PHYSICAL REVIEW B VOLUME 32, NUMBER 1 1 JULY 1985

First-order transitions breaking O(n) symmetry: Finite-size scaling

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(Received 2 January 1985)

The finite-size rounding of a first-order transition is studied in systems representable as n-vector ferromagnets, so that O(n) symmetry ($n \geq 2$) is broken at the bulk transition point. Both "block," $V=L^d$, and "cylinder," $L^{d-1}\times\infty$, geometries are considered for general dimensionality d. Explicit expressions are obtained for the scaling functions describing the rounded transitions and the crossover in shape. Spin-wave effects are shown to be of relative order $1/L^{d-2}$, and are calculated in detail in the block case. For $n=3$ (and $d=3$) this provides an extension of Néel's phenomenological theory of superparamagnetism. The analysis for cylinders involves the formulation of a "degeneracy kernel" to describe the asymptotic rounding of first-order transitions and establishes a general relation between the helicity modulus (or "spin-wave stiffness" or "superfluid density") and the transfer operator spectrum. The relationship to finite-size scaling in the critical region is examined with emphasis on the extra scaling combination, $Vt^{2-\alpha}$, that is needed for $d>d_>=4$. All the results found can be checked in the limit $n\to\infty$ against exact results for spherical models (described elsewhere).

I. INTRODUCTION

In a system with short-range interactions and at most one infinite linear dimension, all thermodynamic phase transitions are rounded off and occur smoothly: the free energy and correlation functions vary analytically with temperature and external fields, and all symmetries of the Hamiltonian are fully respected. However, when the finite dimensions of the system grow without bound, the rounded transition becomes increasingly sharp and, in the full bulk limit, a true phase transition, with nonanalyticities in the free energy, etc., is attained. If the transition is of first order, one (or more) of the symmetries of the Hamiltonian may be spontaneously broken. The aim of finite-size scaling theory is to describe this crossover from analyticity to singularity asymptotically for large length scales, L, and to determine how far it may be described by appropriately scaling thermodynamic and correlation parameters by powers of the linear dimensions, L. The development of the theory to describe critical phenomena in finite systems is now familiar;[1,2] the current status has been reviewed by Barber.[3]

More recently, attention has turned to *first-order transitions*. The present authors[4] (in work to be referred to as I) laid out a systematic and detailed scaling theory of the rounding of first-order transitions in systems with no special symmetries, which can thus be regarded as possessing a single, scalar or ($n=1$)-component order parameter, and thence can most conveniently be pictured as ferromagnetic Ising models. The treatment yields explicit expressions for the scaling functions, of appropriately scaled field variables, for systems shaped both like "blocks" and like "cylinders" (in which one "long" dimension may become indefinitely large). It also describes the crossover between the differing behavior arising in these two limits. The work thus extends an earlier scaling treatment[5] (see also Binder and co-workers[6,7]) and various approaches by other authors.[8–13]

On the other hand, for systems displaying a continuous symmetry which is broken by a first-order transition, only restricted results seem available in the literature.[13–15] Prominent examples in which an O(n) symmetry with $n\geq 2$ is broken are XY-like ($n=2$) and Heisenberg-like ($n=3$) ferromagnets, and superfluids and superconductors ($n=2$) where, however, the appropriate conjugate ordering field is, unfortunately, not physically accessible. Our aim in this paper (denoted as II) is to treat systems of this sort systematically from a scaling viewpoint: as such, this article constitutes a logical continuation of I.[16] However, our presentation will be quite self-contained and, indeed, because of the complications induced by the presence of a continuous symmetry, much of the analysis follows a rather different course. More concretely, we analyze systems which can be represented as ferromagnets composed of n-component spins of fixed length situated on the sites of a d-dimensional lattice and coupled through magnetically isotropic, short-range interactions. It will be convenient, accordingly, to employ "magnetic" language in deriving and describing the results. Both block and cylinder geometries will be considered for general n, including the limit $n=\infty$. We will show that Néel's phenomenological theory of superparamagnetism provides (for $n=3$) the correct leading-order scaling result for block systems in sufficiently small fields: but higher-order corrections can also be determined explicitly. An outline of the contents of the paper follows: a more explicit technical summary is presented in Sec. VII.

In Sec. II the phenomenological scaling theory of the first-order transition is developed following the postulates of I (and Ref. 5) for systems of block (or rectangular) shape with *periodic boundary conditions*. Explicit expressions for the corresponding scaling functions for free energy, magnetization, and susceptibility are derived. The formulas simplify in the asymptotic limit $n\to\infty$ and may then be checked against exact results for general spherical models derived in III (to be published separately).[17]

In the bulk limit it is now well known that the free energy, magnetization, etc. of an isotropic $O(n)$ system ($n \geq 2$) display singularities *as* the first-order transition is approached.[18–22] These arise directly from the spin-wave excitations or, in other language, from the Goldstone modes associated with the broken $O(n)$ symmetry.[18–22] Further, these same fluctuations serve, in a system with short-range interactions, to destroy long-range order and spontaneous magnetization at nonzero temperatures, T, whenever $d \leq 2$.[23] As a result, there is no first-order transition at $T > 0$ for $d \leq 2$. For these reasons all our considerations are restricted to $d > 2$. In a finite system the spin-wave singularities, like the first-order jump in the bulk magnetization, must be rounded off. However, spin waves do not figure in the first-order finite-size scaling formulation expounded in Sec. II (except partially and in disguised fashion through their contribution to the spontaneous magnetization). This poses a problem which has no analog in the Ising-like ($n = 1$) case. To study the issue we recapitulate, in Sec. III, the phenomenological theory[21,22] of the correlations and fluctuations in an ordered system with broken $O(n)$ symmetry. This leads naturally to a concern with the *helicity modulus*, $\Upsilon(T)$ (that is, the "spin-wave stiffness" or, for a superfluid, the superfluid density). On this basis one can see how the spin-wave contributions scale in a finite system and, furthermore, one can elucidate the interference between the rounded spin-wave and first-order singularities. A unified scaling formulation embodies both effects, the spin-wave terms appearing as "corrections to scaling."

The crossover in shape to long cylinders (with periodic boundary conditions) involves a new, longitudinal length scale, $\xi_{\parallel}(T,A)$, which must be identified and calculated. [In I the analogous length for the case $n = 1$ turned out to be related to the interfacial tension, $\Sigma(T)$.] Some pertinent results for this longitudinal correlation length have been described previously.[24–26] We approach the problem in Sec. IV by a novel technique for estimating the largest eigenvalues of the transfer operator (or "matrix") which builds up the system along the cylinder axis. This entails constructing a "degeneracy kernel" which describes the fluctuations of the system on the longest length scales and thus asymptotically mimics the behavior of the full transfer operator. In this way we derive a general formula relating $\xi_{\parallel}(T)$ to the helicity modulus, $\Upsilon(T)$, of any $O(n)$ systems.[24]

Section V develops this approach to describe the leading first-order scaling behavior in the limit of an infinite cylinder. The result entails solving a one-dimensional quantum-mechanical ground-state problem: for $n = 2$ one obtains Mathieu's equation; for $n \to \infty$ a more explicit result can be obtained which checks precisely against the exact results for spherical models found in III.[17] The two-variable scaling function describing the crossover from block to cylinder shape can be expressed in terms of the full set of eigenvalues of the quantum problem.

A first-order transition line quite typically ends in a critical point. Finite-size scaling of the critical behavior *per se* must match the finite-size scaling of the first-order transition as the critical point is approached. The consequences of this matching are discussed in Sec. VI with particular emphasis on the modifications of simple finite-size scaling in the critical region needed for $d > 4$ to account properly for the first-order behavior. Finally, for the convenience of readers, the main findings are summarized and referenced by location in the text in Sec. VII. Some unresolved problems are also mentioned.

II. SCALING FORMS AND ROUNDING FOR BLOCK GEOMETRY

A finite-size "block" lattice geometry is conveniently defined[4] by requiring that a sample of, say, rectangular shape specified by edges of lengths $L_1 \equiv L_{\parallel}, L_2, \ldots, L_d$ retains its proportions in the thermodynamic limit in the sense that while the volume

$$V = \prod_{i=1}^{d} L_i \equiv L_0^d \,,$$

diverges, all the shape ratios $l_j = L_j / L_0 \equiv L_j / V^{1/d}$ approach bounded, nonzero limits. A crossover to a "cylinder" shape, with, possibly, one fully infinite dimension, will then be contemplated by letting $L_1 \equiv L_{\parallel}$ diverge before or more rapidly than $A^{1/(d-1)}$ when the cross-sectional area

$$A = \prod_{i=2}^{d} L_i \equiv L_{\perp}^{d-1} = V / L_{\parallel} \,,$$

becomes infinite while the cross-sectional ratios, $L_i / L_{\perp}$ ($i = 2, \ldots, d$), approach positive constants.

For definiteness we will consider classical n-component spin variables, $\mathbf{s}_i \equiv (s_i^{\lambda})_{\lambda=1,\ldots,n}$, of *unit length* $|\mathbf{s}| = 1$, on a hypercubic lattice of spacing a. The simplest Hamiltonian respecting spin isotropy in zero field has nearest-neighbor ferromagnetic interactions and may be written as

$$-\mathcal{H}/k_B T = K \sum_{\langle ij \rangle} \mathbf{s}_i \cdot \mathbf{s}_j + h a^d \sum_i (\boldsymbol{\sigma} \cdot \mathbf{s}_i) \,, \tag{2.1}$$

where $K \equiv J / k_B T$ is positive while the unit vector $\boldsymbol{\sigma}$ ($|\boldsymbol{\sigma}| = 1$) specifies the direction of the external field,

$$\mathbf{H} \equiv H \boldsymbol{\sigma} \equiv k_B T h \boldsymbol{\sigma} \,.$$

When convenient, we will regard H as a real variable which can take negative as well as positive values. Most of our considerations will apply much more generally to models exhibiting a normal n-vector ferromagnetic bulk first-order transition when $H \to 0$ with $0 < T < T_c$. However, we will assume periodic *boundary conditions* in all directions, unless specified otherwise: different boundary conditions involving free surfaces, boundary fields, etc. may lead to further complications, such as extra scaling variables, nonscaling shifts in the effective location of the transition,[3] etc., which are not discussed here.

Clearly, classical spin systems precisely respecting $O(n)$ symmetry and with periodic boundary conditions represent a theoretical abstraction! But the simplifications allow us to develop (in this section) a detailed scaling theory and to derive (in Sec. III) the leading corrections due to spin-wave fluctuations. As we will demonstrate, a finite system in equilibrium below T_c essentially acts as a single, uniform domain. Physically, assemblies of weakly interacting single-domain ferromagnetic particles dispersed in a nonmagnetic matrix are well known: such systems are customarily termed *superparamagnets*. This topic was reviewed some time ago by Jacobs and Bean;[15] more recently, Stacey and Banerjee[27] have surveyed applications to geophysics; basic experimental studies of superparamagnetic phenomena continue.[28] If the particles are sufficiently small, typically of diameter less than 150 Å, subdomain formation by demagnetization and surface effects is suppressed: the particles then constitute single-domain, Heisenberg-like ($n=3$) finite-sized systems. To observe equilibrium behavior the temperature must exceed the so-called size-dependent "blocking" temperature T_b, above which the thermal fluctuations can overcome the pinning effects of various anisotropic interactions, boundary surfaces, etc. By the same token, when T exceeds T_b the O(3) symmetry becomes valid with reasonable precision. In practice, for small enough particles T_b can be reduced to a few percent of T_c and quite searching experiments can be performed.[15,28] The Néel theory[14,15] and our present study are relevant to such systems when the matrix is solid so that mechanical motion is not possible (in contrast to fluid suspensions).[15]

A. Basic scaling postulate

In our presentation of the scaling formulation for the block geometry, we follow more or less closely Ref. 4, where the scalar, $n=1$ or Ising-like case was analyzed. By considering renormalization-group flows near a discontinuity fixed point,[29,30,13] one is lead generally to the finite-size scaling ansatz[4,5]

$$f_s(H,T;L_j)\equiv F_s/k_BTV \approx A_0(T)V^{-1}W[B(T)HV;L_j/V^{1/d}] , \quad (2.2)$$

where f_s is the *singular part* of the reduced free-energy density at the bulk first-order phase transition occurring in zero field. The bulk ($V=\infty$) spontaneous magnetization, $m_0(T)$, may be defined through

$$m_s=-(\partial f_s/\partial h)_T\approx \pm m_0(T) \quad \text{as } h\to 0\pm . \quad (2.3)$$

To reproduce this, the scaling function must satisfy

$$W(y;l_j)\approx -|y| \quad \text{as } y\to\pm\infty , \quad (2.4)$$

where a convenient normalization has been adopted, which then yields

$$k_BTA_0(T)B(T)=m_0(T) . \quad (2.5)$$

Now, the longitudinal susceptibility, defined via $\chi \equiv(\partial m/\partial H)_T$, is given, for a finite system in *zero* field, by

$$\chi(H=0;L_j)=\frac{a^{2d}}{Vk_BT}\sum_i\sum_j\langle(\boldsymbol{\sigma}\cdot\mathbf{s}_i)(\boldsymbol{\sigma}\cdot\mathbf{s}_j)\rangle_{h=0} . \quad (2.6)$$

To utilize this we argue heuristically, and expect to check later, by various calculations, that the thermodynamically predominant spin configurations in a block sample *at* $H=0$ will have a uniform magnetization vector $\mathbf{m}=m_0\boldsymbol{\mu}$, where $\boldsymbol{\mu}$ is an arbitrary, that is to say, fluctuating, *unit* vector. In accepting this we implicitly adopt the usual arguments[4,14,31–33] which relate the "short long-range order" to the spontaneous magnetization in the form

$$\lim_{|\vec{R}_i-\vec{R}_j|\to\infty}\ \lim_{V\to\infty}\langle\mathbf{s}_i\cdot\mathbf{s}_j\rangle_{h=0}=m_0^2(T) . \quad (2.7)$$

One must also notice the O(n) symmetry in zero field so that in (2.6) one has

$$\langle(\boldsymbol{\sigma}\cdot\mathbf{s}_i)(\boldsymbol{\sigma}\cdot\mathbf{s}_j)\rangle=\langle s_i^\mu s_j^\mu\rangle=\frac{1}{n}\sum_{\lambda=1}^{n}\langle s_i^\lambda s_j^\lambda\rangle =\frac{1}{n}\langle\mathbf{s}_i\cdot\mathbf{s}_j\rangle . \quad (2.8)$$

Estimation of the double sum using (2.7) then yields

$$\chi(H=0;L_j)\approx m_0^2(T)V/nk_BT . \quad (2.9)$$

In assessing (2.2) and (2.9) it is important to note that we have given no account of the spin-wave (or Goldstone mode) singularities[18–22] that characterize the bulk limit of a system with a continuous ordering symmetry when the phase boundary is approached below T_c. Specifically the bulk magnetization, $m_\infty(H,T)$, as a function of the field, H, regarded as a positive or negative scalar, contains a singular piece varying as $|H|^{(d-2)/2}$ with an additional factor $\ln|H|$ when $d\ (>2)$ is an even integer. (See Refs. 18–22 and the next section). For $d\le 4$ this means that the bulk susceptibility, $\chi_\infty(H,T)$, in addition to the usual first-order contribution, $2m_0(T)\delta(H)$, has an additively superimposed divergence: specifically for $\epsilon=4-d>0$ one has

$$\chi_\infty(H,T)\approx X_\infty(T)|H|^{-\epsilon/2} \quad \text{as } H\to 0 , \quad (2.10)$$

when $T<T_c$. *All* these singularities must be rounded in a finite system and one must thus ask whether the spin-wave modes should not interfer in some way and modify the simple finite-size scaling ansatz (2.2): that ansatz was well validated in the $n=1$, scalar case,[4] but the spin-wave singularities are then absent!

The spin-wave singularities also entail a divergence of the bulk ("single-phase") correlation length, $\xi_\infty(H,T)$, as $H\to 0$. By the same token the bulk spin-spin correlations *in* the limit $H=0$ contain slowly decaying, power-law tails (see next section) which, at the very least, must result in a slower convergence of the sum in (2.6) to the asymptotic result (2.9) than in the Ising-like case. We will demonstrate, nevertheless, that corrections to (2.9) involve at most powers $V^{1-\psi}$ with $\psi>0$ and likewise that only weaker powers of V enter into corrections to (2.2). Thus let us accept (2.2) and (2.9) provisionally and proceed.

By differentiating (2.2) twice and using (2.5) and (2.9) we obtain the relation

$$A_0(T)=-nW_0''(l_j) , \quad (2.11)$$

where $W_0''(l_j)=(\partial^2W/\partial y^2)_{y=0}$. From this we may conclude that $A_0(T)$ is actually independent of T and that $W_0''(l_j)$ is independent of the shape ratios $l_j=L_j/L_0$. A further normalization of the scaling function beyond (2.3) is permitted and it is natural to set $W_0''=-1/n$ so that $A_0=1$. Thus we arrive at the final scaling form for block domains, namely[4]

$$f_s(H,T;L_j)\approx V^{-1}W(y_V)\ , \tag{2.12}$$

where, as in the Ising-like case,[4] only the natural dimensionless scaling combination

$$y_V=m_0hV\equiv H/H_V \tag{2.13}$$

enters. However, it must be realized that the scaling function depends explicitly on the symmetry of the ordered state as specified by $n\geq 2$, even though this parameter is not displayed.

B. Explicit scaling functions

If the assumption[14] that uniformly magnetized spin configurations with $\mathbf{m}\approx m_0\boldsymbol{\mu}$ predominate is accepted not only for $H=0$ but also for *small fields* in a finite system, then one may calculate $W(y_V)$ explicitly. The results will be checked in III, for $n\to\infty$, and further substantiated for general $n\geq 2$ by transfer matrix analysis in Sec. V. The assumption itself will be revisited in the next section: it evidently allows us to calculate the overall partition function, $Z(H,T;L_j)$, asymptotically for small H through

$$\frac{Z(H)}{Z(0)}\approx\zeta_n(m_0hV)\equiv\int e^{m_0hV\sigma\cdot\mu}d^{n-1}\mu\Big/\int d^{n-1}\mu\ , \tag{2.14}$$

where the integrations run over the angular coordinates specifying the unit n-vector $\boldsymbol{\mu}$. Since we have $Z\equiv\exp(-Vf)$, the ratio serves to cancel the temperature-dependent "regular part" of the free energy, $f_r\equiv f-f_s$.

The integrals in (2.14) may be evaluated explicitly with the aid of the Funk-Hecke theorem,[34] which yields

$$\begin{aligned}\zeta_n(y)&=\Gamma(\tfrac{1}{2}n)(2/y)^{(n-2)/2}I_{(1/2)n-1}(y)\\&=1+\sum_{k=1}^{\infty}\frac{\Gamma(\frac{1}{2}n)}{\Gamma(k+1)\Gamma(k+\frac{1}{2}n)}\left[\frac{y}{2}\right]^{2k}\ ,\end{aligned} \tag{2.15}$$

where $\Gamma(z)$ and $I_\nu(y)$ denote the standard gamma function and Bessel function of the imaginary argument, respectively.[34,35] In the case $n\to 1$ the previously established Ising-like result,[4,6,7] namely $\zeta_1(y)=\cosh y$, is recovered. For the Heisenberg case, $n=3$, one obtains the simple expression[14] $\zeta_3(y)=(\sinh y)/y$.

Finally, the scaling behavior of the free energy follows as

$$f(H,T;L_j)-f(0,T;L_j)\approx -V^{-1}\ln\zeta_n(m_0hV)\ , \tag{2.16}$$

while the magnetization and susceptibility become

$$m(H,T;L_j)\approx m_0(T)I_{(1/2)n}(y_V)/I_{(1/2)n-1}(y_V) \tag{2.17}$$

and

$$\chi(H,T;L_j)\approx\frac{m_0^2V}{k_BT}\left[\frac{I_{(1/2)n}(y_V)+y_VI_{(1/2)n+1}(y_V)}{y_VI_{(1/2)n-1}(y_V)}-\left[\frac{I_{(1/2)n}(y_V)}{I_{(1/2)n-1}(y_V)}\right]^2\right]\ , \tag{2.18}$$

with $y_V=H/H_V$ and $H_V=k_BT/m_0V$, in accord with (2.13). Evidently, the scaling functions, which can be read off, depend on n but are independent of shape and dimensionality (provided a first-order transition occurs, as it will for $d>2$). The behavior for small fields, i.e., $y_V\to 0$, follows with the aid of the expansion in (2.15). Thus the result (2.9) for the susceptibility in zero field is recovered. For large positive y_V one needs[34]

$$I_\mu(z)\approx e^z/(2\pi z)^{1/2}[1+\tfrac{1}{2}(\mu^2-\tfrac{1}{4})/z+\cdots]\ ,$$

from which one finds, for example,

$$m\approx m_0(T)[1-\tfrac{1}{2}(n-1)y_V^{-1}+\tfrac{1}{8}(n-1)(n-3)y_V^{-2}+\cdots]\ , \tag{2.19}$$

for $n>1$.

The only general result for $n\geq 2$ comparable to (2.16)–(2.18) that has been reported previously in the literature is the conclusion $\chi(H=0)\sim V$ for $T\ll T_c$: this has been derived by Cardy and Nightingale,[13] who considered a renormalization-group transformation of an $L_\perp^{d-1}\times L_\parallel$ cylindrical lattice down to a one-dimensional chain. (See also I and Ref. 3.) However, as mentioned earlier, the results for $n=3$ (with the tacit but harmless assumption $d=3$) are just those of Néel's theory of single-domain, superparamagnetic particles.[14,15] Our analysis thus shows that Néel's phenomenological expressions are valid for fields, $|\mathbf{H}|$, which do not greatly exceed H_V. However, when $|\mathbf{H}|\gg H_V$ the spin-wave singularities must enter (and, as usual, further analytic background contributions must also arise). The spin-wave terms and their corresponding scale, H_S, will be elucidated in the next section (for general n). It will also be seen that the effects are not confined to $|\mathbf{H}|\simeq H_S$: rather, there is an "interference" term present even for $|\mathbf{H}|\lesssim H_V$.

C. Many-component limit

It is instructive to examine the limit of our results in which $n\to\infty$: the integral representation[34]

$$\zeta_n(y)=\frac{\Gamma(\frac{1}{2}n)}{\Gamma(\frac{1}{2})\Gamma(\frac{1}{2}n-\frac{1}{2})}\int_{-1}^{1}e^{\sigma y}(1-\sigma^2)^{(n-3)/2}d\sigma \tag{2.20}$$

is then useful. For large n the method of steepest descents is appropriate, the saddle-point equation being

$$y-(n-3)\sigma/(1-\sigma^2)=0\ , \tag{2.21}$$

which is readily solved. One sees, in fact, that the magnetization, m, is equal to σ *at* the saddle point, and thence one obtains the equation of state

$$m(H,T;L_j)\approx m_0(T)Y^\infty(y_V/n)\ , \tag{2.22}$$

where the scaling function for $n\to\infty$ is simply

$$Y^\infty(\tilde{y})=2\tilde{y}/[1+(1+4\tilde{y}^2)^{1/2}]\ . \tag{2.23}$$

Expressions for the free energy, susceptibility, etc. follow by integration and differentiation. These results for large n correspond precisely with those found in the exact calculations for the spherical model reported in III when the interactions and field are properly scaled: the confirmation represents strong support for the general validity of (2.16)–(2.18).

For convenience, we record here the scaling of variables in terms of n, which yields sensible behavior in the limit $n \to \infty$ and so allows comparison to be made between results obtained here and those found for the spherical model in III. A tilde will denote an appropriately scaled parameter or function which then appears *uninflected* in III. The basic correspondences for the free energy, field, and temperature are

$$\tilde{f}(\tilde{h},\tilde{K};L_j)=n^{-1}f(h,K;L_j)\ , \tag{2.24}$$

$$\tilde{h}=h/n\ ,\quad \tilde{K}=K/n\ ,\quad \text{and } \tilde{J}=J/n\ . \tag{2.25}$$

From these one sees

$$\tilde{m}=m\ ,\quad \tilde{\chi}=n\chi\ ,\quad \text{and } \tilde{\xi}=\xi\ , \tag{2.26}$$

and, by way of example, discovers that the scaled variable $y_V=m_0hV$ goes over to

$$\tilde{y}_V=\tilde{m}_0\tilde{h}V=y_V/n\ , \tag{2.27}$$

in accord with (2.22). Other correspondences follow similarly: we mention only

$$\tilde{\Upsilon}=\Upsilon/n \tag{2.28}$$

for the helicity modulus, which is introduced in the following section.

III. SPIN-WAVE SCALING AND THE HELICITY MODULUS

The simple scaling results for an O(n)-symmetric first-order transition in finite block systems obtained in the preceding section are intuitively appealing. However, one must certainly assess the nature and magnitude of the leading corrections to be expected. The main issue, as already indicated, is to account properly for the role of the spin-wave fluctuations. (We remark, incidentally, that much less guidance from exact analytical and numerical studies is available here, and in the transfer matrix considerations below, than for $n=1$.)

According to (2.2) and (2.18) the first-order peak, $2m_0\delta(H)$, in the bulk susceptibility is rounded on the scale $H_V=(k_BT/m_0)V^{-1}$. To determine the corresponding scale, say H_S, for rounding of the spin-wave singularities, it is reasonable to accept normal scaling ideas and to suppose that deviations from bulk behavior occur when the *bulk correlation length*, $\xi_\infty(H,T)$, which directly reflects the spin waves, attains the linear system dimension, i.e., $\xi_\infty(H_S,T)\approx L_0=V^{1/d}$. Since, as we will check, $\xi_\infty(H)$ diverges when $H\to 0$ while the spin-wave fluctuations are known to be "asymptotically free" (and so governed by a Gaussian fixed point), we can hope to determine ξ_∞ and, hence, the scale H_S by purely phenomenological or "hydrodynamic" considerations. For $d=3$ most of the necessary results have appeared in the literature,[21,22] but we rederive them here in a unified way for general n and d which also serves to introduce important notation. On this basis we will investigate the way in which the rounded spin-wave and first-order singularities combine in a finite system.

A. Phenomenology for an O(n) ordered system

Following Refs. 21 and 22 we first decompose the magnetization density, $\mathbf{m}=(m_l,\mathbf{m}_t)$, into a non-negative "longitudinal" component, m_l, measured parallel to the external magnetic field or, when $\mathbf{H}\to 0$, along the axis of spontaneous order, and an orthogonal, "transverse" vectorial part, $\mathbf{m}_t$. Now, in view of the O(n) symmetry, the free energy, $f(\mathbf{H},T)$, for a finite or infinite system can depend only on

$$|\mathbf{H}|=H_l+\tfrac{1}{2}(|\mathbf{H}_t|^2/H_l)+O(|\mathbf{H}_t|^4/H_l^3)\ . \tag{3.1}$$

It follows directly[21] that the (initial) transverse susceptibility is given *exactly* by

$$\chi_t(\mathbf{H},T;L_j)=m_l(H,T;L_j)/|\mathbf{H}|\ , \tag{3.2}$$

where $|\mathbf{H}|\equiv H_l$ for $\mathbf{H}_t=0$. For low fields in the bulk limit this gives

$$\chi_t^\infty(\mathbf{H},T)\approx m_0(T)/|\mathbf{H}|\ , \tag{3.3}$$

which we will now use (dropping, in most cases, the superscript ∞).

Now if $\mathbf{m}(\vec{\mathrm{R}})$ is the coarse-grained magnetization density, the long-wavelength transverse fluctuations may be described, correct to quadratic order, by the free-energy functional[21]

$$\mathscr{F}_t[\mathbf{m}_t(\vec{\mathrm{R}})]\approx\int d^dR(\tfrac{1}{2}b_t|\nabla\mathbf{m}_t|^2+\tfrac{1}{2}\chi_t^{-1}|\mathbf{m}_t|^2)\ , \tag{3.4}$$

in which $b_t(T)$ is a phenomenological "elasticity coefficient" which measures the "spin-wave stiffness." Since χ_t^{-1} vanishes when $H\to 0$ and since the spin-wave interactions can be shown to be technically irrelevant in this limit[36–38] (the fixed point being asymptotically free), we expect this to yield exact hydrodynamic results. The longitudinal fluctuations, $\delta m_l(\vec{\mathrm{R}})$, may, at the *microscopic*, or *renormalized Hamiltonian* level, be described by a similar functional with b_l replacing b_t and a coefficient r_l in place of χ_t^{-1}. It is crucial to note, however, that such a description does *not* hold in the hydrodynamic limit: there are profound renormalization effects arising, in particular, from a coupling term proportional to $m_t^2(\vec{\mathrm{R}})m_l(\vec{\mathrm{R}})$, and thus r_l cannot be identified with $\chi_l^{-1}\equiv\chi^{-1}$.[21,22]

The correlation function,

$$G_t(\vec{\mathrm{R}})=(n-1)^{-1}\langle\mathbf{m}_t(\vec{0})\cdot\mathbf{m}_t(\vec{\mathrm{R}})\rangle\ ,$$

of the transverse fluctuations, which is what represents the spin waves most directly, follows from (3.4) in the standard way.[21] It Fourier transform at small $\vec{\mathrm{q}}$ is

$$\hat{G}_t(\vec{\mathrm{q}})=k_BT/(\chi_t^{-1}+b_tq^2)\ , \tag{3.5}$$

and reveals the characteristic spin-wave form. From this the bulk correlation length must be identified as

$$\xi_\infty(H,T)\approx[b_t(T)m_0(T)]^{1/2}/|H|^{1/2}\ , \tag{3.6}$$

which, as anticipated, diverges when $H\to 0$. This correlation length might well be termed the *transverse* correlation length. However, as we will see, the longitudinal fluctuations at long wavelengths are driven by the transverse fluctuations and, consequently, ξ_∞ also sets the scale of decay of $G_l(\vec{R})$.[19–22,38] Indeed, as $H \to 0$ (or even when $T \to T_c$) there is no other significant longitudinal correlation length that can be defined.

To substantiate these claims,[19–22,38] note that the reduced bulk free-energy density associated with the spin-wave fluctuations follows from (3.3) and (3.4) as

$$f_S(H,T) \approx \tfrac{1}{2}(n-1)\int_q \ln[(\,|H|/m_0+b_t q^2)/a^d k_B T]\ , \tag{3.7}$$

where we use the notation

$$\int_q \equiv \int \frac{d^d q}{(2\pi)^d} = \lim_{V\to\infty}\frac{1}{V}\sum_{\vec{q}}\ , \tag{3.8}$$

in which the sum runs over those discrete wave vectors compatible with periodic boundary conditions in a finite lattice: thus, a momentum cutoff of order $q_\Lambda = (\pi/a)$ is understood in all integrals on $\vec{q}$. The spin-wave contribution to the longitudinal susceptibility now follows by differentiating once with respect to H to obtain the magnetization, and a second time which yields

$$\chi_S(H,T) \approx \tfrac{1}{2}(n-1)k_B T\int_q (\,|H| + m_0 b_t q^2)^{-2}\ . \tag{3.9}$$

For $2<d\le 4$ this diverges when $H\to 0$ and then represents the dominant contribution to $\chi_\infty \equiv \chi_l^\infty$. The behavior (2.10) is generated, with $\ln|H|^{-1}$ replacing $|H|^{-\epsilon/2}$ when $d=4$; the amplitude is given quite generally by

$$X_\infty(T) = \tfrac{1}{2}(n-1)x_d k_B T/[m_0(T)b_t(T)]^{d/2}\ , \tag{3.10}$$

where x_d is a universal coefficient with $x_3 = 1/8\pi$ and $x_4 = 1/16\pi^2$. For $d>4$ the leading singularity in $\chi_\infty(H)$ is still of the form $|H|^{(d-4)/2}$, with a factor $\ln|H|$ present for $d=6,8,\ldots$, but lower-order *analytic* terms, $\chi_\infty^0 + \chi_\infty'|H| + \cdots$, arise from (3.9) combined with other contributions to χ_l.

On using (3.5), the net longitudinal correlation function corresponding to (3.9) can be identified as[22,38]

$$\hat{G}_l(\vec{q}) \approx \tfrac{1}{2}(n-1)\int_Q \hat{G}_t(\vec{q}-\vec{Q})\hat{G}_t(\vec{Q})/m_0^2(T)\ . \tag{3.11}$$

This inverts to yield

$$G_l(\vec{R}) \approx \tfrac{1}{2}(n-1)[G_t(\vec{R})/m_0(T)]^2\ , \tag{3.12}$$

which confirms the fact that ξ_∞, as given by (3.6), also describes the longitudinal fluctuations (up to a factor of 2 in the regime of exponential decay when $H>0$).

B. Relation to the helicity modulus

Before employing these results to assess the contributions of spin-wave fluctuations to finite-size behavior, it is useful to recall the relation of the coefficient $b_t(T)$ in (3.4) to an important general property of an $O(n)$ ordered state.[21] Specifically, an isotropic system with a nonvanishing spontaneous order, $m_0(T)$ (for $d>2$, $n\ge 2$), is also characterized by a *helicity modulus*, $\Upsilon(T)$, which may be defined[21] by "twisting" the orientation of the order parameter uniformly along the length of a cylinder (say by imposition of ordering fields at the ends). If $\nabla\varphi$ is the gradient of the phase of the mean order-parameter vector, whose orientation may be supposed to rotate uniformly in a plane, the incremental free energy for small gradients should vary as

$$\Delta F = \tfrac{1}{2}\Upsilon(T)(\nabla\varphi)^2 V\ . \tag{3.13}$$

This expression serves to define $\Upsilon(T)$.

A state of uniform twist corresponds to constant $|\nabla \mathbf{m}_t|/m_0 = |\nabla\varphi|$ in (3.4) with $H=0$. Thence we obtain the relation

$$\Upsilon(T) = b_t(T)m_0^2(T)\ , \tag{3.14}$$

first derived by Josephson[21,39] for a superfluid ($n=2$). In the case of a superfluid the helicity modulus is related to the superfluid density by[21] $\rho_s(T) = (m/\hbar)^2\Upsilon(T)$, where m is the helium atom mass. For magnetic systems this expression relates the helicity modulus to the "spin-wave stiffness." By combination with (3.6) we can rewrite the correlation length generally as

$$\xi_\infty(H,T) \approx |\Upsilon(T)/m_0(T)H|^{1/2}\ . \tag{3.15}$$

Likewise, the spin-wave susceptibility amplitude given in (3.10) becomes

$$X_\infty(T) = \tfrac{1}{2}(n-1)x_d k_B T[m_0(T)/\Upsilon(T)]^{d/2}\ . \tag{3.16}$$

Note also that b_t is proportional, in general, to the square of the range, R_0, of the underlying ordering forces. Thus, if $\tilde{J}_0$ is a suitable effective ordering energy, we can write

$$\Upsilon(T) = \tilde{J}_0 R_0^2/a^d\ , \tag{3.17}$$

where a is the lattice spacing (or inverse momentum cutoff). By (3.15) one sees that ξ_∞ varies as R_0, which is just as expected. Furthermore, in the long-range, Kac–van der Waals limit, $R_0\to\infty$, the amplitude X_∞ vanishes, and no spin-wave singularities appear.

We also remark that as $t=(T-T_c)/T_c \to 0$ in the critical region, the helicity modulus, Υ, vanishes as[21,39] $|t|^{2\beta-\eta\nu}$, while the field, H, should scale as $|t|^{-(\beta+\gamma)}$. From (3.15) one then finds that ξ_∞ scales as $|t|^{-\nu}$, as expected. Similarly, by (2.10) and (3.16), the spin-wave susceptibility χ_S scales as $(\,|t|^{d\nu-(2-\alpha)})|t|^{-\gamma}$: for $d\le 4$ the hyperscaling relations hold and the first factor here becomes unity so that χ_S scales like the full susceptibility; above $d=4$, however, one has $d\nu-(2-\alpha) = \tfrac{1}{2}(d-4)>0$ and, as is well known, the spin waves then contribute only *corrections* to the leading critical behavior. All these and the other features discussed above are fully confirmed in the exact solutions for the spherical model (see III).

C. Scaling the spin-wave contributions

We can return now to the issue of finite-size effects. The crossover criterion $\xi_\infty(H_S,T) \approx L_0$ yields the spin-wave scale

$$H_S = \Upsilon(T)/m_0(T)V^{2/d} \tag{3.18}$$

and corresponding putative scaling variable

$$y_S = \frac{|\mathbf{H}|}{H_S} = \frac{m_0 |\mathbf{H}| V^{2/d}}{\Upsilon(T)} = \left[\frac{L_0}{\xi_\infty} \right]^2 > 0 \ . \tag{3.19}$$

This surmise for the rounding scale of the spin-wave singularities is fully confirmed by the analysis of the spherical model in III. It is then clear that the problem involves the *field-independent* scale

$$u_L = \frac{H_V}{H_S} = \frac{y_S}{|y_V|} = \frac{k_B T}{\Upsilon L_0^{d-2}} = \frac{k_B T a^d}{\widetilde{J}_0 R_0^2 L_0^{d-2}} \ , \tag{3.20}$$

where, in the last part, we have used the form (3.17). For L_0 finite, u_L is evidently a measure of the inverse range, R_0^{-1}, which vanishes in the long-range limit; equally, however, u_L vanishes when $L_0 \to \infty$ in any field (provided, of course, one has $d > 2$, to which we are already committed). We may thus conclude that if the limits $V \to \infty$ and $H \to 0$ are taken so that $HV \to \infty$ while $HV^{2/d}$ remains bounded, one should not see the rounded first-order peak in susceptibility as H varies; rather one will see a rounded spin-wave singularity described (for $\frac{1}{2}d$ nonintegral) by a new scaling ansatz that may be written, in the first instance, as

$$\chi_S(H,T;L_j) \approx X_\infty(T) |H|^{-\epsilon/2} Z(y_S;l_j) \ , \tag{3.21}$$

where, in order to reproduce the bulk ($V \to \infty$) result (2.10), we must have $Z(y_S;l_j) \to 1$ when $y_S \to \infty$. Notice that the shape ratios $l_j = L_j / L_0$ must be allowed for. Figure 1 illustrates schematically the separation of the scales H_V and H_S. Note also that in the total susceptibility the same analytic background, $\chi_\infty^0 + \chi'_\infty |H| + \cdots$, must be

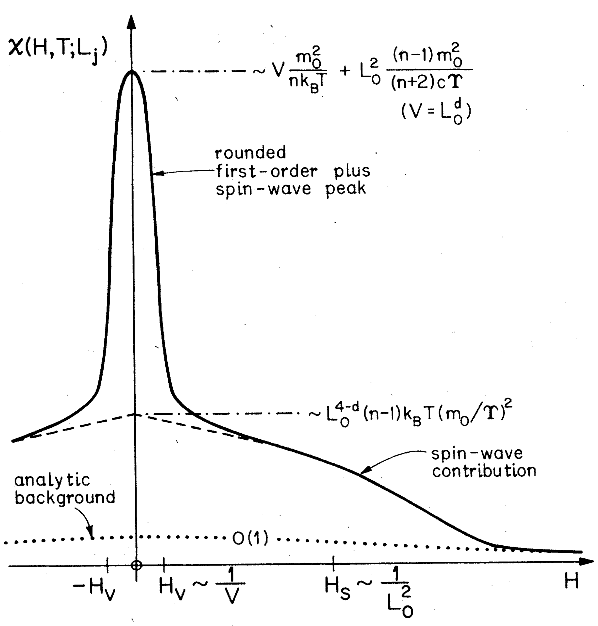

FIG. 1. Schematic plot of the susceptibility vs magnetic field in a block system of finite volume, $V = L_0^d$, for $d > 2$, showing the rounded first-order—plus—spin-wave peak, varying on the scale $H_V = k_B T / m_0 V$, and the superimposed rounded spin-wave contribution characterized by the scale $H_S = \Upsilon / m_0 L_0^2$. An inevitable analytic background, of order unity, is also indicated. The symbol c specifies a shape-dependent constant.

included as remains when $V \to \infty$.

Parallel to (3.21), the net spin-wave contribution to the magnetization must scale as

$$\Delta m_S \approx 2(d-2)^{-1} X_\infty(T) |H|^{(d-2)/2} \widetilde{Y}(y_S;l_j) \ , \tag{3.22}$$

where $\widetilde{Y} \to 1$ when $y_S \to \infty$. But on using (3.16) for X_∞ and recalling the definition (3.20) of u_L, this can be written in the simple form

$$\Delta m_S(H,T;L_j) \approx (n-1) m_0 \operatorname{sgn}(H) u_L Y_S(y_S;l_j) \ , \tag{3.23}$$

where the scaling function diverges for *large* argument as

$$Y_S(y_S) \approx (d-2)^{-1} x_d y_S^{(d-2)/2} \ . \tag{3.24}$$

Note that the scaled range parameter, u_L, appears as a simple prefactor! The corresponding form for the susceptibility, which may be compared with (2.18) and (2.9), is

$$\chi_S(H,T;L_j) \approx (n-1)(V m_0^2 / k_B T) u_L^2 X_S(y_S;l_j) \ , \tag{3.25}$$

where for large arguments

$$X_S(y_S;l_j) \approx \tfrac{1}{2} x_d y_S^{(d-4)/2} \ . \tag{3.26}$$

Note again that the cases $\frac{1}{2}d$ integral are to be excluded in the above expressions since logarithmic factors then appear: these are discussed in III for $d = 4$ when $n \to \infty$. In addition, for $d > 4$ analytic background terms will contribute significantly.

What explicit form should the scaling functions Y_S and X_S take? An answer is gained if one estimates the spin-wave corrections in a finite system for a field *outside* the first-order region $H = O(1/V)$, simply by replacing the integrals, $\int_q$, in (3.7) and (3.9) by discrete sums, $V^{-1} \sum'_{\vec{q}}$, in which the wave vectors $\vec{q} = (q_j)$ run over all the values

$$q_j = 2\pi p_j / L_j, \quad p_j = 0, \pm 1, \pm 2, \ldots, (\bmod N_j) \tag{3.27}$$

where $N_j = L_j / a$, except that $\vec{q} = 0$ is excluded. (Note that the term with $\vec{q} = 0$ corresponds to no spin-wave excitation, but rather would describe a global rotation of the uniformly magnetized state.) One discovers that the scaling forms (3.23) and (3.25) are precisely reproduced with, for $d < 4$,

$$Y_S(y_S;l_j) = D_S(l_j) + \frac{y_S}{2^5 \pi^4} \sum_{\vec{p} \neq 0} \left[\sum_{j=1}^{d} \frac{p_j^2}{l_j^2} \right]^{-1} \times \left[\frac{y_S}{4\pi^2} + \sum_{j=1}^{d} \frac{p_j^2}{l_j^2} \right]^{-1} , \tag{3.28}$$

$$X_S(y_S;l_j) = \frac{1}{2^5 \pi^4} \sum_{\vec{p} \neq 0} \left[\frac{y_S}{4\pi^2} + \sum_{j=1}^{d} \frac{p_j^2}{l_j^2} \right]^{-2} , \tag{3.29}$$

where $\vec{p}$ is an integer vector, now unrestricted in magnitude, of d components. The second expression here is straightforward to derive but the first requires some comment. Specifically, in defining the scaling part of the magnetization, we separate from the total spin-wave contribution which, even for $d < 4$, depends on the details of the cutoff, the value of m_S in the limit $y_S \ll 1$ but with $|y_V| \gg 1$, i.e., for fields, H, much less than $H_S \sim 1/L_0^2$ but much greater than $H_V \sim 1/L_0^d$. The positive coefficient $D_S(l_j) \equiv Y_S(0;l_j)$ thus depends on the asymptotic difference between the sum $\sum'_{\vec{q}}(1/q^2)$ and the corresponding integral: the analysis, which has some subtlety, is presented in an Appendix to III. The result can be written

$$8\pi^2 D_S(l_j) = \int_{-1/2}^{1/2} dx_1 \cdots \int_{-1/2}^{1/2} dx_d \, \mathscr{D}(x_k;l_j) \;, \tag{3.30}$$

$$\mathscr{D}(x_k;l_j) = \frac{1}{\sum_j (x_j/l_j)^2} - \sum_{\vec{p}\neq 0} \frac{\sum_i x_i(2p_i+x_i)/l_i^2}{\sum_j (p_j/l_j)^2 \sum_k (p_k+x_k)^2/l_k^2} \;. \tag{3.31}$$

While this is explicit, it is not very tractable numerically. However, it can be cast in other forms[17,40] and for the symmetric case $l_j=1$ (all j) when $d=3$ we quote[40] $D_S(1) \simeq 0.112\,89$. Physically this term simply represents a finite-size correction to the "spontaneous" magnetization (as observed in fields satisfying $H_V \ll |H| \ll H_S$) due to the discreteness of the spin-wave spectrum. Its sign can be understood since the spin-wave fluctuations always act to reduce the bulk spontaneous magnetization, those at long wavelength being the most effective; but these are cut off in finite systems. For $d \geq 4$ similar subtractions are needed to allow for the analytic background terms and account for the finite-size spin-wave corrections they similarly suffer. The explicit scaling functions are analytic, monotonic functions which are easily seen to satisfy (3.24) and (3.26). The coefficient x_d appears naturally through the appropriate integral which enters its original definition in (3.10).

Finally, these results for the finite-size rounding in the pure spin-wave region, $HV \to \infty$ with $HV^{2/d}$ bounded, can be checked in the spherical model limit obtained explicitly in III: with the correct scaling as $n \to \infty$, all agree precisely.

D. Spin-wave and first-order interference

Owing to the separation of the scales H_V and H_S, we were able to give an account of the rounding of the spin-wave singularities independently of the first-order contribution. However, it remains to address the more challenging question of the effect of the spin-wave fluctuations on the rounding of the first-order transition when H is of order H_V or smaller. The temptation merely to add the two contributions must be resisted since it leads to an unacceptable answer! To see this, note that in a finite system the variation of the magnetization, susceptibility, etc. must remain smooth and analytic as H passes through zero; but the scaling form (3.23) with (3.28) and (3.29) implies contributions to m and χ varying for small H like $\mathrm{sgn}(H)$ and $-|H|$, respectively, which are nonanalytic. (Here again we regard H as a scalar variable which may assume any sign.)

More generally, then, if we recall that $y_S \equiv u_L |y_V|$ we may expect the magnetization to be described by the two-variable scaling form

$$m(H,T;L_j) \approx m_0 Y(y_V,u_L;l_j) \;, \tag{3.32}$$

with, to recapitulate, $y_V = m_0 H L_0^d / k_B T$ and

$$u_L = k_B T/\Upsilon L_0^{d-2} \sim T/R_0^2 L_0^{d-2} \;.$$

When $u_L \to 0$ the spin-wave contributions drop out and the scaling function $Y(y,u;l_j)$ should reduce to

$$Y_0(y) = I_{(1/2)n}(y)/I_{(1/2)n-1}(y) \;, \tag{3.33}$$

as implied by (2.17). Evidently, T/R_0^2 acts as an irrelevant variable scaling as L_0^{d-2}, by contrast to h, which is relevant and scales as L_0^{-d}. The exponents here may be recognized as the accepted renormalization-group eigenvalues or scaling exponents, $\lambda_h = d$ and $\lambda_T = 2-d$, at a discontinuity fixed point in a system with $n \geq 2$.[13,29,30] Furthermore, our analysis here, and also in Sec. V below, indicates that $m_0 h \equiv m_0(T) H/k_B T$ and $u_L L_0^{d-2} \equiv k_B T/\Upsilon(T)$ are appropriate *nonlinear scaling fields* near the ferromagnetic phase boundary. In the opposite limit when $|y_V| \to \infty$ the pure spin-wave region should be attained, so $Y_0 \to \mathrm{sgn}(y)$ and we expect to find

$$Y(y,u;l_j) \approx \mathrm{sgn}(y)[1+(n-1)uY_S(u|y|;l_j)] \;, \tag{3.34}$$

where omitted terms should represent the onset, as H is reduced, of interference between the spin-wave and first-order contributions. Again, these plausible arguments do yield the correct results in the spherical model limit.

Some insight into the interference between spin-wave and first-order terms may be obtained by another route if we focus on $H=0$. Thus, one contribution to the deviation,

$$\Delta\chi_0(T;L_j) \equiv \chi(0,T;L_j) - m_0^2 V/nk_B T \;, \tag{3.35}$$

from the first-order scaling result (2.9), can be estimated heuristically by appealing to (3.12) and (3.5). It follows that the summand in (2.6) should, ultimately, decrease to its limit, given in terms of m_0^2 by (2.7), like $G_l(\vec{R}_{ij}) \sim 1/R_{ij}^{2(d-2)}$; at least this description should be valid for $L_0 \gg R_{ij} \gg a$. Now one sum may be performed by using translational invariance and the other can then be approximated reasonably by an integral cutoff at $R_{ij} \simeq L_0$. This yields an additive spin-wave correction to $\chi(0,T;L_j)$, proportional to

$$(n-1)k_B T(m_0/\Upsilon)^2 L_0^{4-d} = (n-1)(m_0^2 V/k_B T)u_L^2 \sim V^{\epsilon/d} \;, \tag{3.36}$$

where $\epsilon = 4-d$. (Again $\frac{1}{2}d$ must be nonintegral: for $d=4$ one finds a divergence as $\ln V$.) Note that this is just of the scaling form (3.25) if the scaling function $X_S(y_S)$ approaches a finite limit when $y_S \to 0$, as it does according to (3.29). This would, in fact, be consistent with a mere addition of the first-order and spin-wave forms, but this, as we have seen, cannot actually be quite correct.

Indeed, another source contributing to $\Delta\chi_0$ is readily identified if the significance of the term $D_S(l_j)$ in (3.28) is recalled. This represented a finite-size enhancement of the spontaneous magnetization by an amount $\Delta m_0 = (n-1)D_S m_0 u_L$. If this correction is allowed for in (2.9) in the heuristic derivation of $\Delta\chi_0$, it clearly leads to a further additive term: naively one gets

$$\Delta\chi_0^{(1)} \simeq 2D_S(n-1)(Vm_0^2/nk_BT)u_L \sim V^{2/d} . \tag{3.37}$$

This is of lower order in u_L than (3.36) and hence dominates; but it is *not* consistent with a purely additive spin-wave scaling expression (3.25) if (3.29) is accepted. Clearly, then, concrete interference effects between the spin-wave and first-order scaling behavior are to be expected. [The guess (3.37) will be confirmed up to a factor $n/(n+2)$.]

To proceed further, notice that when H approaches H_V from above in a finite system we can no longer accept the bulk result (3.3) for the transverse susceptibility, $\chi_t(\mathbf{H},T)$, which controls the spin waves. Rather it seems appropriate to use the general result (3.2) instead. This suggests that to describe the spin-wave free energy, f_S, in a finite system, we should not only discretize the momentum integral in (3.7) as above, but we should *also* replace $|H|/m_0$ by $H/m(H,T;L_j)$. We may then form an estimate for the total free energy by adding f_S to the pure first-order contribution, say f_0, as given by (2.16). Differentiating this with respect to H to obtain $m(H,T;L_j)$ evidently leads to an unpleasant implicit equation, also entailing $\chi(H,T;L_j)$, whose general validity might well be questioned. However, we have seen that the spin-wave term will be proportional to u_L which may always be regarded as small. Thus, to leading order in u_L it should suffice to replace $H/m \approx H/m_0Y(y_V,u_L)$ by $H/m_0Y_0(y_V)$ in the spin-wave free energy [see (3.7)]. Doing this leads, after some algebra, to the two-variable scaling form (3.32) with the explicit scaling function

$$Y(y_V,u_L;l_j)=Y_0(y_V)+(n-1)u_Lz'(y_V)Y_S[u_Lz(y_V)] , \tag{3.38}$$

where $z(y)=y/Y_0(y)$. This result should, if the arguments are correct, be valid to order u_L in *all* regimes (for $d<4$). It may be compared with the limiting result (3.34) to which it reduces for large y_V since, as $|y|\to\infty$, we have, from (2.19),

$$z(y)\equiv y/Y_0(y)=|y|+\tfrac{1}{2}(n-1)[1+O(y^{-1})] , \tag{3.39}$$

$$z'(y)\equiv(dz/dy)=\mathrm{sgn}(y)[1-\tfrac{1}{8}(n^2-1)/y^2+\cdots] . \tag{3.40}$$

The behavior of these two functions can be determined simply for $n\gg1$ by using (2.23), which yields

$$z(y)\approx\tfrac{1}{2}n+(y^2+\tfrac{1}{4}n^2)^{1/2} , \tag{3.41}$$

$$z'(y)\approx y/(y^2+\tfrac{1}{4}n^2)^{1/2} . \tag{3.42}$$

Evidently the replacement of y by $z(y)$ removes the spin-wave scaling function singularities for small fields since $z(y)\gtrsim n$. Similarly, $z'(y)$ acts as a cutoff factor which vanishes at $y=0$ and damps out the spin-wave contribution for fields up to $|H|\simeq H_V$. The qualitative behavior for all $n\geq2$ is very similar.

Although the arguments presented here for the effects of the spin-wave fluctuations might be characterized as "naively optimistic," they are fully adequate in the large-n limit since the form (3.38) is exactly confirmed by the spherical model calculations in III. We suspect, accordingly, that (3.38) is actually correct for all $n\geq2$.

The behavior of the susceptibility follows by a further differentiation with respect to H (or y_V). The overall scaling function, $X(y_V,u_L;l_j)\approx k_BT\chi/m_0^2V$, may be written as a sum of (i) a first-order piece, $X_0(y_V)$, following from (2.18), (ii) a pure spin-wave piece following from (3.25) and (3.29) with $y_S\equiv u_L|y_V|$, and (iii) interference term which, for $d<4$, may be written

$$\begin{aligned}\Delta X(y_V,u_L;l_j)=(n-1)u_L\{&z''(y_V)Y_S(y_Lz)\\&-u_L[1-(z')^2]X_S(y_Lz)\\&-[X_S(u_L|y_V|)-X_S(u_Lz)]\} ,\end{aligned} \tag{3.43}$$

where $z''=(d^2z/dy^2)$, $z'=z'(y_V)$, and $z=z(y_V)$. For large y_S the last term is essentially proportional to $u_LX_S'(y_S)\sim X_S/|y_V|$, where (3.26) has been invoked, while $1-(z')^2$ and z'' decay as $1/y_V^2$ and $1/|y_V|^3$, respectively. Thus all the interference terms are small. For small y_V, the dominant contribution, leading in u_L, comes from $Y_S(0;l_j)=D_S$, which was identified before as the source of the leading correction to the zero-field susceptibility. For small y_S, the corresponding interference correction to the first-order peak is thus

$$\Delta\chi^{(1)}\approx\frac{(n-1)m_0^2L_0^2}{\Upsilon(T)}D_S(l_j)z''(y_V) , \tag{3.44}$$

which, for large n, reduces to

$$\Delta\chi^{(1)}\approx\frac{m_0^2V}{nk_BT}\frac{k_BT}{\Upsilon L_0^{d-2}}\frac{2(n-1)D_S(l_j)}{[1+(2m_0HV/nk_BT)^2]^{3/2}} . \tag{3.45}$$

The field variation for finite $n\geq2$ is qualitatively very similar. In zero field, however, (3.44) yields the shift

$$\Delta\chi_0^{(1)}\approx\frac{2(n-1)m_0^2L_0^2}{(n+2)\Upsilon(T)}D_S(l_j) , \tag{3.46}$$

which differs from the naive result (3.37) by a factor of $n/(n+2)$. Note that we cannot check this factor against the spherical model results. Indeed, for the present, the validity of this and our other specific and general conjectures for $n<\infty$ must remain unchecked by a more rigorous argument.

IV. LONGITUDINAL CORRELATION LENGTH, THE TRANSFER OPERATOR, AND THE HELICITY MODULUS

Consider now the case of a long, ultimately infinitely long, $A\times L_{\parallel}$ cylinder. The order parameter, $\mathbf{m}(\vec{\mathrm{R}})$, within a long cylinder in zero field, cannot reasonably be supposed to have a uniform orientation as proved to be effectively the case in a block geometry: rather, owing to the gain in entropy available, the dominant configurations will involve relative *rotations* of the order parameter along the cylinder on a length scale, say $\xi_{\parallel}(T)$. Since $\xi_{\parallel}$ must evidently measure the spatial extent of the correlations in the orientation of $\mathbf{m}(\vec{\mathrm{R}})$, it can be identified[41] with the *longitudinal correlation length* of an infinitely long cylinder of finite cross section, A: as such it must depend sensitively on both A and T. Our aim in this section is to elucidate this dependence.

A. The degeneracy kernel

In order to find a phenomenological description of the rotational fluctuations of the order parameter in zero field on the longest length scales, let us divide up the $A\times L_{\parallel}$ cylinder into $L_{\parallel}/b$ successive *slices* or *layers* of lengthwise thickness, b, with, possibly, $b\to 0$. The magnetization $\mathbf{m}(\vec{R})$ within a slice may, since we suppose $b \ll \xi_{\parallel}$, be regarded as uniform with an (average) orientation specified by a unit vector $\boldsymbol{\mu}$. For the present the *magnitude* of this layer magnetization will not play a role, but one would presume it is close to m_0 if $L_\perp$ is not too small. Now between one layer and the next, with orientations $\boldsymbol{\mu}$ and $\boldsymbol{\mu}'$, there will, in a typical configuration, be a mismatch in orientation of phase, $\Delta\varphi$, and an associated increment in free energy, $\Delta F(\boldsymbol{\mu},\boldsymbol{\mu}')$. But by the definition (3.13) of the helicity modulus, $\Upsilon(T)$, this increment should be $\Delta F\approx\frac{1}{2}\Upsilon(\nabla\varphi)^2Ab$, where $V_b=Ab$ is the volume of a slice. Since $\cos(\Delta\varphi)=\boldsymbol{\mu}\cdot\boldsymbol{\mu}'$, we may use the discrete approximation

$$\tfrac{1}{2}(\nabla\varphi)^2\simeq\tfrac{1}{2}(\Delta\varphi/b)^2\simeq(1-\boldsymbol{\mu}\cdot\boldsymbol{\mu}')/b^2 \tag{4.1}$$

when b is not too large. Apart from an orientation-independent factor, the Boltzmann factor for the coupling of two adjacent slices in zero field thus becomes

$$\mathscr{K}_0(\boldsymbol{\mu},\boldsymbol{\mu}')=\exp\left[\frac{\Upsilon(T)A}{k_BTb}\boldsymbol{\mu}\cdot\boldsymbol{\mu}'\right]. \tag{4.2}$$

Note that this form is rotationally invariant in $\boldsymbol{\mu}$ space as it must be: clearly this dictates the dot product form of coupling.

Now it is evident that we may regard the function $\mathscr{K}_0(\boldsymbol{\mu},\boldsymbol{\mu}')$ as specifying the kernel of an *effective* transfer operator or "matrix" which can be used in the standard way to build up the n-vector cylinder slice by slice. The spectrum of this operator should, in the usual way,[4,41] provide information on the correlations and order. Since, however, the derivation has allowed only for the longest length scales associated with the buildup of long-range order and, thence, with asymptotic degeneracy in the full transfer operator spectrum, we may term $\mathscr{K}_0(\boldsymbol{\mu},\boldsymbol{\mu}')$ the *degeneracy kernel.* The limits of validity and the more precise interpretation of $\mathscr{K}_0(\boldsymbol{\mu},\boldsymbol{\mu}')$ will be discussed further below and in the following section.

Now the eigenvalues of the degeneracy kernel (4.2) are well known.[34,42] With $l=0,1,2,\dots$ one finds

$$\Lambda_l=(2\pi)^{n/2}K_A^{(2-n)/2}I_{l-1+n/2}(K_A)\ , \tag{4.3}$$

where the effective nearest-neighbor coupling is

$$K_A\equiv\Upsilon(T)A/k_BTb\ . \tag{4.4}$$

The lth eigenvalue is manyfold degenerate, the eigenfunctions being the n-dimensional hyperspherical harmonics,[34] $Y_{l\tau}(\boldsymbol{\mu})$, in which the second label is $\tau=1,\dots,g(l;n)$, the degeneracy $g(l;n)$ being given explicitly by

$$g(l;n)=\frac{(2l+n-2)(l+n-3)!}{(n-2)!\,l!}\ , \tag{4.5}$$

for $l=0,1,2,\dots$ and $n=2,3,\dots$, except for the case $l=0$, $n=2$, for which one has $g(0;2)=1$. When A/b and, hence, K_A are large, one can use the asymptotic approximation[35]

$$\ln\Lambda_l=\ln\Lambda_0(K_A;n)-\tfrac{1}{2}l(l+n-2)K_A^{-1}+O(K_A^{-2})\ , \tag{4.6}$$

where $\ln\Lambda_0$ is independent of l and thereby has no interest for us here.

B. Correlation length and helicity modulus

Now the lengthwise or longitudinal correlation length of an infinite cylinder is given, in terms of the eigenvalues as usual, by

$$\xi_{\parallel}=b/\ln(\Lambda_0/\Lambda_1)\ . \tag{4.7}$$

For $K_A\gg 1$, or as $A/b\to\infty$, we thence obtain the relation[24]

$$\xi_{\parallel}(T;A)\approx 2\Upsilon(T)A/(n-1)k_BT\ . \tag{4.8}$$

This result is the analog for $n\geq 2$ of the formula relating the interfacial or surface tension, $\Sigma(T)$, in a scalar, $n=1$ system to the transfer matrix eigenvalues.[4,41] It can be rewritten as[24]

$$\Upsilon(T)=\tfrac{1}{2}(n-1)k_BT\lim_{A\to\infty}\frac{b}{A\ln[\Lambda_0(T;A,b)/\Lambda_1(T;A,b)]}\ , \tag{4.9}$$

which is an explicit expression for the helicity modulus in terms of the largest, Λ_0, and second largest, Λ_1, eigenvalues of the transfer operator. Note that the eigenvalues depend on the slice or layer thickness, b, but the result in the limit $A\to\infty$ will not! The original derivation[24] of (4.9) for the case $n=2$ (where the spectrum and eigenfunctions of $\mathscr{K}_0$ are simple) followed a somewhat different route: see further below.

One may note that a low-temperature approximation[26] for $\xi_{\parallel}(T;A)$ when $n=2$ gives $\xi_{\parallel}\simeq 2KA/a^{d-2}$ for a $(d=3)$-dimensional simple-cubic lattice with lattice spacing a. This result does, indeed, agree with (4.8) since, by using the original definition (3.13), one easily finds $\Upsilon(0)=J/a^{d-2}$.

One knows,[21,39,43] as remarked before, that Υ vanishes quite generally as $|t|^{2\beta-\eta\nu}$ when $t=(T-T_c)/T_c\to 0$. Accordingly the longitudinal correlation length is characterized by

$$\xi_{\parallel}/A\sim(\tilde{J}_0R_0^2/a^d)\,|t|^{2\beta-\eta\nu}\ , \tag{4.10}$$

when $T\to T_c^-$, where (3.17) has been invoked. On the other hand, Brézin[25] has conjectured, on the basis of his exact calculations for the limit $n\to\infty$, that one should have $\xi_{\parallel}/A\sim|t|^{(d-2)\nu}$ as $t\to 0$. For $d\leq d_>=4$ hyperscaling relations such as $d\nu=2\beta+\gamma$ hold and Brézin's exponent agrees with (4.10); however, the conjecture is not valid for $d>4$.

In writing (4.9) we have considered only the eigenvalues of the degeneracy kernel, (4.2); but as the bulk limit is approached these should reflect accurately the *most degenerate* part of the spectrum of the full lattice transfer matrix, or kernel. (For nearest-neighbor coupling, one may simply set b equal to the lattice spacing, a; recall that the limit relating $\xi_{\parallel}$ to Υ involves $A/b \to \infty$ so b may be held fixed.) To see the limitations entailed in describing the spectrum by the degeneracy kernel, note that the successive "mass gaps" or inverse "higher" correlation lengths defined by

$$\xi_l^{-1}(T;A) \equiv b^{-1}\ln(\Lambda_0/\Lambda_l) \tag{4.11}$$

are given roughly by $l^2/(n-1)\xi_{\parallel}$ for $l > n$. However, as already discussed, one must not forget the spin-wave modes that must be present in the bulk, single-phase system. Here it is primarily the transverse spin-wave modes *within* a single slice or layer that matter. (The longitudinal modes should be accounted for, in a first approximation, by the degeneracy kernel itself.) The transverse modes must be associated with new spectral features determined by the transverse dimension $L_\perp = A^{1/(d-1)}$. The scale of these may be estimated via $\xi_j \approx L_\perp$. (Compare with the spacing of levels in a "single-particle band" for $n=1$ as discussed in I.) By equating $l^2/(n-1)\xi_{\parallel}$ to $L_\perp^{-1}$, we conclude that $\mathscr{K}_0(\boldsymbol{\mu},\boldsymbol{\mu}')$ can describe *at best* of order $(\Upsilon/k_BT)^{1/2}L_\perp^{(d-2)/2}$ of the largest eigenvalues (not counting the degeneracies) of the full transfer matrix in zero field. Nevertheless, as $A \to \infty$ an unbounded number of eigenvalues should be well represented.

For $n=2$ one can regard $\boldsymbol{\mu}$ and $\boldsymbol{\mu}'$ as phase angles φ and φ' and, by symmetry, the eigenfunctions are simply $e^{\pm il\varphi}$. The spectrum is quadratic and can be written

$$b/\xi_l \approx -\tfrac{1}{2}l^2/K_A \quad (n=2)\,, \tag{4.12}$$

which might now be regarded as a *definition* of K_A. Then one can reverse the arguments.[24] Specifically, one may postulate (4.12) and use the character of the eigenfunctions to compute for an $A \times L_{\parallel}$ cylinder the incremental free energy, $\Delta F(\theta)$, associated with a *twist* in the order imposed by the symmetry-breaking boundary conditions $\varphi=0$ at one end of the cylinder and $\varphi=\theta$ ($|\theta|<\pi$) at the other end. One finds that $\Delta F(\theta)$ varies as $\theta^2 A/L_{\parallel}$; but through (3.13) the coefficient is related[21] to $\Upsilon(T)$ and thence (4.9) is recaptured (for $n=2$).

This argument suggests that if (4.12) is valid for $d=2$, $n=2$ (i.e., for the two-dimensional XY model), then the helicity modulus in the Kosterlitz-Thouless, critical phase[44,45,46] below T_c should also be given by (4.9); or, to put the matter alternatively, that the longitudinal correlation length in an $L_\perp \times \infty$ two-dimensional XY model strip with periodic boundary conditions should be given by (4.8). In fact, this answer is correct! This follows by combining the famous relation[44–46]

$$\eta(T) = k_BT/2\pi\Upsilon(T) \tag{4.13}$$

for the decay exponent of the bulk correlations with the recent result of Pichard and Sarma,[26,47]

$$L_\perp/\xi_{\parallel}(T,L_\perp) = \pi\eta(T)\,, \tag{4.14}$$

which has been rederived elegantly by Cardy, who invokes conformal covariance of the critical correlation functions.[48]

While the conclusion (4.8) is thus valid for $d=2$ and $n=2$, the quadratic nature, (4.12), of the transfer matrix spectrum has not been checked in detail. It must, however, reflect the asymptotically free spin-wave character of the Kosterlitz-Thouless phase.[47] (See Refs. 49–51 for various studies of the transfer matrix for the $d=2$ XY-model.) It is also true, in the absence of a spontaneous magnetization ($m_0 \equiv 0$), that the physical picture leading to the degeneracy kernel (4.2) might be considered deficient. Recall, however, that m_0 does *not* actually enter into the specification of $\mathscr{K}_0(\boldsymbol{\mu},\boldsymbol{\mu}')$ and one may, following current ideas, regard Υ as measuring the long-wavelength, renormalized coupling between coarse-grained or renormalized "block" spins representing a layer.

The arguments used by Pichard and Sarma[26] for (4.14) are rather formal and of a somewhat peculiar character. However, it is worth remarking that they also apply for $d>2$. Specifically, they construct a fluxlike integral based on the logarithmic derivative of the total correlation function

$$G_{\rm tot}(\vec{\mathbf{R}}) = \langle \mathbf{s}_{\vec{0}}\cdot\mathbf{s}_{\vec{\mathbf{R}}}\rangle = m_0^2 + G_l(\vec{\mathbf{R}}) + (n-1)G_t(\vec{\mathbf{R}}) \tag{4.15}$$

in zero field. In a cylinder their method relates this to $\xi_{\parallel}$. Then if (4.8) is accepted, one obtains, for the *bulk* correlation function, the relation

$$\frac{d}{dR}\ln G_{\rm tot}(\vec{\mathbf{R}}) \approx -\tfrac{1}{2}(n-1)k_BT\Gamma(\tfrac{1}{2}d)/\pi^{d/2}\Upsilon(T)R^{d-1}\,, \tag{4.16}$$

as $|\vec{\mathbf{R}}| \to \infty$. This can be integrated using (4.15) to yield an asymptotic expression for $G_t(\vec{\mathbf{R}})$ in zero field, which is in complete accord with the phenomenological result (3.5) with (3.6) and (3.14).

V. ROUNDING AND SCALING FOR CYLINDER GEOMETRIES

A. Scaling forms

Since, as we have demonstrated, a new length scale, $\xi_{\parallel}(T,A)$, appears in cylinder geometries when $L_{\parallel}$ exceeds $L_\perp$, it is natural to extend the first-order scaling ansatz (2.12) to

$$f_s(H,T;L_j) \approx V^{-1}\widetilde{W}[m_0(T)hV; L_{\parallel}/\xi_{\parallel}(T,A)]\,, \tag{5.1}$$

in which, now, $L_1 \equiv L_{\parallel}$ may grow at the same or a faster rate than $L_2,\ldots,L_d$, which all diverge at comparable rates measured by

$$A = L_\perp^{d-1} = \prod_{i=2}^{d} L_i = V/L_{\parallel} = L_0^d/L_{\parallel}\,.$$

The longitudinal correlation length diverges like A according to (4.8). For $L_{\parallel} \ll \xi_{\parallel}$ we must regain the results for a block geometry so that one has

$$\widetilde{W}(y_V;0) = W(y_V)\,, \tag{5.2}$$

where the latter scaling function follows explicitly from (2.15) and (2.16). On the other hand, in the limit $L_{\parallel} \gg \xi_{\parallel}$, which includes an infinite cylinder, we expect the dependence on $L_{\parallel}$ to drop out. This occurs provided

$$\widetilde{W}(y_V;x) \approx xW_\infty(y_V/x) \quad \text{as } x \to \infty\,. \tag{5.3}$$

In this *cylinder limit*, therefore, we expect

$$f_s(H,T;L_j)\approx(\xi_{\parallel}A)^{-1}W_{\infty}(y_A)\ , \tag{5.4}$$

where the new scaled field variable is

$$y_A=m_0h\xi_{\parallel}A\simeq 2m_0(T)\Upsilon(T)HA^2/(n-1)k_B^2T^2\ . \tag{5.5}$$

The first-order scaling behavior of the magnetization and susceptibility in the cylinder limit follow by differentiation as

$$m(H,T;L_j)\approx m_0Y_{\infty}(y_A)\ , \tag{5.6}$$

$$\chi(H,T;L_j)\approx 2[m_0^2\Upsilon A^2/(n-1)k_B^2T^2]X_{\infty}(y_A)\ . \tag{5.7}$$

Evidently the initial (or zero-field) susceptibility, $\chi_0(T;L_j)$, diverges as $A^2\sim L_{\perp}^{2(d-1)}$ for all $n\geq 2$; this contrasts with the exponential divergence of χ_0 with A in the scalar, $n=1$ case as found in I. The behavior $\chi_0(T)\sim A^2$ has been observed previously for $T\to 0$ by Cardy and Nightingale.[13] The rounding of the susceptibility peak occurs on the scale

$$H_A=\tfrac{1}{2}(n-1)(k_BT)^2/m_0\Upsilon A^2\ , \tag{5.8}$$

which, given $d>2$, is much smaller than the block scale H_V.

B. Extended degeneracy kernel

In order to explore the foundations of the scaling expressions (5.1) and (5.4), let us introduce an external field into the considerations leading to the formulation of the degeneracy kernel (4.2). A field $\mathbf{H}=k_BTh\boldsymbol{\sigma}$ must couple to the total magnetization, say $\mathbf{m}Ab$, of a layer or slice. As mentioned originally, it is reasonable to suppose that $\mathbf{m}\simeq m_0\boldsymbol{\mu}$; but, as seen in Sec. III, there should be some spin-wave corrections to this. However, we will suppose, here, in analogy to what was established in Sec. III, that these corrections are of higher order in $1/L_{\perp}$ and so do not affect the leading first-order scaling behavior. Thus we are lead to expect that the degeneracy kernel

$$\mathscr{K}(\boldsymbol{\mu},\boldsymbol{\mu}')=\exp[\tfrac{1}{2}(n-1)\xi_{\parallel}\boldsymbol{\mu}\cdot\boldsymbol{\mu}'/b]\exp(m_0hAb\boldsymbol{\sigma}\cdot\boldsymbol{\mu}) \tag{5.9}$$

will provide an asymptotically exact account of the largest eigenvalues of the full transfer operator for $d>2$. In writing this, following (4.2), we have used (4.8) to introduce $\xi_{\parallel}$. [The kernel has been written in unsymmetric form merely for convenience: it may be symmetrized by replacing $\boldsymbol{\mu}$ by $\frac{1}{2}(\boldsymbol{\mu}+\boldsymbol{\mu}')$.]

To analyze the degeneracy kernel, let us denote the angular part of the Laplace operator in n dimensions, $\nabla_{(n)}^2$, by $\Omega_{(n)}$: if r is the n-dimensional radius, $\Omega_{(n)}$ is defined via

$$\nabla_{(n)}^2=r^{-(n-1)}\frac{\partial}{\partial r}\left[r^{n-1}\frac{\partial}{\partial r}\right]+r^{-2}\Omega_{(n)}\ , \tag{5.10}$$

and acts only on the $n-1$ angular coordinates[34] specifying the orientation $\boldsymbol{\mu}$: more concretely, we will denote the angle between $\boldsymbol{\mu}$ and the fixed field direction, $\boldsymbol{\sigma}$, by θ, so that $\boldsymbol{\sigma}\cdot\boldsymbol{\mu}=\cos\theta$. The eigenfunctions of $\Omega_{(n)}$ are the hyperspherical harmonics, $Y_{l\tau}(\boldsymbol{\mu})$ for $l=0,1,2,\ldots$ and $\tau=1,\ldots,g(l;n)$, as described in Sec. IV: see (4.5). The eigenvalues are given by

$$\Omega_{(n)}Y_{l\tau}(\boldsymbol{\mu})=-l(l+n-2)Y_{l\tau}(\boldsymbol{\mu})\ . \tag{5.11}$$

If one compares this with the result (4.6) for the eigenvalues of $\mathscr{K}_0$, one sees that $\mathscr{K}_0$ can be approximated for $A/b\to\infty$ by an exponential of $\Omega_{(n)}$. In fact, using (4.6) and (5.5) we can, more generally, rewrite the degeneracy kernel as

$$\mathscr{K}(\boldsymbol{\mu},\boldsymbol{\mu}')\approx\delta(\boldsymbol{\mu}-\boldsymbol{\mu}')\exp[(y_Ab/\xi_{\parallel})\cos\theta]\times\exp[b\Omega_{(n)}'/(n-1)\xi_{\parallel}]\ , \tag{5.12}$$

when $\xi_{\parallel}/b\sim A/b\to\infty$, where $\Omega_{(n)}'$ acts on the $\boldsymbol{\mu}'$ dependence only. Now, in this same limit with $y_A=O(1)$, the commutators entailed in replacing a product of operator exponentials by an exponential of an operator sum can be neglected as of higher order in $b/\xi_{\parallel}$. Thus our extended degeneracy kernel is equivalent, as the bulk limit $L_{\perp}\to\infty$ is approached, to the differential operator

$$\tilde{\mathscr{K}}=\exp\{(b/\xi_{\parallel})[(n-1)^{-1}\Omega_{(n)}+y_A\cos\theta]\}\ . \tag{5.13}$$

C. The cylinder limit

To proceed further, consider the Schrödinger equation

$$[-(n-1)^{-1}\Omega_{(n)}-y_A\cos\theta]\psi(\boldsymbol{\mu})=E\psi(\boldsymbol{\mu})\ , \tag{5.14}$$

where $\psi(\boldsymbol{\mu})$ is a continuous function on the unit sphere ($|\boldsymbol{\mu}|=1$) in n dimensions. This equation specifies a discrete spectrum of eigenvalues $E_0(y_A)<E_1(y_A)\leq E_2(y_A)\leq\cdots$. For $n=2$ it is simply Mathieu's equation,

$$\frac{d^2\psi}{d\theta^2}+(E+y_A\cos\theta)\psi(\theta)=0\ , \tag{5.15}$$

which is well studied. Here one seeks periodic solutions with $\psi(0)=\psi(2\pi)$.

For $n=3,4,\ldots$, a reduction to a single-variable Schrödinger equation follows from the identity

$$\Omega_{(n)}=(\sin\theta)^{2-n}\frac{\partial}{\partial\theta}\left[(\sin\theta)^{n-2}\frac{\partial}{\partial\theta}\right]+(\sin\theta)^{-2}\Omega_{(n-1)}\ , \tag{5.16}$$

in which $\Omega_{(n-1)}$ acts on the set Θ, of $(n-2)$ remaining angular coordinates beyond θ: see Ref. 34, Sec. 11.1 for further details and a description of a convenient choice of Θ, the hyperspherical polar coordinate system. Then, if $Y_{\lambda\tau}(\Theta)$ now represents the $(n-1)$-dimensional hyperspherical harmonics with $\lambda=0,1,\ldots$ and $\tau=1,\ldots,g(\lambda;n-1)$, setting

$$\psi(\theta;\Theta)=(\sin\theta)^{-(n-1)/2}u(\theta)Y_{\lambda\tau}(\Theta) \tag{5.17}$$

leads to the ordinary differential equation

$$-\frac{d^2u}{d\theta^2}-\frac{1}{2}(n-2)\left[1-\frac{n-4}{2\tan^2\theta}\right]u+\frac{\lambda(\lambda+n-3)}{\sin^2\theta}u=(n-1)(E+y_A\cos\theta)u\ . \tag{5.18}$$

This must be solved subject to the boundary conditions that $\psi(0)$ and $\psi(\pi)$ be finite: by (5.17) the boundary conditions for $u(\theta)$ thus depend on n. It is now evident that the eigenvalues in (5.14) may be labeled by three quantum numbers: the "principal" quantum number, say, $\kappa=0,1,2,\ldots$ runs over the eigenstates of (5.18) for fixed λ. The full eigenfunction, $\psi_{\kappa\lambda\tau}$, is given by (5.17) in terms of $u_{\kappa\tau}(\theta)$ and $Y_{\lambda\tau}(\Theta)$, and has energy $E_{\kappa\lambda\tau}\equiv E_{\kappa\lambda}$ given by (5.18), each level being $g(\lambda;n-1)$-fold degenerate. However, when $y_A=0$ the degeneracy is higher: multiplets merge into degenerate sets of $g(l;n)$ levels, where $l=0,1,2,\ldots$. Finally, notice that since the "centrifugal" term, $\propto 1/\sin^2\theta$, is positive, the ground state of (5.14) always lies in the $\lambda=0$ sector.

Now if $E_0(y_A)$ is the ground-state eigenvalue of (5.14) [or (5.18)], the largest eigenvalue of the degeneracy kernel, $\mathscr{K}$, is, asymptotically, given simply by $\Lambda_0\approx\exp[-bE_0(y_A)/\xi_{\|}]$ and should represent accurately the dominant field dependence of the largest eigenvalue of the full transfer operator. For an infinite cylinder of finite cross section the first-order transition should thus be described by

$$f_s(H,T;L_j)\approx-(bA)^{-1}\ln\Lambda_0\approx(\xi_{\|}A)^{-1}E_0(y_A)\;, \tag{5.19}$$

which thus confirms the scaling postulate (5.4) and shows that the scaling function is given by $W_\infty(y_A)=E_0(y_A)$. One can easily check that $E_0(y_A)$ is an even function of y_A, which varies as $-|y_A|$ when $y_A\to\pm\infty$. [Compare with (2.4).] Likewise, the scaling functions Y_∞ and X_∞ entering in (5.6) and (5.9) are equal to the derivatives $-E_0'$ and $-E_0''$. As an example, we have evaluated $E_0''(0)$ by standard perturbation theory for $n=2$. This gives the height of the rounded first-order susceptibility peak as

$$\chi_0(T;L_j)\approx4\pi m_0^2(T)\Upsilon(T)(A/k_BT)^2\quad(n=2,\;L_1\to\infty)\;. \tag{5.20}$$

D. Infinite-component limit

The degeneracy kernel arguments yielding (5.19) are, we believe, convincing, but they are certainly not rigorous. In order to check them against exact calculations, let us examine the limit $n\to\infty$. To this end, return to (5.18) with $\lambda=0$ and set

$$E(y_A)=n\tilde{E}(\tilde{y})\quad\text{and}\quad y_A=n\tilde{y}\;. \tag{5.21}$$

For large n the Schrödinger equation then becomes

$$\frac{1}{n^2}\frac{d^2u}{d\theta^2}+[\tilde{E}-U(\theta)]u=0\;, \tag{5.22}$$

in which the potential is given by

$$U(\theta)=1/4\tan^2\theta-\tilde{y}\cos\theta\;, \tag{5.23}$$

while terms of relative order $1/n$ have been dropped. But (5.22) is simply a Schrödinger equation for a particle with a mass proportional to n^2 in a fixed potential. As n becomes large, therefore, the ground-state wave function peaks at the (unique) minimum of the potential, and, correspondingly, the ground-state energy, $\tilde{E}_0$, approaches

$$\tilde{E}_0^\infty(\tilde{y})=\min_{0\le\theta\le\pi}U(\theta)\equiv U(\theta_0)\;. \tag{5.24}$$

These physically obvious statements can, of course, be fully justified analytically.

To obtain a more explicit expression for the scaling function, note that the scaling function for the magnetization in (5.6) now corresponds to

$$\frac{m}{m_0}\approx Y_\infty=-\frac{dE_0}{dy}=-\frac{d\tilde{E}_0}{d\tilde{y}}=\langle\cos\theta\rangle_0\;, \tag{5.25}$$

where $\langle\cos\theta\rangle_0$ denotes an average in the ground state and so approaches $\cos\theta_0$ when $n\to\infty$. The substitution $\cos\theta_0=Y_\infty$ in (5.24) then yields

$$\tilde{E}_0^\infty(\tilde{y})=\tfrac{1}{4}Y_\infty^2(1-Y_\infty^2)-\tilde{y}Y_\infty\;, \tag{5.26}$$

while minimization leads to

$$Y_\infty/(1-Y_\infty^2)^2=2\tilde{y}\;. \tag{5.27}$$

This latter relation is an algebraic equation for the magnetization scaling function $Y_\infty(\tilde{y})$ valid for large n (in the cylinder limit). For small $\tilde{y}\equiv y_A/n$, one can solve to obtain

$$Y_\infty(y_A;n)\approx2\tilde{y}[1-8\tilde{y}^2+O(\tilde{y}^4)]\;. \tag{5.28}$$

In terms of this function the scaling function for the free energy for large n follows via (5.21) and (5.19). With $\tilde{y}\equiv y_A/n$ it can be written more explicitly as

$$W_\infty(y_A;n)\approx-\tfrac{1}{4}nY_\infty^2(1+Y_\infty^2)/(1-Y_\infty^2)^2\;, \tag{5.29}$$

$$\approx-n\tilde{y}^2[1-4\tilde{y}^2+O(\tilde{y}^4)]\quad\text{as }\tilde{y}\to0\;, \tag{5.30}$$

$$\approx-n|\tilde{y}|[1-1/\sqrt{2|\tilde{y}|}+O(\tilde{y}^{-1})]\quad\text{as }|\tilde{y}|\to\infty\;. \tag{5.31}$$

A crucial point, however, is that the first-order behavior in the cylinder limit may be calculated exactly for the spherical model: see III. One finds that the scaling functions W_∞ and Y_∞, for free energy and magnetization, are precisely as given by (5.27) and (5.29). Thus the degeneracy kernel approach is certainly correct for large n. Incidentally, in making this check, one needs the explicit value of the helicity modulus in the spherical model which has been calculated by Barber and Fisher.[52]

E. Finite cylinders

For a cylinder of finite length, $L_{\|}$, with periodic boundary conditions, the partition function may, as regards the field dependence, be approximated by

$$\begin{aligned}\mathscr{Z}&=\mathrm{Tr}\{\tilde{\mathscr{K}}^{L_{\|}/b}\}\\&=\mathrm{Tr}\{\exp[(L_{\|}/\xi_{\|})(n-1)^{-1}\Omega_{(n)}+m_0hV\cos\theta]\}\;,\end{aligned} \tag{5.32}$$

where $\mathrm{Tr}\{\;\}$ represents a normalized integration over the orientational coordinates specifying $\boldsymbol{\mu}$ as in (2.14). The associated free energy, $-V^{-1}\ln\mathscr{Z}$, has precisely the two-variable scaling form anticipated in (5.1). The result can also be written asymptotically as

$$f_s\approx-V^{-1}\ln\sum_{k=0}^{\infty}\exp[-(L_{\|}/\xi_{\|})E_k(y_A)]\;, \tag{5.33}$$

where the $E_k(y_A)$ are the eigenvalues of the full Schrödinger equation (5.14), where k denotes, collectively, all the quantum numbers. For long cylinders with $L_{\parallel} \gg \xi_{\parallel}(T;A)$ the term with E_0 dominates and the result (5.19) is reproduced. Evidently the leading correction to this is of relative order $\exp[-(L_{\parallel}/\xi_{\parallel})\Delta E_1(y_A)]$, where the energy gap $\Delta E_1 = E_1 - E_0$ takes the value 1 when $y_A \to 0$. In the other limit, $L_{\parallel} \ll \xi_{\parallel}(T;A)$, one may neglect the derivative term in (5.32) and the original block scaling result (2.16) is correctly recaptured. In between, (5.33) provides a leading-order description of the crossover from block to cylinder geometries.

In the scalar case, $n=1$, it was shown in I that only the two leading eigenvalues of the transfer matrix were necessary to describe the first-order transition in the block limit, in the cylinder limit, *and* in the full crossover region between them. The situation here is not so simple. In the first case, it is clear that once $L_{\parallel} \lesssim \xi_{\parallel}$, successive terms in the series (5.33) decrease only by factors $\exp[-(L_{\parallel}/\xi_{\parallel})\Delta E_k]$, with $\Delta E_k = E_k - E_{k-1}$, which are of order unity (for bounded k) and hence cannot be neglected.

More physical insight can be gained, however, if we note that the crucial scaled combination can be written, using (4.8) and (5.8), as

$$x = L_{\parallel}/\xi_{\parallel}(T;A) = H_A/H_V = \tfrac{1}{2}(n-1)k_B T L_{\parallel}^2/\Upsilon L_0^d$$
$$= \tfrac{1}{2}(n-1)u_L l_{\parallel}^2 \,. \qquad (5.34)$$

Here we have $l_{\parallel} = L_{\parallel}/L_0 \equiv l_1$, while $u_L = k_B T/\Upsilon L_0^{d-2}$ is the parameter, introduced in (3.20), which measures the strength of the spin-wave contributions in the block limit relative to the leading first-order terms scaling with $y_V = m_0 h V$. It is then clear that the derivative term in (5.32), while vital in the cylinder limit, $l_{\parallel} \to \infty$, represents essentially only a spin-wave correction in the block limit, $l_{\parallel} = O(1)$. Furthermore, since terms proportional to $l_2^2, l_3^2, \ldots$, which must be anticipated on the grounds of symmetry, do *not* appear, it is clear that spin-wave modes "propagating" transversely to the cylinder axis have not been properly accounted for. Recall that the leading effects of all the spin-wave modes in the block limit are represented by the scaling-with-corrections expression (3.38) and the associated results. Since, by construction, the degeneracy kernel took direct account only of the spin-wave modes with wave vectors parallel to the cylinder axis, the absence of the other contributions is hardly surprising. Furthermore, as the check in the spherical model limit confirmed, their absence is no loss as regards *leading* behavior either in the limit of a long cylinder with $l_{\parallel}^2 \gg 1$ or in the block situation. Nonetheless, as $l_{\parallel}^2$ decreases and crossover occurs one will reach a final region in which the degeneracy kernel partition function (5.32) successfully represents the leading first-order behavior but is numerically inaccurate as regards the spin-wave terms of order u_L in which the shape dependence enters and out of which the crossover to the cylinder limit develops.

One might attempt to go further by adapting the lines of argument used in Sec. III to elucidate the spin-wave interference effects in the block limit. Some improvement is probably to be had by modifying the value, m_0, assumed for the layer magnetization, in the formulation of the degeneracy kernel in order to allow for the truncated spin-wave enhancement of m for small H as found in Sec. III. However, a less *ad hoc* treatment would have to account for the propagation of spin waves from one slice to the next in constructing a suitably expanded degeneracy kernel. It is not clear how that could be done in general without substantially complicating the formalism. (In the limit $n \to \infty$ the results can, of course, be found analytically by direct analysis: see III.)

Despite the restriction to $|\mathbf{H}| \ll H_S$ in the approximation (5.33), it is worth exploring a little further to show that some important spin-wave features *are* nevertheless represented in qualitatively correct fashion. Thus, consider the field dependence and note that when $y_A = H/H_A$ is large (and, say, positive), one may use $\cos\theta \approx 1 - \frac{1}{2}\theta^2$, $\tan\theta \approx \theta$, and expand around the potential minimum to approximate (5.18) as an equation for a harmonic oscillator. Leaving aside pure numerical factors, the first energy gap then varies as

$$\Delta E_1(y_A;n) = E_1 - E_0 \sim [m_0 H \xi_{\parallel} A/(n-1)k_B T]^{1/2} \,. \qquad (5.35)$$

But this corresponds to a correlation length

$$\xi_1(H,T) = \xi_{\parallel}/\Delta E_1 \propto [\Upsilon(T)/m_0(T)H]^{1/2} \,. \qquad (5.36)$$

Comparison with (3.15) reveals precise agreement with the variation of the isotropic bulk correlation length, $\xi_\infty(H,T)$, which in turn represents a direct manifestation of the spin waves. Despite this, the fact that the degeneracy kernel, as formulated, does not fully include the spatially transverse spin-wave fluctuations shows up even in an infinite cylinder. The resulting first-order crossover scaling function, e.g., for the limit $n \to \infty$ in (5.26)–(5.31), is correct on the scale $H_A \sim 1/A^2$ (as checked for $n \to \infty$), but clearly contains no structure on the spin-wave scale $H_S \sim 1/L_0^2$. [See (3.18).] One should note, however, that $H_A/H_S = \frac{1}{2}(n-1)u_L^2 l_{\parallel}^2$ so that, as in the block case, the residual spin-wave effects must be regarded only as corrections to the leading scaling behavior—and the leading behavior *is* given correctly by the degeneracy kernel!

Similar considerations apply if one views (5.1) as a scaling relation at a renormalization-group discontinuity fixed point[13,29,30] at $h=0$, $T=0$. Indeed, by (5.34) the ratio $L_{\parallel}/\xi_{\parallel}$ is just a product of the two scaling combinations $l_{\parallel}^2$ and u_L. The cylinder scaling result (5.33), which satisfies (5.2) and (5.3), describes correctly that part of the u_L dependence of the *full* two-variable scaling form, as in (3.32), which is singular or "dangerous" when the product $l_{\parallel}^2 u_L$ becomes large. In the opposite limit of small $l_{\parallel}^2 u_L$, the u_L dependence is reproduced correctly only to order $(u_L)^0$ in an expansion of the *full* scaling function in powers of the irrelevant combination u_L: happily, such an expansion is quite legitimate in this, the block limit (see Sec. III), even though the $(u_L)^1$ terms are needed to see the leading spin-wave corrections.

VI. FIRST-ORDER SCALING IN THE CRITICAL REGION

Near the critical point ($H \simeq 0$, $T \simeq T_c$), thermodynamic properties and the correlation functions, etc. should obey the usual, "critical" finite-size scaling theory.[1-3] For the singular part of the free energy (as defined, in particular, in Ref. 53), one adopts the hypothesis

$$f_c(H,T;L_j) \approx |t|^{2-\alpha} W_c^{\pm}(h/|t|^{\Delta}, L_0|t|^{\nu}; l_j) , \tag{6.1}$$

for $h \to 0$ and $t=(T-T_c)/T_c \to 0\pm$ with $\Delta = \beta+\gamma$. This embodies the assertion that all unbounded lengths should be scaled asymptotically by the bulk correlation length, ξ_∞, say, in zero field above T_c, where it diverges as $t^{-\nu}$. Now, as observed in I, the critical and first-order scaling regimes have overlapping domains of validity, specifically, small, *fixed* $t<0$ with $h \to 0\pm$ and large L_0. Then, in the first-order scaling expressions, one should take

$$m_0(T) \approx B|t|^{\beta} \text{ and } \Upsilon(T)/k_BT \approx D|t|^{2\beta-\eta\nu} . \tag{6.2}$$

Inasfar as the scaling behavior matches, so too must the first-order and critical scaling functions correspond, as demonstrated in I. We will not enter into any details here since they parallel closely those presented in I and in Ref. 54; however, we will examine the degree to which the simple scaling form (6.1) and its natural extension

$$\xi(H,T;L_j) \approx |t|^{-\nu} Z^{\pm}(h/|t|^{\Delta}, L_0|t|^{\nu}; l_j) \tag{6.3}$$

for correlation lengths defined in various ways are actually valid. As pointed out by Brézin[25] and discussed in I (and Ref. 54), finite-size first-order behavior is *not* adequately represented by (6.3) when hyperscaling fails. This happens for $d>4$ when, in particular, the combination

$$d\nu-(2-\alpha) \equiv \omega^*\nu \tag{6.4}$$

fails to vanish identically: for ordinary O(n) critical points one has $\omega^*=0$ for $d \le 4$, but $\omega^*=d-4$ for $d \ge 4$.

To discuss this issue, note that (6.1) and (6.3) entail only the scaled variables

$$y=h/|t|^{\Delta} \text{ and } z_0=L_0|t|^{\nu},\ \ z_{\|}=L_{\|}|t|^{\nu}, \text{ etc.} \tag{6.5}$$

Our first-order scaling results for the block limit involve

$$y_V=m_0hV=ByV|t|^{2-\alpha}=Byz_0^d|t|^{-\omega^*\nu} , \tag{6.6}$$

where the standard scaling relation $\alpha+2\beta+\gamma=2$ (valid for all d) has been used. As anticipated, the first-order scaling is encompassed by (6.1) when $\omega^*=0$, as for $d \le 4$, but fails when $\omega^*>0$. (We ignore logarithmic factors present at the borderline $d_>=4$.) As commented in I, the *extra* finite-size variable

$$z_V=V|t|^{2-\alpha} \equiv L_0^d|t|^{2-\alpha} \tag{6.7}$$

thus enters for $d>d_>$; for $d \le d_>$ one has $z_V=z_0^d$.

If, following Brézin[25] (and I), we define an *overall* size-dependent correlation length via

$$\xi_V(H,T;L_j) \equiv a(k_BT\chi/a^d)^{\nu/\gamma} , \tag{6.8}$$

it is natural to postulate that ξ_V scales, in the first-order region, only with z_V, rather than with z_0. Accepting this yields

$$\xi_V(0,T;L_j) \approx |t|^{-\nu} Z_V^{\pm}(z_V;l_j) , \tag{6.9}$$

and then the critical point value must vary as

$$\xi_{V,c} \equiv \xi_V(0,T_c;L_j) \approx L_0^{d/(d-\omega^*)} Z_V^c(l_j) . \tag{6.10}$$

Thus ξ_c diverges as L_0 for $d \le 4$, but like $L_0^{d/4}$ for $d>4$. Except for a logarithmic factor at $d=4$, these conjectures agree precisely with Brézin's exact calculations for $n \to \infty$.

In the case of a block which becomes a long cylinder, a second first-order scaling parameter entered, namely

$$x=\frac{L_{\|}}{\xi_{\|}}=\tfrac{1}{2}(n-1)\frac{k_BTL_{\|}^2}{\Upsilon V} \approx \frac{(n-1)}{2D}\frac{z_{\|}^2}{z_0^d}t^{\omega^*\nu} = \frac{(n-1)}{2D}\frac{z_{\|}^2}{z_V} , \tag{6.11}$$

where the relation $\gamma=(2-\eta)\nu$ has been invoked. Once again, simple scaling holds only if ω^* vanishes. However, no *new* scaling variable is needed beyond z_V, which already entered in the block limit. [In I it was suggested, following the analogous reasoning involving the surface tension, that one would also require $z_A=A|t|^{\mu}(=A|t|^{3/2}$ for $d \ge 4$); but one easily checks that $z_A=z_V/z_{\|}$ holds for all d so z_A is not separately needed.]

The scaling of the correlation length $\xi_{\|}$ defined through the gap in the transfer matrix spectrum can only depend on the transverse dimensions since this is a feature of an infinite cylinder ($L_{\|} \to \infty$). Thus only the scaled combination $z_A=z_V/z_{\|}=L_{\perp}^{d-1}|t|^{2-\alpha-\nu}$ should enter. Following an argument parallel to that used for ξ_V then yields

$$\xi_{\|,c}(L_j) \approx L_{\perp}^{(d-1)/(d-1-\omega^*)} Z_{\|}^c(l_j) . \tag{6.12}$$

For $\omega^*=0$, i.e., $d \le 4$, one has again $\xi_{\|,c} \sim L_{\perp}$, but for $d>4$ one finds $\xi_{\|,c} \sim L_{\perp}^{(d-1)/3}$. These results are clearly independent of n (even encompassing $n=1$) and they agree with Brézin's exact calculations for $n \to \infty$ (up to a logarithmic factor at $d=4$).

When *only* the scaling combination z_V or $z_V/z_{\|}$ enters, one can rewrite scaling expressions to use L as the primary variable and thence explicitly exhibit the modified powers $L^{d/(d-\omega^*)}$, etc. In general, however, one must expect *both* z_0 (or the individual $z_{\|} \equiv z_1, z_2, \ldots$) *and* z_V to enter. We should also recall, as explained in I, that in renormalization-group theory the breakdown of simple finite-size scaling is associated with the appearance (for $d>4$) of a dangerous irrelevant variable.[55] This enters directly into first-order scaling quantities like the total free energy, the helicity modulus and, for $n=1$, the interfacial tension.

The corrections to first-order scaling in the block limit due to spin waves entail the correlation length $\xi_\infty(H,T)$ defined in (3.15) and the new scaled field variable y_S introduced in (3.19). As regards the former, we have

$$\xi_\infty \approx |\Upsilon/m_0H|^{1/2} \sim 1/|y|^{1/2}|t|^{\nu} ,$$

which satisfies the expectations of simple scaling, as remarked earlier: We also have $y_S=(L_0/\xi_\infty)^2 \sim |y|z_0^2$, for which the same is true. But the "irrelevant" spin-wave parameter of (3.20) reduces to $u_L \approx z_0^2/Dz_V$, which involves z_V. This is a reflection of the fact that for $d>4$

the spin waves actually enter into the asymptotic critical free energy only as corrections to the leading scaling behavior, which is otherwise fully classical and independent of n.

VII. SUMMARY AND FURTHER DEVELOPMENTS

For convenience we present here a brief overview of our results referencing the most important expressions. We also raise some questions that remain to be answered.

First, we have shown, for the block limit, that a finite system of volume $V=L_0^d$ should behave, in leading order, as a single, fully magnetized domain which is, however, free to reorient in the external field. As a result, the one and only basic scaling variable is

$$y_V \equiv H/H_V = m_0 HV/k_B T \ , \tag{7.1}$$

where $m_0(T)$ is the spontaneous magnetization. The corresponding scaling behavior of free energy, magnetization, and susceptibility is independent of shape and can be expressed explicitly for general n in terms of Bessel functions: see (2.16)—(2.18). For large n the results—see (2.22)—may be checked against exact results for the spherical model presented in III.[17] The precise correspondences needed to do this in the limit $n \to \infty$ are given in (2.24)—(2.28).

The leading-order scaling results do not allow for the bulk singularities associated with spin-wave fluctuations as observed, say, in the susceptibility: see (2.10). To discuss this, a phenomenological treatment based on the free-energy functional (3.4) is appropriate. This yields explicit expressions for the bulk correlation functions [in (3.5), (3.6), (3.11), and (3.12)] in terms of the spin-wave stiffness parameter, b_t; this, in turn, may be related, via (3.14), to the helicity modulus, $\Upsilon(T)$, which is defined in (3.13). Thereby the bulk correlation length, $\xi_\infty(H,T)$, for small fields below T_c depends only on Υ and m_0: see (3.15). The proper scale for the rounding of the spin-wave singularities is thence found to be

$$y_S \equiv |\mathbf{H}|/H_S = m_0 |\mathbf{H}| L_0^2/\Upsilon \ ; \tag{7.2}$$

see (3.18) and (3.19). From this one sees that the relative magnitude of the spin-wave terms, which now appear as *corrections* to the leading behavior, is determined by the asymptotically small parameter

$$u_L = H_V/H_S = k_B T/\Upsilon(T) L_0^{d-2} \ . \tag{7.3}$$

The rounding of the spin-wave singularities in the domain $H_V \ll H \simeq H_S$ is now described by scaling functions $Y_S(y_S)$ and $X_S(y_S)$, which make contributions to the magnetization and susceptibility, respectively, proportional to u_L and u_L^2. [See (3.23), (3.25), (3.28), and (3.29).] Finally, the full scaling behavior of the magnetization for the block situation including the "interference" terms between first-order and spin-wave rounding, is described by a scaling function of two variables, namely $Y(y_V,u_L)$. [See (3.32) *et seq.*] To first order in u_L, the function is given exactly in (3.38). Among its principal consequences is a finite-size correction to the susceptibility peak in small fields (of order H_V) arising directly from the spin-wave fluctuations: the expression (3.44) shows this is of order u_L relative to the leading result (2.18). Figure 1 depicts these various conclusions schematically.

For cylinder geometries with cross-sectional area $A=L_\perp^{d-1}$, the longitudinal correlation length enters: this is related to the two largest eigenvalues of the transfer operator and to the helicity modulus via

$$\xi_{\parallel}(T,A) = b/\ln(\Lambda_0/\Lambda_1) = 2\Upsilon(T)A/(n-1)k_B T \ . \tag{7.4}$$

This formula follows by construction of a "degeneracy kernel" [(4.2) and (5.9)] which asymptotically approximates the transfer matrix. This also serves to establish the correct scaling behavior in a field, which is postulated in (5.1) and entails the previous variable y_V and the new combination

$$x = L_{\parallel}/\xi_{\parallel}(T,A) = \tfrac{1}{2}(n-1)u_L(L_{\parallel}/L_0)^2 \ . \tag{7.5}$$

In addition, it yields expressions for the scaling functions: see (5.32) and (5.33). For a long cylinder it proves necessary only to compute the ground-state energy $E_0(y_A)$ of the Schrödinger equation (5.18), in terms of which (5.19) yields the free energy as a function of

$$y_A \equiv H/H_A = m_0 H \xi_{\parallel} A/k_B T \equiv y_V/x \ . \tag{7.6}$$

It follows that rounding now occurs only on the scale $H_A \sim 1/A^2$. The quantal problem simplifies in the limit $n \to \infty$ to yield (5.27)—(5.31), which agree with the exact spherical model results in III. Although the scaling formulas for cylinder geometry entail the spin-wave parameter u_L and reproduce some important spin-wave effects, they are valid only to leading order since the residual bulk spin-wave singularities are not accounted for: to do so remains a task for the future.

Finally, in the critical region, first-order scaling proves fully consonant with the simplest critical finite-size scaling formulation, provided $d \le 4$ when the hyperscaling relation $d\nu = 2-\alpha$ is valid. This fails above $d=4$, however, and then one finds, in agreement with Brézin,[25] that $\xi_{\parallel}(H=0,\ T=T_c,\ L_\perp)$ varies as $L_\perp^{(d-1)/3}$ in a cylinder geometry, while for blocks an appropriately defined "overall" correlation length, $\xi_V(H=0,\ T=T_c,\ L_0)$, diverges as $L_0^{d/4}$. [See (6.8), (6.10), and (6.12).]

Of course, all the results described pertain only to true equilibrium conditions. In real experiments or practical simulations one may, owing to strong pinning or to insufficient observation times, see hysteresis and other nonequilibrium effects near a first-order transition, even in a finite system. Indeed, as mentioned, to ensure equilibrium for a given particle size in superparamagnetic materials, the temperature must exceed the size-dependent blocking temperature. But even then, it is clear that periodic boundary conditions are not realized in nature! Nevertheless, with due precautions, the effects predicted should be observable in Monte Carlo simulations of adequate length.[6,7,56]

As to other further, not fully resolved aspects of first-order finite-size scaling, the most important is, surely, to relax the constraint of periodic boundary conditions. If the boundary conditions respect the O(n) symmetry and do not enhance the surface interactions, rather few changes are likely to occur: by symmetry, there will be no finite-size shift in the transition point and no independent surface ordering will occur. The spin-wave boundary conditions will change, so the corresponding scaling functions must change, but the quantitative effects should be minor and the spin waves and other boundary effects should still appear only as higher-order corrections. These considerations apply, of course, to $d>2$ and should provide a reasonable account of various practical situations. For $d=2$ and $n=2$, however, there arises the interesting problem of finite-size effects on Kosterlitz-Thouless phases; but since those exhibit algebraic decay of correlation, the task is really one of *critical* finite-size scaling, which is probably much harder.

If the interactions on the boundary are sufficiently enhanced, one will encounter incipient ordering of the surface *before* the bulk tends to order. A high degree of order, reflecting near broken symmetry on the surface, may clearly affect the internal region of a system significantly. Consequently, the formulation of the finite-size effects could be considerably more complicated. Similar issues arise when the boundary conditions actually break the O(n) symmetry. If there is a true ordering field on the boundary, the effective transition point in a finite system will shift.[4,5] But the boundary interactions might merely serve to *lower* the symmetry from O(n) to, say, O(1), rather than to destroy it entirely. The resulting anisotropies will certainly affect the scaling behavior. However, one may again hope that with appropriate shifts in the scaling variables all the boundary effects will remain as higher-order scaling corrections. More detailed considerations, however, are essential to confirm such a speculation and estimate the actual nature and magnitude of these effects.

ACKNOWLEDGMENTS

We wish to thank K. Binder, E. Brézin, J. L. Cardy, M. Nauenberg, R. Pandit, J. Rudnick, A. M. Szpilka, and A. P. Young for instructive discussions and correspondence. Our work has enjoyed financial support from the National Science Foundation, through the Condensed Matter Theory Program and, in part, through the Materials Science Center at Cornell University. M.E.F. is grateful to the California Institute of Technology for hospitality during his visit and for support from the Sherman Fairchild Foundation; V.P. acknowledges support at Caltech through the Myron A. Bantrell Fund.

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