2$ and

$$\delta^d(\vec{q}_1, \vec{q}_2, \vec{q}_3, \vec{q}_4) = (2\pi)^{d-1}\delta^{d-1}(\vec{p}_1 + \vec{p}_2 + \vec{p}_3 + \vec{p}_4)\Delta(k_1, k_2, k_3, k_4), \tag{2.14}$$

where

$$\Delta(k_1, k_2, k_3, k_4) = \frac{\pi}{4}\sum \epsilon_1\epsilon_2\epsilon_3\epsilon_4\delta(\epsilon_1 k_1 + \epsilon_2 k_2 + \epsilon_3 k_3 + \epsilon_4 k_4) \times \cos(\epsilon_1\varphi_1 + \epsilon_2\varphi_2 + \epsilon_3\varphi_3 + \epsilon_4\varphi_4), \tag{2.15}$$

where $\epsilon_i = \pm 1$ and the sum is over all 16 combinations of ϵ. $R(\vec{q}_1, \vec{q}_2, \vec{q}_3, \vec{q}_4)$ is a complicated function which is evaluated in Appendix B. It contains only irrelevant potentials and will, therefore, not be included in our model Hamiltonian below.

Critical properties are expected to depend only on long-wavelength fluctuations and not on details of short-wavelength terms in the Hamiltonian or on the detailed shape of the Brillouin zone. For convenience, we, therefore, restrict $\vec{q}$ to be in a domain D_Λ which is a cylinder of radius Λ and height of 2Λ. Λ is a cutoff parameter which we choose to satisfy $\Lambda \le \min(1, \lambda^{-1})$. In this case, $\sum_{\vec{\delta}}(1 - \cos\vec{q}\cdot\vec{\delta})$ can be replaced by q^2, and because of Eq. (2.11), $\cos(\epsilon_1\varphi_1 + \epsilon_2\varphi_2 + \epsilon_3\varphi_3 + \epsilon_4\varphi_4)$ can be replaced by unity. Our model reduced Hamiltonian on which subsequent calculations will be based is then

$$\mathcal{H} = \frac{1}{2}\int_{\vec{q}\in D_\Lambda}(r_0 + q^2)\vec{\sigma}(\vec{q})\cdot\vec{\sigma}(-\nu\vec{q}) \times u_0\int_{\vec{q}_1,\ldots,\vec{q}_4\in D_\Lambda}\vec{\sigma}(\vec{q}_1)\cdot\vec{\sigma}(\vec{q}_2)\vec{\sigma}(\vec{q}_3)\cdot\vec{\sigma}(\vec{q}_4) \times\delta^d(\vec{q}_1, \vec{q}_2, \vec{q}_3, \vec{q}_4), \tag{2.16}$$

where $\delta^d(\vec{q}_1, \vec{q}_2, \vec{q}_3, \vec{q}_4)$ is given by Eq. (2.15) without the cosine factor. A final comment on Eq. (2.16) is in order. We can define the region D_Λ only for some fixed value of λ^{-1}. If λ^{-1} is allowed to go to zero, D_Λ must shrink to zero. Thus the renormalization calculations in this paper are not intended to treat the cross over from $\lambda^{-1} = 0^+$ to $\lambda^{-1} = 0^-$. This will be treated in Papers II and III.

The extrapolation length λ is a number which is determined by the strength of the surface interaction, Δ_s, in the initial Hamiltonian. It appears in the wave functions $\psi_{\vec{q}}(\vec{x})$ but not in the model Hamiltonian Eq. (2.15) except via the cutoff Λ. It is, thus, unaffected by any renormalizations which will be applied to $\mathcal{H}$ and only resurfaces with its initial value when spatial correlation functions are calculated from momentum correlation functions. λ appears in scaling theories[12,19] via the requirement that the magnetization $M(z, t)$ at reduced temperature t vanish at $z = -\lambda$,

$$M(z, t) = |t|^\beta f[(z+\lambda)/\xi(t)], \tag{2.17}$$

where $\xi(t) = \xi_0|t|^{-\nu}$ is the correlation length and

$$f(w) \to \begin{cases} 0 & \text{as } w \to 0^+ \\ 1 & \text{as } w \to \infty \end{cases}. \tag{2.18}$$

The second condition ensures that the bulk magnetization is regained as $z \to \infty$. The surface magnetization $m_1(t)$ is then

$$m_1(t) = |t|^\beta f[\lambda/\xi(t)] \sim |t|^{\beta_1}, \tag{2.19}$$

where β_1 is the surface magnetization critical exponent. $f(w)$ can either be analytic or nonanalytic for small w. In the first case,

$$m_1(t) \sim |t|^\beta \lambda\xi^{-1} f'(0) \sim |t|^{\beta_1} \tag{2.20}$$

and λ must diverge as $|t|^{\beta_1 - \beta - \nu}$ near $|t| = 0$. This is the form suggested by Fisher.[12] Alternatively, $f(w) \sim w$ for small w, and

$$m_1(t) \sim |t|^{\beta + \sigma\nu}\lambda^\sigma. \tag{2.21}$$

In this case, originally suggested by Wolfram *et al.*,[19] λ remains constant and $\beta_1 = \beta + \sigma\nu$. The latter description is more compatible with the renormalization group analysis presented here. σ is tabulated in Table I.

III. ε EXPANSION

A. Renormalization procedure

The renormalization-group transformation R_b is defined by

$$R_b = R_b^s R_b^i, \tag{3.1}$$

where R_b^i is an integration over intermediate wavevectors and R_b^s is a change of scale. The operation R_b^i consists of writing $\vec{\sigma}(\vec{q}) = \vec{\sigma}^<(\vec{q}) + \vec{\sigma}^>(\vec{q})$, where

$$\vec{\sigma}^<(\vec{q}) = \begin{cases} \vec{\sigma}(\vec{q}), & \vec{q}\in D_{b^{-1}\Lambda} \\ 0, & \vec{q}\notin D_{b^{-1}\Lambda} \end{cases} \tag{3.2}$$

where b is a number greater than unity. $\vec{\sigma}^>(\vec{q})$ is now eliminated by evaluating the trace in the partition function over degrees of freedom $\vec{q}\notin D_{b^{-1}\Lambda}$. This yields a new Hamiltonian which is a function of $\vec{\sigma}^<(\vec{q})$. The operation R_b^s consists of a nonlocal renormalization of $\vec{\sigma}^<(\vec{q})$ followed by a change of scale $\vec{q}\to b\vec{q}$. The spin renormalization is defined by

$$\vec{\sigma}^<(\vec{q}) = \int_{\vec{q}'}^{<}\zeta(\vec{q}, \vec{q}')\vec{\sigma}'(b\vec{q}'), \tag{3.3}$$

where $\int_{\vec{q}'}^{<}$ signifies an integral over $\vec{q}'\in D_{b^{-1}\Lambda}$. This operation yields a Hamiltonian which is a function of $\vec{\sigma}'(b\vec{q})$. Finally, the change of scale yields a Hamiltonian which is a function of $\vec{\sigma}'(\vec{q})$ with $\vec{q}\in D_\Lambda$.

The only difference between this problem and the bulk problem is the form of the spin renormalization. In the bulk case, the renormalization is local, i.e., $\zeta(\vec{q}, \vec{q}') = \zeta(2\pi)^d\delta^d(\vec{q} - \vec{q}')$; and the calculated value of ζ yields the exponent η since the cor-

TABLE I. Critical exponents.

	ϵ expansion	MF[a]	3D Ising	3D Heisenberg	2D Ising	Spherical $d=3$	Spherical $d=4-\epsilon$
$\eta_\perp$	$\left(1-\frac{n+2}{2(n+8)}\epsilon\right)$[b]	1	0.64[c]		$\frac{5}{8}$[c]	1[d]	1[d]
$\eta_\parallel$	$2\left(1-\frac{n+2}{2(n+8)}\epsilon\right)$[b]	2	<1[c] 0.8		1[e]	2[d]	2[d]
γ_1	$\left(\frac{1}{2}+\frac{n+2}{2(n+8)}\epsilon\right)$[c]	$\frac{1}{2}$	7/8[f]		$\frac{11}{8}$[c]	1[g]	$\frac{1}{2-\epsilon}$[h]
$\gamma_{1,1}$	$\left(-\frac{1}{2}+\frac{n+2}{4(n+8)}\epsilon\right)$[c]	$-\frac{1}{2}$	<0.1[i] >−0.1		$o(\log)$[e]	−1[g]	$-\frac{1}{2-\epsilon}$[h]
β_1	$\left(1-\frac{3}{2(n+8)}\epsilon\right)$[c]	1	2/3[f]	0.75[j]	$\frac{1}{2}$[e]	3/2[g]	$\frac{4-\epsilon}{2(2-\epsilon)}$[c]
Δ_1	$\left(\frac{1}{2}+\frac{n-4}{4(n+8)}\epsilon\right)$[c]	$\frac{1}{2}$	<0.79[c] >0.67		$\frac{1}{2}$[c]	1/2[c]	1/2[c]
σ	$\left(1-\frac{n+2}{2(n+8)}\epsilon\right)$[c]	1	0.51[c]		$\frac{3}{8}$[c]	1[c]	1[c]

[a]From Refs. 1–5 and 19.
[b]Calculated in this paper from ϵ expansion.
[c]Obtained by scaling relation from calculated quantities.
[d]Exact calculation, Ref. 18.
[e]Exact calculation, Ref. 14.
[f]Series extrapolation, Refs. 4 and 5. All quantities have an error of ± 0.1.
[g]Exact calculation, Ref. 17.
[h]Exact calculation, reported in Ref. 13, but details unpublished.
[i]Series extrapolation, Ref. 4 and scaling Ref. 5.
[j]Monte Carlo, Ref. 5 and low T, Ref. 9.

relation function

$$\delta_{ij}\Gamma(\vec{q},\vec{q}\,') = \langle\sigma_i(\vec{q})\sigma_j(\vec{q}\,')\rangle \qquad (3.4)$$

must satisfy the scaling equation

$$\Gamma^*(\vec{q},\vec{q}\,') = \zeta^2\Gamma^*(b\vec{q}, b\vec{q}\,') \qquad (3.5)$$

at the fixed point. This is possible if and only if $\Gamma^*(\vec{q},\vec{q}\,')\sim q^{2-\eta}\delta(\vec{q}+\vec{q}\,')$ and $\zeta = b^{(d+2-\eta)/2}$. In the semi-infinite case, the equation analogous to (3.5) is

$$\Gamma^*(\vec{q},\vec{q}\,') = \int_{\vec{Q}}^{<}\int_{\vec{Q}'}^{<} \zeta(\vec{q},\vec{Q})\zeta(\vec{q}\,',\vec{Q}')\Gamma^*(b\vec{Q}, b\vec{Q}') \,. \qquad (3.6)$$

The task of this paper is to find a function $\Gamma^*(\vec{q},\vec{q}\,')$ which satisfies (3.6) for the calculated form of $\zeta(\vec{q},\vec{q}\,')$. $\Gamma^*(\vec{q},\vec{q}\,')$ will then give the exponents characterizing spin correlation functions at the critical point in the semi-infinite system.

B. Transformation R_b^i

To obtain $\hat{\mathcal{H}} = R_b^i\mathcal{H}$, it is convenient to introduce the symbol $\mathrm{Tr}_>$ signifying an integral over all $\sigma_i^>(\vec{q})$. $\hat{\mathcal{H}}[\vec{\sigma}^<]$ is then defined via

$$e^{-(\hat{\mathcal{H}}+\hat{C})} \equiv \mathrm{Tr}_> e^{-(\mathcal{H}_0+\mathcal{H}_1)} \,, \qquad (3.7)$$

where $\hat{C}$ is a constant independent of $\vec{\sigma}^<$. Equation (3.7) can be expanded for small values of u,

$$e^{-(\hat{\mathcal{H}}+\hat{C})} = Z^0(1 - \langle\mathcal{H}_1\rangle + \tfrac{1}{2}\langle\mathcal{H}_1^2\rangle + \cdots) \,, \qquad (3.8)$$

where $Z^0 = Z^0(\vec{\sigma}^<) = \mathrm{Tr}_> e^{-\mathcal{H}_0}$, and $\langle\hat{A}\rangle = (Z^0)^{-1}\mathrm{Tr}_> e^{-\mathcal{H}_0}A$ for any operator A. $\hat{\mathcal{H}}$ can then be expressed in the form

$$\hat{\mathcal{H}} = \frac{1}{2}\int_{\vec{q}}^{<}\int_{\vec{q}'}^{<} \hat{V}_2(\vec{q},\vec{q}\,')\vec{\sigma}^<(\vec{q})\cdot\vec{\sigma}^<(\vec{q}\,') + \int_{\vec{q}_1}^{<}\int_{\vec{q}_2}^{<}\int_{\vec{q}_3}^{<}\int_{\vec{q}_4}^{<} \hat{V}_4(\vec{q}_1,\vec{q}_2,\vec{q}_3,\vec{q}_4) \times\vec{\sigma}^<(q_1)\cdot\vec{\sigma}^<(\vec{q}_2)\vec{\sigma}^<(q_3)\cdot\vec{\sigma}^<(\vec{q}_4) \,. \qquad (3.9)$$

Higher-order terms in $\vec{\sigma}^<$ have been omitted in Eq. (3.9) because their associated potentials are irrelevant. $\hat{V}_2$ and $\hat{V}_4$ are potentials which contain nonlocal parts. We evaluate these to lowest order in u (we use r and u rather than r_0 and u_0 to distinguish between the initial Hamiltonian and the one obtained after one or more applications of R_b), using the diagrams in Fig. 1,

$$\hat{V}_2(\vec{q}_1,\vec{q}_2) = (2\pi)^d(r+q^2)\delta(\vec{q}_1+\nu\vec{q}_2) + \hat{V}_2^{(1)}(\vec{q}_1,\vec{q}_2) \,, \qquad (3.10)$$

where from Fig. 1(a),

$$\hat{V}_2^{(1)}(\vec{q}_1,\vec{q}_2) = 4u(n+2)\int_{\vec{q}}^{>} \frac{1}{q^2+r}\delta^d(\vec{q}_1,\vec{q}_2,\vec{q},-\nu\vec{q}) \,, \qquad (3.11)$$

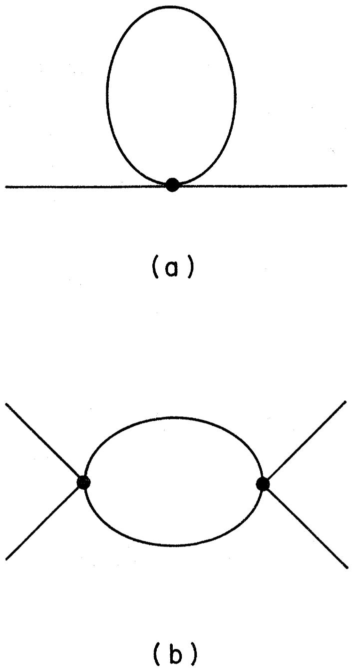

FIG. 1. (a) First-order graph used to calculate the nonlocal spin renormalization. (b) Second-order graph for the quartic potential.

where $\int_{\vec{q}}^{>}$ signifies an integral over $\vec{q}\in D_{b^{-1}\Lambda}$ and where the superscript (1) refers to the order in u. This can be decomposed into a local and a nonlocal part using Eq. (2.15),

$$\hat{V}_2^{(1)}(\vec{q}_1,\vec{q}_2)=(2\pi)^d 4u(n+2)C_1(r)\times\delta^d(\vec{q}_1+\nu\vec{q}_2)-X_2^{(1)}(\vec{q}_1,\vec{q}_2)\,, \qquad (3.12)$$

where

$$X_2^{(1)}(\vec{q}_1,\vec{q}_2)=-(2\pi)^{d-1}\delta^{d-1}(\vec{p}_1+\vec{p}_2)4(n+2)u\times\int_{\vec{q}}^{>}\frac{1}{q^2+r}[2\pi\delta(k_1+k_2+2k)-2\pi\,\delta(k_1-k_2+2k)] \qquad (3.13)$$

and $C_1(r)=\int_{\vec{q}}^{>}1/(q^2+r)$. The first term in Eq. (3.12) is the local term which appears in infinite systems. $X_2^{(1)}(\vec{q}_1,\vec{q}_2)$ is a nonlocal term which results from reflections off the surface. $\hat{V}_4$ can be evaluated to lowest order in u using the diagram shown in Fig. 1(b),

$$\hat{V}_4(\vec{q}_1,\vec{q}_2,\vec{q}_3,\vec{q}_4)=u\delta^d(\vec{q}_1,\vec{q}_2,\vec{q}_3,\vec{q}_4)+\hat{V}_4^{(2)}(\vec{q}_1,\vec{q}_2,\vec{q}_3,\vec{q}_4)\,, \qquad (3.14)$$

where

$$\hat{V}_4^{(2)}(\vec{q}_1,\vec{q}_2,\vec{q}_3,\vec{q}_4)=-4(n+8)u^2\times\int_{\vec{q}}^{>}\int_{\vec{q}'}^{>}\frac{1}{q^2+r}\,\frac{1}{q'^2+r}\,\delta^d(\vec{q}_1,\vec{q}_2,\vec{q},\vec{q}')\times\delta^d(\vec{q}_3,\vec{q}_4,-\nu\vec{q},-\nu\vec{q}')\,. \qquad (3.15)$$

Again, this can be decomposed into a local and a nonlocal part

$$\hat{V}_4^{(2)}(\vec{q}_1,\vec{q}_2,\vec{q}_3,\vec{q}_4)=-4(n+8)u^2C_2\delta^d(\vec{q}_1,\vec{q}_2,\vec{q}_3,\vec{q}_4)+X_4^{(2)}(\vec{q}_1,\vec{q}_2,\vec{q}_3,\vec{q}_4)\,, \qquad (3.16)$$

where $C_2=\int_q^{>}(q^2+r)^{-2}$ and $X_4^{(2)}(\vec{q}_1,\vec{q}_2,\vec{q}_3,\vec{q}_4)$ is the nonlocal four-point potential which is evaluated in Appendix C.

The transformation R_b^i which we have just described takes us from a potential of the form of Eq. (2.16) with only local interactions to Eq. (3.9) with nonlocal interactions. Since the renormalization transformation is to be iterated many times to locate the fixed point, one might argue that the nonlocal Hamiltonian equation (3.9) should be used as the input to R_b^i in order to obtain a new Hamiltonian of the form of Eq. (3.9). We shall see, however, that the nonlocal two-point potential X_2 will be removed by the scale transformation on $\vec{\sigma}^<$. We show in Appendix C that the nonlocal four-point function X_4 is irrelevant. Hence after application of the transformation R_b^s and elimination of irrelevant variables, we end up with a Hamiltonian of the form of Eq. (2.16) with renormalized r and u which can again be transformed by R_b^i.

C. Transformation R_b^s

The relevant terms in $\mathcal{H}$ are, therefore,

$$\mathcal{H}=\frac{1}{2}\int_{\vec{q}}^{<}\{[r+4u(n+2)C_1]+q^2\}\vec{\sigma}^<(\vec{q})\cdot\vec{\sigma}^<(-\nu\vec{q})-\frac{1}{2}\int_{\vec{q}_1}^{<}\int_{\vec{q}_2}^{<}X_2^{(1)}(\vec{q}_1,\vec{q}_2)\vec{\sigma}^<(\vec{q}_1)\cdot\vec{\sigma}^<(\vec{q}_2)+[u-4(n+8)u^2C_2]\int_{\vec{q}_1,\vec{q}_2,\vec{q}_3,\vec{q}_4}^{<}\vec{\sigma}^<(\vec{q}_1)\cdot\vec{\sigma}^<(\vec{q}_2)\times\vec{\sigma}^<(\vec{q}_3)\cdot\vec{\sigma}^<(\vec{q}_4)\,\delta^d(\vec{q}_1,\vec{q}_2,\vec{q}_3,\vec{q}_4)\,. \qquad (3.17)$$

We now choose the spin renormalization operator $\zeta(\vec{q}_1,\vec{q}_2)$ to eliminate the quadratic nonlocal term $X_2^{(1)}(\vec{q}_1,\vec{q}_2)$. To first order in u,

$$\zeta(\vec{q}_1,\vec{q}_2)=\zeta\left((2\pi)^d\delta^d(\vec{q}_1-\vec{q}_2)+\frac{1}{2q_1^2}X_2^{(1)}(\vec{q}_1,-\nu\vec{q}_2)\right). \qquad (3.18)$$

Here, we have used the fact that $r\sim u\sim\epsilon=d-4$ near the fixed point. Hence Eq. (3.18) gives rise to second-order terms in Eq. (3.17) proportional to $[r+4u(n+2)C_1]X_2^{(1)}$ which must be eliminated along with second-order contributions to X_2 by second-order terms in $\zeta(\vec{q}_1,\vec{q}_2)$, and so on. In this paper, we calculate only to first order in ϵ so Eq. (3.18) suffices. The coefficient ζ is chosen so that the coefficient of q^2 in the quadratic term remains $\frac{1}{2}$ after the scale transformation $\vec{q}\to b\vec{q}$ and is the same as ζ in the bulk problem $\zeta=b^{(d+2-\eta)/2}$, where $\eta=0$ to first order in ϵ.

The Hamiltonian $\mathcal{H}'=R_b^sR_b^i\mathcal{H}$ is then

$$\mathcal{H}'[\vec{\sigma}'] = \mathcal{H}[r', u', \vec{\sigma}'] , \tag{3.19}$$

where $\mathcal{H}$ is given by Eq. (2.16), and r' and u' are related to r and u by the bulk recursion relations

$$r' = b^{2-\eta}[r + 4K_d(n+2)u(D - r\ln b)] ,$$
$$u' = b^{\epsilon-2\eta}[u - 4K_d(n+8)u^2 \ln b] , \tag{3.20}$$

where $D = K_d^{-1}C_1(0)$, $\epsilon = 4-d$, and $K_d = 2^{-(d-1)}\pi^{-d/2} \times[\Gamma(\frac{1}{2}d)]^{-1}$. These equations have the standard bulk non-Gaussian fixed point,[22,24,26] with $u^* = [1/4K_d(n+8)]\epsilon$ and $r^* = -\epsilon[(n+2)/(n+8)][D/(1-b^{-2})]$ and exponent[22,24]

$$\nu = \tfrac{1}{2} + [(n+2)/4(n+8)]\epsilon . \tag{3.21}$$

Thus, in the semi-infinite system, there is only one divergent correlation length with the same exponent as in the infinite system. Furthermore, all information about critical behavior of the surface is contained in the spin or wave-function renormalization.

D. Correlation function to order ϵ

We now look for a scaling solution to Eq. (3.6) to order ϵ. We write

$$\Gamma^*(\vec{q}, \vec{q}') = \Gamma_0^*(\vec{q}, \vec{q}') + \Gamma_1^*(\vec{q}, \vec{q}') , \tag{3.22}$$

where Γ_0 is the Gaussian solution at the critical point

$$\Gamma_0^*(\vec{q}, \vec{q}') = \frac{(2\pi)^d}{2} \frac{1}{q^2} [\delta^d(\vec{q} + \nu\vec{q}') - \delta^d(\vec{q} + \vec{q}')] \tag{3.23}$$

and Γ_1^* is of order ϵ. Substituting Eq. (3.18) and (3.22) into (3.6) gives to order ϵ,

$$\Gamma_0^*(\vec{q}, \vec{q}') + \Gamma_1^*(\vec{q}, \vec{q}') = \zeta^2\Gamma_0^*(b\vec{q}, b\vec{q}') + \zeta^2\Gamma_1^*(b\vec{q}, b\vec{q}') + \zeta^2 b^{-d-2}(1/q^2 q'^2) X_2^{*(1)}(\vec{q}, \vec{q}') , \tag{3.24}$$

where we have made use of the symmetry properties of $X^{*(1)}(\vec{q}, \vec{q}')$ as displayed in Eq. (3.13): $X_2^{*(1)}(\vec{q}, \vec{q}') = X_2^{*(1)}(\vec{q}', \vec{q}) = -X_2^{*(1)}(\vec{q}, -\nu\vec{q}')$. Now $\zeta^2\Gamma_0^*(b\vec{q}, b\vec{q}') = \Gamma_0^*(\vec{q}, \vec{q}')$, since $\zeta = b^{d/2+1}$, so we are left with

$$\Gamma_1^*(\vec{q}, \vec{q}') - b^{d+2}\Gamma_1^*(b\vec{q}, b\vec{q}') = (1/q^2 q'^2) X_2^{*(1)}(\vec{q}, \vec{q}') . \tag{3.25}$$

We may rewrite $X_2^{*(1)}(\vec{q}, \vec{q}')$ as

$$X_2^{*(1)}(\vec{q}, \vec{q}') = T_1^{(1)}(\vec{q}, \vec{q}') - T_b^{(1)}(\vec{q}, \vec{q}') \tag{3.26}$$

by writing the integral in Eq. (3.13) as an integral over D_Λ minus an integral over $D_{b^{-1}\Lambda}$, i.e., $\int_{\vec{q}}^{>} = \int_{\vec{q}} - \int_{\vec{q}}^{<}$ so

$$T_b^{(1)}(\vec{q}, \vec{q}') = -(2\pi)^{d-1}\delta^{(d-1)}(\vec{p} + \vec{p}')2(n+2)u^* \times \int_{\vec{q}_1}^{<} \frac{1}{q_1^2} [2\pi\delta(k + k' + 2k_1) - 2\pi\delta(k - k' + 2k_1)] . \tag{3.27}$$

Noting that

$$T_1^{(1)}(b\vec{q}, b\vec{q}') = T_b^{(1)}(\vec{q}, \vec{q}')b^{-2-d} ,$$

we have

$$\Gamma_1^*(\vec{q}, \vec{q}') - b^{2+d}\Gamma_1^*(b\vec{q}, b\vec{q}') = \frac{1}{q^2 q'^2} T_1^{(1)}(\vec{q}, \vec{q}') - b^{2+d} \frac{1}{(b^2q^2)(b^2q'^2)} T_1^{(1)}(b\vec{q}, b\vec{q}') ,$$

and finally,

$$\Gamma_1^*(\vec{q}, \vec{q}') = (1/q^2 q'^2) T_1^{(1)}(\vec{q}, \vec{q}') . \tag{3.28}$$

Therefore, in the limit of small q, q' we have a scaling solution.

Setting $d=4$, we have

$$\Gamma_1^*(\vec{q}, \vec{q}') = -(2\pi)^3\delta^{(3)}(\vec{p} + \vec{p}')\frac{n+2}{n+8}\epsilon t^{(1)}(k, k')\frac{1}{q^2 q'^2} , \tag{3.29}$$

$$t^{(1)}(k, k') = \int_0^\Lambda dp_1\, p_1^2\left(\frac{1}{p_1^2 + \frac{1}{4}(k+k')^2} - \frac{1}{p_1^2 + \frac{1}{4}(k-k')^2}\right) , \tag{3.30}$$

or

$$t^{(1)}(k, k') = \tfrac{1}{4}(k-k')^2 \int_0^\Lambda \frac{dp_1}{p_1^2 + \frac{1}{4}(k-k')^2} - \tfrac{1}{4}(k+k')^2 \int_0^\Lambda \frac{dp_1}{p_1^2 + \frac{1}{4}(k+k')^2} .$$

Evaluating the integrals, we find

$$t^{(1)}(k, k') = \tfrac{1}{2}(k-k')\tan^{-1} 2\Lambda/(k-k') - \tfrac{1}{2}(k+k')\tan^{-1} 2\Lambda/(k+k') , \tag{3.31}$$

which reduces to

$$t^{(1)}(k, k') = \tfrac{1}{4}\pi(|k-k'| - |k+k'|) \tag{3.32}$$

for $k, k' \ll \Lambda$. Eq. (3.29) is cutoff independent which indicates that the renormalization procedure presented here makes sense. Finally, we have

$$\Gamma_1^*(\vec{q}, \vec{q}') = (2\pi)^3\delta^3(\vec{p} + \vec{p}')\gamma_1^*(\vec{q}, \vec{q}') , \tag{3.33}$$

with

$$\gamma_1^*(\vec{q}, \vec{q}') = \frac{n+2}{n+8}\epsilon\frac{1}{q^2 q'^2} t^{(1)}(k, k') . \tag{3.34}$$

IV. CRITICAL EXPONENTS

A. Exponents from $\Gamma^*(\vec{x}, \vec{x}')$

In this section, we evaluate $\Gamma^*(\vec{x}, \vec{x}')$ to first order in ϵ. From this, we obtain the exponents $\eta_\parallel$ and $\eta_\perp$ introduced by Binder and Hohenberg[4] and an exponent $\tilde{\eta}$ describing the approach to the bulk correlation function as $z, z' \to +\infty$. To first order in ϵ, only one of these exponents is independent. In Sec. IVB, we argue that this feature should be general.

Fourier transformation of Eq. (3.22) yields

$$\Gamma^*(\vec{x}, \vec{x}') = \Gamma_0^*(\vec{x}, \vec{x}') + \Gamma_1^*(\vec{x}, \vec{x}') , \tag{4.1}$$

where $\Gamma_0^*(\vec{x}, \vec{x}')$ is the Gaussian correlation function obtained from Eq. (3.23),

$$\Gamma_0^*(\vec{x},\vec{x}')=G_d(\vec{x}-\vec{x}')-G_d(\vec{x}-\nu\vec{x}'+2\lambda\hat{e}_\perp)\ , \qquad (4.2)$$

where

$$G_d(\vec{R})=\frac{\Gamma(\frac{1}{2}d-1)}{4\pi^{(d/2)}}\frac{1}{|\vec{R}|^{d-2}}\ , \qquad (4.3)$$

where $\nu\vec{x}=(\vec{\rho},-z)$ and $\hat{e}_\perp$ is a unit vector perpendicular to the surface. [No confusion should result from the Γ function appearing in Eq. (4.3) and the correlation function Γ^* in Eq. (4.2).]

In Appendix C, we evaluate $\Gamma_1^*(\vec{x},\vec{x}')$ from Eq. (3.33) for $\Gamma_1^*(\vec{q},\vec{q}')$,

$$\Gamma_1^*(\vec{x},\vec{x}')=\frac{1}{2}\frac{n+2}{n+8}\epsilon\frac{1}{4\pi^2|\vec{x}-\vec{x}'|^2}\left(\ln\frac{|\vec{x}-\nu\vec{x}'+2\lambda\hat{e}_\perp|^2}{4(z+\lambda)(z'+\lambda)}-E_1[2\Lambda(z+\lambda)]-E_1[2\Lambda(z'+\lambda)]\right)$$
$$-\frac{1}{2}\frac{n+2}{n+8}\epsilon\frac{1}{4\pi^2|\vec{x}-\nu\vec{x}'+2\lambda\hat{e}_\perp|^2}\left(\ln\frac{|\vec{x}-\vec{x}'|^2}{4(z+\lambda)(z'+\lambda)}-E_1[2\Lambda(z+\lambda)]-E_1[2\Lambda(z'+\lambda)]\right)\ , \qquad (4.4)$$

where E_1 is the exponential integral. To obtain this equation, we have used Eq. (3.31) which includes cutoff dependence. In general, there are other unimportant cutoff-dependent terms which are discussed at the end of Appendix D. Note $\Gamma_1^*(\vec{x},\vec{x}')$ is antisymmetric under interchange of $|x-x'|$ and $|x-\nu x+2\lambda\hat{e}_\perp|$ as expected. Combining Eqs. (4.4) and (4.3) and exponentiating, we obtain

$$\Gamma^*(\vec{x},\vec{x}')=\frac{\Gamma(\frac{1}{2}d-1)}{4\pi^{d/2}}\left(\frac{1}{a(z)a(z')}\right)^{\tilde{\eta}}\left[\frac{1}{|\vec{x}-\vec{x}'|^{2-\epsilon}}\left(\frac{|\vec{x}-\nu\vec{x}'+2\lambda\hat{e}_\perp|^2}{4(z+\lambda)(z'+\lambda)}\right)^{\tilde{\eta}}-\frac{1}{|\vec{x}-\nu\vec{x}'+2\lambda\hat{e}_\perp|^{2-\epsilon}}\left(\frac{|\vec{x}-\vec{x}'|^2}{4(z+\lambda)(z'+\lambda)}\right)^{\tilde{\eta}}\right]\ , \qquad (4.5)$$

where $a(z)=\exp\{E_1[2\Lambda(z+\lambda)]\}$ and

$$\tilde{\eta}=\tfrac{1}{2}\epsilon(n+2)/(n+8)\ . \qquad (4.6)$$

Note that all cutoff dependence is incorporated into an over-all prefactor which tends to unity rapidly as z and z' go into the bulk

$$a(z)\sim\begin{cases}\dfrac{e^{2(z+\lambda)\Lambda+\gamma}}{2\Lambda(z+\lambda)} & \text{for } (z+\lambda)\Lambda\ll 1\ ,\\[2ex] \exp\left(\dfrac{1}{2\Lambda(z+\lambda)}e^{-2\Lambda(z+\lambda)}\right) & \text{for } (z+\lambda)\Lambda\gg 1\ ,\end{cases} \qquad (4.7)$$

where γ is Euler's constant. This indicates that we cannot determine the variation of the overall coefficient from the ϵ expansion when z and z' are near the surface. However, when z and z' are of order a few times λ, this coefficient becomes independent of z and Λ.

We now consider various limiting forms for $\Gamma^*(\vec{x},\vec{x}')$. To obtain these, note that $|\vec{x}-\nu\vec{x}'+2\lambda\hat{e}_\perp|^2=|\vec{x}-\vec{x}'|^2+4(z+\lambda)(z'+\lambda)$. First, consider what happens when z and z' go into the bulk with $|\vec{x}-\vec{x}'|$ large and fixed. In this case, the bulk correlation function Eq. (4.2) should be retrieved. Noting that $4(z+\lambda)(z'+\lambda)=(z+z'+2\lambda)^2-(z-z')^2$, we obtain

$$\Gamma^*(\vec{x},\vec{x}')-\Gamma_B^*(\vec{x},\vec{x}')\sim(z+z')^{-(d-2+2\tilde{\eta})}\ . \qquad (4.8)$$

Thus, the approach to the bulk value of the correlation function behaves like a power law and occurs more rapidly than in the mean-field theory. Next, allow $|x-x'|^2$ to be much greater than $4(z+\lambda)\times(z'+\lambda)$, then

$$\Gamma^*(\vec{x},\vec{x}')\sim\frac{1}{|\vec{x}-\vec{x}'|^{2-\epsilon}}\left(\frac{4(z+\lambda)(z'+\lambda)}{|\vec{x}-\vec{x}'|^2}\right)^{1-\tilde{\eta}}\ , \qquad (4.9)$$

where we have not included the (z-dependent) prefactor. Two limits of this equation are of interest. In the first, z and z' are fixed and $|\vec{\rho}-\vec{\rho}'|$ becomes large; in the second, z' is fixed and $|\vec{x}-\vec{x}'|$ becomes large. In these limits, $\Gamma^*(\vec{x},\vec{x}')$ obtains the forms introduced by Binder and Hohenberg[4]

$$\Gamma^*(\vec{x},\vec{x}')\sim\begin{cases}\dfrac{1}{|\vec{x}-\vec{x}'|^{d-2+\eta_\parallel}}, & z,z' \text{ fixed}\ ,\\[2ex] \dfrac{A(\theta)}{|\vec{x}-\vec{x}'|^{d-2+\eta_\perp}}, & z' \text{ fixed}\ ,\end{cases} \qquad (4.10)$$

where $\cos\theta=(z-z')/|\vec{x}-\vec{x}'|$ and

$$\eta_\parallel=2-2\tilde{\eta}=2-[(n+2)/(n+8)]\epsilon\ , \qquad (4.11)$$

$$\eta_\perp=1-\tilde{\eta}=1-\tfrac{1}{2}[(n+2)/(n+8)]\epsilon\ , \qquad (4.12)$$

$$A(\theta)=(\cos\theta)^{1-\tilde{\eta}}\ . \qquad (4.13)$$

B. Exponents from scaling

There are a variety of exponents describing surface critical properties which have been described by several authors.[4,5,11–13] All of these exponents can be obtained from our $\eta_\parallel$ and $\eta_\perp$ combined with scaling relations implied by simple homogeneity assumptions. If the shift exponent λ introduced by Fisher[11] is greater than unity as most evidence indicates,[5–7] the scaling from the surface free energy can be written[4,5,11,13]

$$F_s=|t|^{2-\alpha_s}f(|t|^{-\Delta}h,\ |t|^{-\Delta_1}h_1)\ , \qquad (4.14)$$

where h is the bulk magnetic field, h_1 is the magnetic field on the surface layer, α_s the surface specific-heat exponent, Δ is the bulk gap exponent, and Δ_1 is the surface gap exponent. α_s satisfies

$$\alpha_s=\alpha+\theta^{-1}\ , \qquad (4.15)$$

where α is the bulk specific-heat exponent and θ the rounding exponent.[11] If one argues[7] that the crossover from d- to $(d-1)$-dimensional critical behavior occurs when $\xi_d \sim L$, where ξ_d is the correlation length and L the finite length along one direction, one obtains $\theta^{-1}=\nu$, in which case

$$\alpha_s = \alpha + \nu \; . \tag{4.16}$$

Using Eq. (4.14), one can introduce new exponents γ_s for the surface susceptibility $\chi_s = -\partial^2 F_s/\partial h^2$; β_s for the surface magnetization $m_s = -\partial F_s/\partial h$; β_1 for the layer magnetization $m_1 = -\partial F_s/\partial h_1$; γ_1 for the layer susceptibility $\chi_1 = -\partial^2 F_s/\partial h_1 \partial h$; $\gamma_{1,1}$ for the local susceptibility $\chi_{1,1} = -\partial^2 F_s/\partial h_1^2$, etc. The exponents γ_1 and $\gamma_{1,1}$ can be obtained from the scaling relations derived by Binder and Hohenberg[4]

$$\gamma_1 = \nu(2-\eta_\perp) \; , \tag{4.17}$$

$$\gamma_{1,1} = \nu(1-\eta_\parallel) \; . \tag{4.18}$$

The second relation follows from the assumption that correlations on the surface obey scaling in a $(d-1)$-dimensional system with $\eta_s = 1+\eta_\parallel$. The values of these exponents to first order in ϵ along with other exponents that follow from scaling are listed in Table I. We also list, for comparison, the relevant exponents from: (i) mean-field (MF) theory,[1,2,4] (ii) exact calculations for two-dimensional (2D) Ising systems by McCoy and Wu,[14] (iii) exact calculations for a spherical model by Fisher and Barber[17] and by Watson,[18] and (iv) numerical calculations for the Ising and Heisenberg models in three dimensions (3D) by Binder and Hohenberg.[4,5] Note that the $n=\infty$ values obtained from the present work do not agree with exact calculations on the spherical model (e.g., $\eta_\perp$ is $1-\frac{1}{2}\epsilon$ from the $n=\infty$ limit of ϵ expansion and $\eta_\perp$ is 1 for all ϵ in the spherical model). For bulk systems the spherical and the $n=\infty$ model are equivalent in the critical region. In finite systems, the $n=\infty$ limit most likely corresponds to a spherical model in which a spherical constraint is applied individually to each layer[27] rather than to the spherical model considered by Fisher, Barber,[17] and Watson[18] in which the spherical constraint is applied to all of the spins. It is difficult to make meaningful comparison between the exponents calculated for two- and three-dimensional systems and those calculated to first order in ϵ in this paper. One can say however that the general qualitative trend of the ϵ expansion is in agreement with the lower-dimensional exponents. For example, the ϵ expansion says that $\eta_\perp$ should decrease from 1 as ϵ increases from 0. Both the numerical calculations in three dimensions ($\eta_\perp = 0.64$) and exact calculations in two dimensions ($\eta_\perp = \frac{5}{8}$) yield an $\eta_\perp$ which is less than 1. Similar considerations apply to all of the surface exponents listed in Table I.

The Barber[13] surface exponent relation

$$2\gamma_1 - \gamma_{1,1} = \gamma_s = \gamma + \nu = \gamma + \theta^{-1} \tag{4.19}$$

can be combined with the Binder-Hohenberg relations, Eqs. (4.17) and (4.18), and the bulk-scaling relation $\gamma = \nu(2-\eta)$ to obtain a useful relation for the η's,

$$\eta_\parallel = 2\eta_\perp - \eta \; . \tag{4.20}$$

This relationship is satisfied exactly by the mean-field theory, the 2D Ising model and to first order in ϵ in the ϵ expansion; and it is satisfied within estimated error in the 3D Ising model. A form for the spin correlation function which gives exponents which always satisfy this relation is

$$\Gamma^*(\vec{x},\vec{x}\,') = \frac{1}{|\vec{x}-\vec{x}\,'|^{d-2+\eta}}\left(\frac{|\vec{x}-\nu\vec{x}\,'+2\lambda\hat{e}_\perp|^2}{4(z+\lambda)(z'+\lambda)}\right)^{\tilde{\eta}} - \frac{1}{|\vec{x}-\nu\vec{x}\,'+2\lambda\hat{e}_\perp|^{d-2+\eta}}\left(\frac{|\vec{x}-\vec{x}\,'|^2}{4(z+\lambda)(z'+\lambda)}\right)^{\tilde{\eta}} . \tag{4.21}$$

This is the same form as Eq. (4.5) with $\eta = 0$ and predicts

$$\eta_\perp = 1+\eta-\tilde{\eta} \; , \tag{4.22a}$$

$$\eta_\parallel = 2+\eta-2\tilde{\eta} \; , \tag{4.22b}$$

which trivially satisfies Eq. (4.20). A calculation to second order in ϵ should verify Eq. (4.21). Such a calculation now seems feasible and is currently being considered.

ACKNOWLEDGMENTS

We are grateful to Kenneth Wilson for pointing out to us the presence of the singular terms in the potential discussed in Appendix B.

APPENDIX A

In this appendix, we will show that the functions $\psi_{\vec{q}}(\vec{x})$ defined in Eq. (2.7) form an orthonormal basis which diagonalizes the Gaussian Hamiltonian $\mathcal{H}_0$, Eq. (2.5). To show that $\psi_{\vec{q}}(\vec{x})$ diagonalizes $\mathcal{H}_0$, we note that $\delta\mathcal{H}_0/\delta s_i(\vec{x})$ is a linear operator on $s_i(\vec{x})$ which we denote by $\hat{O}$;

$$\frac{\delta\mathcal{H}_0}{\delta s_i(\vec{x})} = \begin{cases} s_i(\vec{x}) - \frac{1}{2}K\sum_{\vec{\delta}}[s_i(\vec{x}+\vec{\delta})+s_i(\vec{x}+\vec{\delta})], & z>0 \\ s_i(\vec{\rho},0) - Ks_i(\vec{\rho},1) - \frac{1}{2}K\Delta_s\sum_{\vec{\delta}}[s_i(\vec{\rho}+\vec{\delta}_\parallel,0)+s_i(\vec{\rho}-\vec{\delta}_\parallel,0)], & z=0 \end{cases}$$

$$\equiv \hat{O} s_i(\vec{x}). \tag{A1}$$

Now, consider the effect of $\hat{O}$ on $\psi_{\vec{q}}(\vec{x})$,

$$O\psi_{\vec{q}}(\vec{x}) = \begin{cases} \left(1 - K\sum_{\vec{\delta}} \cos\vec{q}\cdot\vec{\delta}\right)\psi_{\vec{q}}(\vec{x}), & z>0 \\ \left[\left(1 - K(1+\Delta_s)\sum_{\vec{\delta}_\parallel} \cos\vec{p}\cdot\vec{\delta}_\parallel - K\cos k\right) - K\sin k \cot\varphi\right]\psi_{\vec{q}}(\vec{p}, 0), & z=0. \end{cases} \tag{A2}$$

Hence

$$\hat{O}\psi_{\vec{q}}(\vec{x}) = \epsilon(\vec{q})\psi_{\vec{q}}(\vec{x}) \tag{A3}$$

for all $\vec{x}$ where

$$\epsilon(\vec{q}) = 1 - K\sum_{\vec{\delta}} \cos\vec{q}\cdot\vec{\delta} = (1-2dK) + Kq^2 + O(q^4), \tag{A4}$$

provided

$$\left(1 - K(1+\Delta_s)\sum_{\vec{\delta}_\parallel} \cos\vec{p}\cdot\vec{\delta}_\parallel - K\cos k - K\sin k\cot\varphi\right) = \epsilon(\vec{q}), \tag{A5}$$

Equation (A5) is satisfied if

$$\tan\varphi = \sin k \Big/ \left(\cos k - \Delta_s \sum_{\vec{\delta}} \cos\vec{p}\cdot\vec{\delta}_\parallel\right). \tag{A6}$$

We must now show that the functions $\psi_{\vec{q}}(\vec{x})$ form a complete orthonormal set on the semi-infinite lattice for $-\pi < q_j \le \pi$, $j = 1, 2, \ldots, d$.

1. *Orthogonality*

The orthogonality condition is

$$\sum_{\vec{x}} \psi^*_{\vec{q}}(\vec{x})\psi_{\vec{q}}(\vec{x}')$$

$$= \tfrac{1}{2}\left[(2\pi)^d \delta^d(\vec{q} - \vec{q}\,') - (2\pi)^d \delta^d(\vec{q} - \nu\vec{q}\,')\right], \tag{A7}$$

which follows from

$$\sum_{\vec{p}} e^{i(\vec{p}-\vec{p}\,')\cdot\vec{\rho}} = (2\pi)^{d-1}\delta^{d-1}(\vec{p} - \vec{p}\,') \tag{A8}$$

and

$$\sum_{z=0}^{\infty} 2\sin(kz+\varphi)\sin(k'z+\varphi') = \pi\delta(k-k') - \pi\delta(k+k'), \tag{A9}$$

where $\varphi = \varphi(k, \vec{p})$ and $\varphi' = \varphi(k', \vec{p})$ are defined through Eq. (A6). Equation (A8) is a standard result and we will not demonstrate it here. Equation (A9) requires some work so we will prove it:

$$\sum_{z=0}^{\infty} 2\sin(kz+\varphi)\sin(k'z+\varphi')$$

$$= \sum_{z=0}^{\infty} \{\cos[(k-k')z + \varphi - \varphi'] - \cos[(k+k')z + \varphi + \varphi']\}. \tag{A10}$$

Now

$$\sum_{z=0}^{\infty} \cos(\alpha z + \beta) = \lim_{L\to\infty} \mathrm{Re}\sum_{z=0}^{L} e^{i\alpha z} e^{i\beta} = \lim_{L\to\infty}\left(\cos\beta \frac{\sin\alpha\frac{1}{2}(L+1)\cos\alpha\frac{1}{2}L}{\sin\frac{1}{2}\alpha} - \sin\beta\frac{\sin\alpha\frac{1}{2}(L+1)\sin\alpha\frac{1}{2}L}{\sin\frac{1}{2}\alpha}\right)$$

$$= \lim_{L\to\infty}\left[\cos\beta\left(\frac{\sin\alpha(L+\frac{1}{2})}{2\sin\frac{1}{2}\alpha} + \frac{1}{2}\right) + \sin\beta\left(\frac{\cos\alpha(L+\frac{1}{2})}{2\sin\frac{1}{2}\alpha} - \frac{\cos\frac{1}{2}\alpha}{2\sin\frac{1}{2}\alpha}\right)\right]. \tag{A11}$$

If $\alpha \ne 0$, the limit of Eq. (A11) is

$$J(\alpha,\beta) = \tfrac{1}{2}(\cos\beta - \sin\beta\cot\tfrac{1}{2}\alpha). \tag{A12}$$

If $\alpha = 0$, the limit is

$$\pi\delta(\alpha)\cos\beta. \tag{A13}$$

Substituting these results in Eq. (A10) gives

$$\sum_{z=0}^{\infty} 2\sin(kz+\varphi)\sin(k'z+\varphi') = \pi\delta(k-k') - \pi\delta(k+k') + H(k,k'), \tag{A14}$$

where we have used the fact that $\varphi = \varphi'$ when $k = k'$ and $\varphi = -\varphi'$ when $k = -k'$ and where $H(k,k') = J(k-k', \varphi - \varphi') - J(k+k', \varphi+\varphi')$. It is not difficult to show using Eq. (A6) that H vanishes.

2. *Completeness*

The completeness relation we must prove is

$$\int_{\vec{q}} \psi_{\vec{q}}(\vec{x})\psi^*_{\vec{q}}(\vec{x}\,') = \delta_{\vec{x}\vec{x}'}, \tag{A15}$$

where $\vec{x}$ and $\vec{x}\,'$ are points on the semifinite lattice. Since

$$\int_{\vec{q}} e^{i\vec{p}\cdot(\vec{\rho}-\vec{\rho}')} = \delta_{\vec{\rho}\vec{\rho}'} , \quad \text{(A16)}$$

it remains to show that

$$\int_{-\pi}^{\pi} \frac{dk}{2\pi} 2\sin(kz+\varphi)\sin(kz'+\varphi) = \delta_{zz'} . \quad \text{(A17)}$$

Now

$$\int_{-\pi}^{\pi} \frac{dk}{2\pi} 2\sin(kz+\varphi)\sin(kz'+\varphi)$$

$$= \int_{-\pi}^{\pi} \frac{dk}{2\pi}[\cos k(z-z') - \cos(k(z+z')+2\varphi)]$$

$$= \delta_{zz'} - \mathrm{Re} I , \quad \text{(A18)}$$

$$I = \int_{-\pi}^{\pi} \frac{dk}{2\pi} e^{ik(z+z')} e^{2i\varphi} . \quad \text{(A19)}$$

From Eq. (A6), we have

$$e^{2i\varphi} = \frac{[e^{ik} - f(\vec{p})]^2}{1 - 2f(\vec{p})\cos k + f^2(\vec{p})} , \quad \text{(A20)}$$

where $f(\vec{p}) = \Delta_s \sum_{\vec{q}} \cos\vec{p}\cdot\delta_{\parallel}$. If we now introduce the change of variables $\zeta = e^{ik}$, we find

$$I = -\frac{1}{f(\vec{p})} \oint \frac{d\zeta}{2\pi i} \zeta^{z+z'} \frac{\zeta - f(\vec{p})}{\zeta - 1/f(\vec{p})} , \quad \text{(A21)}$$

where the contour is the unit circle in the complex ζ plane. Thus, we see that I vanishes provided $|f(\vec{p})| < 1$ for all $\vec{p}$. Since $|f(\vec{p})| \le 2\Delta_s(d-1)$, we have $I=0$ if $2\Delta_s(d-1)<1$. Thus for $\Delta_s < [2(d-1)]^{-1}$ we obtain Eq. (A15).

Hence, we can expand $\vec{s}(\vec{x})$ in terms of $\psi_{\vec{q}}(\vec{x})$,

$$s(\vec{x}) = G\int_{\vec{q}} \vec{\sigma}(\vec{q})\psi_{\vec{q}}(\vec{x}) . \quad \text{(A22)}$$

Inserting this into $\mathcal{H}_0$, we obtain

$$\mathcal{H}_0 = G^2 \int_{\vec{q}} \epsilon(\vec{q})\vec{\sigma}(\vec{q})\cdot\vec{\sigma}(-\nu\vec{q}) . \quad \text{(A23)}$$

If we now choose $G = K^{-1/2}$, we obtain Eqs. (2.9) and (2.10).

APPENDIX B: EVALUATION OF $R(\vec{q}_1,\vec{q}_2,\vec{q}_3,\vec{q}_4)$

To obtain Eq. (2.13), we express $\vec{s}(\vec{x})$ in terms of $\psi_{\vec{q}}(\vec{x})$ in $\tilde{\mathcal{H}}_1 = \tilde{u}\sum|\vec{s}(\vec{x})|^4$,

$$\tilde{\mathcal{H}}_1 = \frac{\tilde{u}}{K^2}\int \vec{\sigma}(\vec{q}_1)\cdot\vec{\sigma}(\vec{q}_2)\vec{\sigma}(\vec{q}_3)\cdot\vec{\sigma}(\vec{q}_4)(2\pi)^{d-1}$$

$$\times\delta(\vec{p}_1+\vec{p}_2+\vec{p}_3+\vec{p}_4)S(\vec{q}_1,\vec{q}_2,\vec{q}_3,\vec{q}_4) , \quad \text{(B1)}$$

where

$$S = 4\sum_{z\ge0}\prod_{j=1}^{4}\sin(k_jz+\varphi_j)$$

$$= 4\sum_{z\ge0}\prod_{j=1}^{4}(\sin k_jz\cos\varphi_j + \cos k_jz\sin\varphi_j) , \quad \text{(B2)}$$

where φ_j is given by Eq. (A6). Equation (B2) can be expanded term by term and evaluated. Terms involving an even number of factors of $\sin k_jz$ are all proportional to $\delta(\sum_{\epsilon_j=\pm1}\epsilon_jk_j)$ with the exception of $4\sum_{z\ge0}\prod_{j=1}^{4}\cos k_jz\sin\varphi_j$ which has an additional contribution, $2\prod_j\sin\varphi_j$. Terms involving an odd number of factors of $\sin k_jz$ can all be reduced to sums involving

$$\sum_{z\ge0}\sin\alpha z = \lim_{L\to\infty}\mathrm{Im}\sum_{z=0}^{L} e^{i\alpha z}$$

$$= \lim_{L\to\infty}\left(\tfrac{1}{2}\cot\tfrac{1}{2}\alpha - \frac{1}{2}\frac{1}{\sin\frac{1}{2}\alpha}\cot\alpha(L+\tfrac{1}{2})\right)$$

$$= \begin{cases} 0, & \alpha=0, \\ \tfrac{1}{2}\cot\tfrac{1}{2}\alpha, & \alpha\ne0, \end{cases} \quad \text{(B3)}$$

where $\alpha = \sum_{\epsilon_j=\pm1}\epsilon_jk_j$. Following the above prescription, we obtain after much tedious algebra

$$S = \frac{\pi}{4}\sum_{\epsilon_j=\pm1}\epsilon_1\epsilon_2\epsilon_3\epsilon_4\delta\left(\sum_j\epsilon_jk_j\right)\cos\left(\sum_j\epsilon_j\varphi_j\right)$$

$$+ Q(\vec{q}_1,\vec{q}_2,\vec{q}_3,\vec{q}_4) , \quad \text{(B4)}$$

where $Q = Q_1 + Q_2$ and

$$Q_1 = 2\sin\varphi_1\sin\varphi_2\sin\varphi_3\sin\varphi_4 , \quad \text{(B5a)}$$

$$Q_2 = -\frac{1}{8}\sum_{\epsilon_j=\pm1}\epsilon_1\epsilon_2\epsilon_3\epsilon_4\cot\left(\frac{1}{2}\sum_j\epsilon_jk_j\right)\sin\left(\sum_j\epsilon_j\varphi_j\right) . \quad \text{(B5b)}$$

Plugging Eq. (B4) into Eq. (B1), we obtain Eq. (2.13) with

$$R(\vec{q}_1,\vec{q}_2,\vec{q}_3,\vec{q}_4) = (2\pi)^{d-1}\delta(\vec{p}_1+\vec{p}_2+\vec{p}_3+\vec{p}_4)$$

$$\times Q(q_1,q_2,q_3,q_4) . \quad \text{(B6)}$$

If $\Delta_s=0$ ($\lambda=1$), we have $\varphi_j=k_j$. We can then easily evaluate Q_2 using $\cot\frac{1}{2}\theta = (1+\cos\theta)/\sin\theta$:

$$\frac{1}{8}\sum_{\epsilon_j}\epsilon_1\epsilon_2\epsilon_3\epsilon_4\cot\frac{1}{2}\left(\sum_j\epsilon_jk_j\right)\sin\sum_j\epsilon_jk_j$$

$$= \frac{1}{8}\sum_{\epsilon_j}\epsilon_1\epsilon_2\epsilon_3\epsilon_4\cos\left(\sum_j\epsilon_jk_j\right) = 2\prod_j\sin\varphi_j . \quad \text{(B7)}$$

Therefore, $Q=0$ when $\Delta_s=0$ in agreement with the treatment in Ref. 20. If $\Delta_s\ne0$, we need to determine whether or not Q can lead to any relevant potentials. From Eq. (A6), we have

$$\sin\varphi_j = \frac{\sin k_j}{(1-2\cos k_jf_j+f_j^2)^{1/2}} , \quad \text{(B8)}$$

where $f_j = \Delta_s\sum_{\delta_{\parallel}}\cos\vec{p}\cdot\vec{\delta}_{\parallel}$. If $\lambda<\infty$, we expand Q for $k\lambda\ll1$ and $p\ll1$. Equation (B8) yields

$$\varphi_j = k_j\lambda[1 - \tfrac{1}{6}k_j^2(1-3\lambda+2\lambda^2) - \Delta_sp^2\lambda] . \quad \text{(B9)}$$

Using this in Eq. (B5), we obtain

$$Q=\tfrac{2}{15}k_1k_2k_3k_4(1-10\lambda^2+9\lambda^4)+\frac{\lambda}{24}\sum_{\epsilon_j=\pm1}\epsilon_1\epsilon_2\epsilon_3\epsilon_4\left(\sum_i\epsilon_ik_i[k_i^2(1-3\lambda+2\lambda^2)+6\lambda\Delta_sp_i^2+O(q^4)]\Big/\sum\epsilon_ik_i\right). \quad (B10)$$

This reduces to zero when $\lambda=1$ as required. The second term has a singularity at $\sum\epsilon_ik_i=0$. It is, however, integrable and less singular than a δ function. Let W_1 and W_2 be the potentials arising, respectively, from the first and second term of Eq. (B10). Then under renormalization, we have

$$W_1'\sim b^{-4d}\zeta^4b^{d-1}b^{-4}W_1=b^{-1-d}W_1\ ,$$
$$W_2'\sim b^{-4d}\zeta^4b^{d-1}b^{-2}W_2=b^{1-d}W_1\ . \quad (B11)$$

Thus both W_1 and W_2 are irrelevant and can be ignored. When $\lambda=\infty$, $f_i=1-\Delta_sp_i^2+O(p_i^4)$ and

$$\sin\varphi_i=(k_i/|k_i|)[1+O(q^2)]\ . \quad (B12)$$

Then we have

$$Q_1=2k_1k_2k_3k_4/|k_1k_2k_3k_4|\ . \quad (B13)$$

Q_2 is much more complicated. It is possible to show after much tedious algebra that Q_2 contains terms of the form of Eq. (B13) and singular terms

$$Q_2\sim A\frac{k_1k_2k_3k_4}{|k_1k_2k_3k_4|}+\sum_{\epsilon_j}\frac{B(\vec q_1,\vec q_2,\vec q_3,\vec q_4)}{|k_1k_2k_3k_4|(\sum\epsilon_ik_i)}\ , \quad (B14)$$

where B is of order q^5. There are *no* terms of the form $|k_1k_2k_3k_4|^{-1}(\sum_i\epsilon_ik_i)^{-1}p_l^2k_m$. Therefore, all terms in Q_1 and Q_2 are of order unity and the potential W, resulting from Q, is irrelevant above three dimensions

$$W'\sim b^{-4d}\zeta^4b^{d-1}W=b^{3-d}W\ . \quad (B15)$$

This result will be useful in the third paper in this series.

APPENDIX C: EVALUATION OF DIAGRAM 1(b)

In this appendix, we will evaluate the contribution to diagram 1(b) to the recursion relation for $\hat V_4$. In particular, we will show that $X_4^{(2)}$ is irrelevant.

$$V_4(\vec q_1,\vec q_2,\vec q_3,\vec q_4)=-4(n+8)u^2\int_{\vec q_5}^{>}\int_{\vec q_6}^{>}\frac{1}{q_5^2+r}\frac{1}{q_6^2+r}\delta^d(\vec q_1,\vec q_2,\vec q_5,\vec q_6)\delta^d(-\nu\vec q_5,-\nu\vec q_6,\vec q_3,\vec q_4)\ , \quad (C1)$$

where

$$\delta^d(\vec q_1,\vec q_2,\vec q_5,\vec q_6)\delta^d(-\nu\vec q_5,-\nu\vec q_6,\vec q_3,\vec q_4)=(2\pi)^{2(d-1)}\delta^{d-1}(\vec p_1+\vec p_2+\vec p_5+\vec p_6)\delta^{d-1}(-\vec p_5-\vec p_6+\vec p_3+\vec p_4)\Delta(k_1,k_2,k_5,k_6)\times\Delta(k_5,k_6,k_3,k_4) \quad (C2)$$

and

$$\Delta^2\equiv\Delta(k_1,k_2,k_5,k_6,)\Delta(k_5,k_6,k_3,k_4)=\left(\frac{\pi}{4}\right)^2\sum\epsilon_1\epsilon_2\epsilon_5\epsilon_6\epsilon_5'\epsilon_6'\epsilon_3\epsilon_4\delta(\epsilon_1k_1+\epsilon_2k_2+\epsilon_5k_5+\epsilon_6k_6)\delta(\epsilon_5'k_5+\epsilon_6'k_6+\epsilon_3k_3+\epsilon_4k_4)\ , \quad (C3)$$

where as usual, we have taken $|k|\lambda\ll1$. This sum can be decomposed into four parts:

$$\text{(i)}\ \epsilon_5'=-\epsilon_5;\ \ \epsilon_6'=-\epsilon_6,\quad \text{(ii)}\ \epsilon_5'=\epsilon_5;\ \ \epsilon_6'=\epsilon_6,\quad \text{(iii)}\ \epsilon_5'=-\epsilon_5;\ \ \epsilon_6'=\epsilon_6,\quad \text{(iv)}\ \epsilon_5'=\epsilon_5;\ \ \epsilon'_6=-\epsilon_6\ . \quad (C4)$$

Hence,

$$\Delta^2=2\left(\frac{\pi}{4}\right)^2\sum\epsilon_1\epsilon_2\epsilon_3\epsilon_4\delta(\epsilon_1k_1+\epsilon_2k_2+\epsilon_3k_3+\epsilon_4k_4)\delta(\epsilon_5k_5+\epsilon_6k_6-\epsilon_3k_3-\epsilon_4k_4)$$
$$-\left(\frac{\pi}{4}\right)^2\sum\epsilon_1\epsilon_2\epsilon_3\epsilon_4\delta(\epsilon_1k_1+\epsilon_2k_2+\epsilon_3k_3+\epsilon_4k_4+2\epsilon_6k_6)\delta(-\epsilon_5k_5+\epsilon_6k_6+\epsilon_3k_3+\epsilon_4k_4)$$
$$-\left(\frac{\pi}{4}\right)^2\sum\epsilon_1\epsilon_2\epsilon_3\epsilon_4\delta(\epsilon_1k_1+\epsilon_2k_2+\epsilon_3k_3+\epsilon_4k_4+2\epsilon_6k_6)\delta(\epsilon_5k_5-\epsilon_6k_6+\epsilon_3k_3+\epsilon_4k_4)\ . \quad (C5)$$

The first term comes from parts (i) and (ii) and the last two from (iii) and (iv). In the limit that k_1, k_2, k_3 and k_4 become much smaller than k_5 and k_6, this becomes

$$\Delta^2=\Delta(k_1,k_2,k_3,k_4)\frac{\pi}{2}\sum\delta(\epsilon_5k_5+\epsilon_6k_6)-\left(\frac{\pi}{4}\right)^2\sum\epsilon_1\epsilon_2\epsilon_3\epsilon_4[\delta(2\epsilon_6k_6)\delta(-\epsilon_5k_5+\epsilon_6k_6)+2\delta(\epsilon_5k_5)\delta(\epsilon_5k_5-\epsilon_6k_6)]\ . \quad (C6)$$

The last term is zero since $\sum\epsilon_1\epsilon_2\epsilon_3\epsilon_4=0$. Combining Eqs. (C1), (C2) and (C6) we find

$$\hat{V}_4^{(2)}(\vec{q}_1,\vec{q}_2,\vec{q}_3,\vec{q}_4) = -4(n+8)u^2\delta^d(\vec{q}_1,\vec{q}_2,\vec{q}_3,\vec{q}_4)\int_{\vec{q}_5}^{>}\frac{1}{(q_5^2+r)^2} + X_4^{(2)}(\vec{q}_1,\vec{q}_2,\vec{q}_3,\vec{q}_4)\ . \tag{C7}$$

This is the result quoted in Eq. (3.16) in the text.

$X_4^{(2)}$ can be divided into two parts. The first part is preceded by a δ function in the k's [coming from the first term in Eq. (C5)]; the second term has no δ function in the k's [coming from the second and third terms of Eq. (C5)]:

$$X_4^{(2)}(\vec{q}_1,\vec{q}_2,\vec{q}_3,\vec{q}_4,) = (2\pi)^{d-1}\delta^{d-1}(\vec{p}_1+\vec{p}_2+\vec{p}_3+\vec{p}_4)\sum \epsilon_1\epsilon_2\epsilon_3\epsilon_4\delta(\epsilon_1k_1+\epsilon_2k_2+\epsilon_3k_3+\epsilon_4k_4)y^{(2)}(\vec{q}_1,\vec{q}_2,\vec{q}_3,\vec{q}_4) + (2\pi)^{d-1}\delta^{d-1}(\vec{p}_1+\vec{p}_2+\vec{p}_3+\vec{p}_4)Z^{(2)}(\vec{q}_1,\vec{q}_2,\vec{q}_3,\vec{q}_4)\ . \tag{C8}$$

$y^{(2)}(\vec{q}_1,\vec{q}_2,\vec{q}_3,\vec{q}_4)$ is proportional to a linear combination of q_1^2, q_2^2, q_3^2, and q_4^2 with coefficients that depend on k_1/p, etc., for small $\vec{q}$'s. Hence

$$y_{l+1}^{(2)} \sim b^{-3d}\zeta^4 b^{-2}y_l^{(2)} \sim b^{\epsilon-2}y_l^{(2)}\ , \tag{C9}$$

where l refers to the number of renormalization iterations. Thus $y^{(2)}$ is an irrelevant variable. $Z^{(2)}(\vec{q}_1, \vec{q}_2,\vec{q}_3,\vec{q}_4)$, is odd under $k_i \to -k_i$ for all $i=1,2,3,4$. Furthermore, it is analytic in k_i for small k. Hence

$$Z^{(2)} \sim k_1k_2k_3k_4 \tag{C10}$$

and is irrelevant just as W_1, Eq. (B11), in Appendix B is irrelevant.

APPENDIX D

In this appendix, we evaluate $\Gamma_1^*(\vec{x},\vec{x}')$. From Eq. (3.33),

$$\Gamma_1^*(\vec{x},\vec{x}') = \int_{\vec{q}}\int_{\vec{q}'}(2\pi)^3\delta^3(\vec{p}+\vec{p}')\gamma_1^*(\vec{q},\vec{q}')\psi_{\vec{q}}(\vec{x})\psi_{\vec{q}'}(\vec{x}')\ , \tag{D1}$$

where $\psi_{\vec{q}}(\vec{x})$ is defined in Eq. (2.7), and the integrals are over D_Λ. Substituting in the expression for $\gamma_1^*(\vec{q},\vec{q}')$ from Eq. (3.34) gives

$$\Gamma_1^*(\vec{x},\vec{x}') = -\frac{n+2}{n+8}\epsilon\int_0^\Lambda\frac{d^3p}{(2\pi)^3}\,e^{i\vec{p}\cdot(\vec{\rho}-\vec{\rho}')}\times\int_{-\Lambda}^{\Lambda}\frac{dk}{2\pi}\int_{-\Lambda}^{\Lambda}\frac{dk'}{2\pi}\left(\frac{1}{p^2+k^2}\,\frac{1}{p^2+k'^2}\times t^{(1)}(k,k')2\sin k(z+\lambda)\sin k'(z'+\lambda)\right). \tag{D2}$$

Using Eq. (3.29) for $t^{(1)}$ and exploiting the symmetry in k and k', we obtain after performing the angular integrations over $\vec{p}$,

$$\Gamma_1^*(\vec{x},\vec{x}') = \frac{1}{4\pi^2}\,\frac{n+2}{n+8}\epsilon\,\frac{1}{|\rho-\rho'|}A(\vec{x},\vec{x}')\ , \tag{D3}$$

where

$$A(\vec{x},\vec{x}') = \frac{1}{2\pi^2}\int_0^\Lambda dp\int_{-\Lambda}^{\Lambda}dk\int_{-\Lambda}^{\Lambda}dk'p\sin p\rho_1\,2\sin kz_1\times\sin k'z_1'\,\frac{1}{p^2+k^2}\,\frac{1}{p^2+k'^2}(k+k')\tan^{-1}\frac{2\Lambda}{k+k'}\ , \tag{D4}$$

where $\vec{\rho}_1 = |\vec{\rho}-\vec{\rho}'|$ and $z_1 = z+\lambda$. We now extend the upper limits of integration to ∞ and obtain

$$A(\vec{x},\vec{x}') = \frac{1}{4\pi^2}\mathrm{Im}\int_{-\infty}^{\infty}dp\,p\,e^{ip\rho_1}\times\int_{-\infty}^{\infty}dk\int_{-\infty}^{\infty}dk'\left(\frac{1}{p^2+k^2}\,\frac{1}{p^2+k'^2}\times(k+k')\tan^{-1}\frac{2\Lambda}{k+k'}2\sin kz_1\sin k'z_1'\right). \tag{D5}$$

The p integration can be done by closing the contour in the upper half-plane

$$A(\vec{x},\vec{x}') = \frac{1}{4\pi}P\int_{-\infty}^{\infty}dk\int_{-\infty}^{\infty}dk'\frac{k+k'}{k^2-k'^2}\tan^{-1}\frac{2\Lambda}{k+k'}\times(e^{-|k'|\rho_1}-e^{-|k|\rho_1})2\sin kz_1\sin k'z_1'$$
$$= \frac{1}{4\pi}\left(P\int_{-\infty}^{\infty}dk\int_{-\infty}^{\infty}dk'\frac{k+k'}{k^2-k'^2}\times\tan^{-1}\frac{2\Lambda}{k+k'}e^{-|k'|\rho_1}2\sin kz_1\sin k'z_1' + (z_1\to z_1')\right). \tag{D6}$$

Using the integral representation for $\tan^{-1}$

$$\tan^{-1}\frac{2\Lambda}{k+k'} = (k+k')\int_0^{2\Lambda}\frac{dx}{x^2+(k+k')^2} \tag{D7}$$

and transforming the k' integral to go from 0 to ∞, we obtain

$$A(\vec{x},\vec{x}') = \frac{1}{\pi}\left(\int_0^{2\Lambda}dx\int_0^\infty dk'\,e^{-k'\rho_1}\sin kz_1\times B(k',x,z_1) + (z_1\to z_1')\right)\ , \tag{D8}$$

where

$$B(k',x,z_1) = P\int_{-\infty}^{\infty}dk\,\frac{k+k'}{k-k'}\,\frac{1}{(k+k')^2+x^2}\sin kz_1 = \pi\,\mathrm{Re}\left(\frac{1}{ix-2k'}e^{-ik'z_1-xz_1} + \frac{2k'}{4k'^2+x^2}e^{ik'z_1}\right)\ . \tag{D9}$$

Hence, after some rearrangement, we obtain

$$A(\vec{x},\vec{x}')=\tfrac{1}{2}[J_+(\rho_1+i(z_1+z_1'),z_1)-J_+(\rho_1+i(z_1-z_1'),z_1)+J_+(\rho_1+i(z_1+z_1'),z_1')-J_+(\rho_1-i(z_1-z_1'),z_1')-J_+(\rho-i(z_1+z_1'),0)+J_-(\rho-i(z_1+z_1'),0)]\ , \qquad \text{(D10)}$$

where

$$J_\pm(\eta,z)=\mathrm{Re}\int_0^{2\Lambda}dx\int_0^\infty dk'\,e^{-xz}\frac{e^{-k'\eta}}{x\pm 2ik'}\equiv\pm\frac{1}{2i}\int_0^{2\Lambda}dx\,e^{-x(z\mp\eta/2i)}E_1\left(\pm\frac{x\eta}{2i}\right)\ , \qquad \text{(D11)}$$

where E_1 is the exponential integral.[28] The integral in Eq. (D11) has been evaluated[29]

$$J_\pm(\eta,z)=\frac{1}{\eta\mp 2iz}\left[\ln\frac{\pm\eta}{2iz}+e^{-2\Lambda(z\mp\eta/2i)}\times E_1\left(\pm\frac{\Lambda\eta}{2i}\right)-E_1(2\Lambda z)\right]\ . \qquad \text{(D12)}$$

We are interested in the limit $|\vec{x}-\vec{x}'|\to\infty$. In this case $|\eta|\Lambda\gg 1$ for all η's appearing in Eq. (D10), and we have

$$J_\pm(\eta,z)\sim\frac{1}{\eta\mp 2iz}\left(\ln\frac{\pm\eta}{2iz}-E_1(2\Lambda z)\right)\ . \qquad \text{(D13)}$$

Therefore, from Eqs. (D3), (D10), and (D13), we have

$$\Gamma_1^*(\vec{x},\vec{x}')=\frac{1}{4\pi^2}\frac{1}{2}\frac{n+2}{n+8}\,\epsilon\left[\frac{1}{|\vec{x}-\vec{x}'|^2}\left(\ln\frac{|\vec{x}-\nu\vec{x}'+2\lambda\hat{e}_\perp|^2}{4(z+\lambda)(z'+\lambda)}-E_1[2\Lambda(z+\lambda)]-E_1[2\Lambda(z'+\lambda)]\right)-\frac{1}{|\vec{x}-\nu\vec{x}'+2\lambda\hat{e}_\perp|^2}\left(\ln\frac{|\vec{x}-\vec{x}'|^2}{4(z+\lambda)(z'+\lambda)}-E_1[2\Lambda(z+\lambda)]-E_1[2\Lambda(z'+\lambda)]\right)\right]\ . \qquad \text{(D14)}$$

We have kept the cutoff dependence coming from $\tan^{-1}[2\Lambda/(k+k')]$ because it leads to cutoff-dependent corrections for small z and z' but large $|\vec{\rho}-\vec{\rho}'|$ as discussed in Sec. IV. There are other cutoff-dependent terms arising from the finite upper limit to the integrals in Eq. (D4). These corrections oscillate at large $|\vec{x}-\vec{x}'|$ and presumably become unimportant as $\Lambda|\vec{x}-\vec{x}'|$ become large. We have not verified this point in detail. We note however that troubles arise even in the Gaussian problem if Λ is allowed to have a value other than π. If $\Lambda=\pi$, the correct asymptotic form for the spin correlation length is obtained. For $\Lambda<\pi$, however, there are terms which behave like

$$\frac{1}{(z-z')^2}\cos\Lambda(z-z')-\frac{1}{(z+z'+2\lambda)^2}\cos\Lambda(z+z'+2\lambda)$$

as $|\vec{x}-\vec{x}'|$ tends to infinity perpendicular to these surfaces. These terms die off less rapidly than the correct solution and are clearly unphysical.

---

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

[1]D. L. Mills, Phys. Rev. B 3, 3887 (1971).

[2]M. I. Kaganov and A. M. Omelyanchouk, Zh. Eksp. Teor. Fiz. 61, 1679 (1971) [Sov. Phys.-JETP 34, 895 (1972)]; M. I. Kaganov, *ibid.* 62, 1196 (1972) [*ibid.* 35, 631 (1972)].

[3]M. T. Béal-Monod, Pradeep Kumar, and H. Suhl, Solid State Commun. 11, 855 (1972); R. A. Weiner, M. T. Béal-Monod, and D. L. Mills, Phys. Rev. B 7, 3399 (1973).

[4]K. Binder and P. C. Hohenberg, Phys. Rev. B 6, 3461 (1972).

[5]K. Binder and P. C. Hohenberg, Phys. Rev. B 9, 2194 (1974).

[6]G. A. T. Allan, Phys. Rev. B 1, 352 (1970).

[7]D. S. Ritchie and M. E. Fisher, Phys. Rev. B 7, 480 (1973).

[8]K. Binder, Phys. Rev. Lett. A 30, 273 (1969); H. Müller-Krumbhaar and K. Binder, Z. Phys. 254, 269 (1972).

[9]M. N. Barber, J. Phys. C 6, L262 (1973).

[10]K. Binder, Physica (Utr.) 62, 508 (1972), and references therein.

[11]M. E. Fisher, in *Critical Phenomena*, edited by M. S. Green (Academic, New York, 1971), p. 1 ff.

[12]M. E. Fisher, J. Vac. Sci. Technol. 10, 665 (1973).

[13]M. N. Barber, Phys. Rev. B 8, 407 (1973).

[14]B. M. McCoy and T. T. Wu, Phys. Rev. 162, 436 (1967).

[15]M. E. Fisher and A. E. Ferdinand, Phys. Rev. Lett. 19, 169 (1967); A. E. Ferdinand and M. E. Fisher, Phys. Rev. 185, 832 (1969).

[16]H. Au-Yang, J. Math. Phys. 14, 937 (1973).

[17]M. E. Fisher and M. N. Barber, Phys. Rev. Lett. 28, 1516 (1972); Ann. Phys. (N.Y.) 77, 1 (1973); and M. N. Barber, J. Stat. Phys. 10, 59 (1974).

[18]P. G. Watson, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and M. S. Green (Academic, New York, 1972), Vol. II, p. 101 ff.

[19]T. Wolfram, R. E. DeWames, W. F. Hall, and P. W. Palmberg, Surf. Sci. 28, 45 (1971).

[20]T. C. Lubensky and Morton H. Rubin, Phys. Rev. Lett. 31, 1469 (1973).

[21]K. G. Wilson, Phys. Rev. B 4, 3174 (1971); 4, 3184 (1971).

[22]K. G. Wilson and J. Kogut, Phys. Rept. 12, 75 (1974).

[23]S. Ma, Rev. Mod. Phys. 45, 589 (1973).

[24]K. G. Wilson and M. E. Fisher, Phys. Rev. Lett. 28, 240 (1972).

[25]T. C. Lubensky and Morton H. Rubin (unpublished).

[26]Γ^* depends on the shape of the Brillouin zone. The value quoted here is thus slightly different from that usually quoted for a spherical zone.

[27]The first terms in a high-temperature series indicate that the system with $n=\infty$ and the system with constraints on each layer are equivalent and distinct from the system with the spin constraint applied to the entire sys-

tem. A. B. Harris (private communication).

[28]We use the convention for the exponential integral found in *Handbook of Mathematical Functions*, edited by Milton Abramowitz and Irene A. Stegun (U. S. GPO, Washington, D.C., 1965).

[29]I. S. Gradshteyn and I. M. Ryzhik, *Tables of Integrals, Series and Products* (Academic, New York, 1965), No. 5.221.