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Interface Formation and a Structural Phase Transition for the Spherical Model of Ferromagnetism

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A detailed analysis is reported examining the local magnetic susceptibility $\chi(\mathbf{r})$, in relation to the correlation function $G(\mathbf{R})$ and correlation length ξ, of a spherical model ferromagnet confined to geometry $\Omega = L^{d-d'} \times \infty^{d'}$ ($d' \leqslant 2$, $d > 2$) under a continuous set of *twisted* boundary conditions. The "twist" parameter $\underline{\tau}$ in this problem may be interpreted as a measure of the geometry-dependent doping level of interfacial impurities (or antiferromagnetic seams) in the *extended* system at various temperatures. For $\tau_j \to 0$, $\forall j \in d-d'$, no seams are present except at infinity, whereas if $\tau_j = 1/2$, impurity saturation occurs. For $0 < \tau_j < 1/2$ the physical domain $\Omega_{\text{phys}} = D^{d-d'} \times \infty^{d'}$ ($D > L$), defining the region between seams containing the origin, depends on temperature above a certain threshold ($T > T_0$). Below that temperature ($T < T_0$), seams are frozen at the same position ($D \approx L/2\tau$, $d - d' = 1$), revealing a smoothly varying large-scale structural phase transition.

KEY WORDS: Twisted boundary conditions; local susceptibility; spherical model; finite-size scaling.

1. INTRODUCTION

Local effects in a variety of response functions are known to exist for systems subject to boundary conditions that somehow pin a well-defined order parameter field $\langle \sigma(\mathbf{r}) \rangle$—or wavefunction—near an interface.(1),[2] In such situations the system may possess spatially varying interactions (due to the presence of a surface,(2–5),[3] membrane, (6–8),[4] or wall,(9) etc.), giving

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[2] For rigorous and exact results see ref. 2. A recent review of subsequent developments is given in ref. 3.

[3] For a field-theoretic approach see ref. 5.

[4] See also the review articles by Fisher(7) and Liebler.(8)

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rise to rather complicated local thermodynamic behavior. Often an interface can be described more simply by a sharp defect plane of broken bonds brought about by nonperiodic boundary conditions in Ising-type systems[10] or, for example, an inhomogeneity[11] separating domains in a spherical ferromagnet under antiperiodic boundary conditions (APBC)—both of which do not affect the spatial interactions. Recently, local variational free energy functionals have been constructed with success in determining the spatial ($\mathbf{r}$) dependence of the near-critical energy density for a ferromagnetic Ising model in the vicinity of a wall and grain boundary;[9] however, similar progress for corresponding $O(n)$ systems exhibiting continuous symmetry ($n \geqslant 2$) is quite limited.[11–14] The main difficulty with these systems is the apparent lack of analytical and numerical tractability due to interference of spin-wave (Goldstone) excitations. A particularly important exception to this trend is in the spherical limit ($n \to \infty$), where analytical solutions can be derived, and yet even for this model, only limited results with "realistic" boundary conditions (and interactions[15,16]) have emerged.[11–14,17–20]

It is an established fact (due to Stanley in 1968) that in the limit $n \to \infty$, the bulk $O(n)$ model with translationally invariant interactions reduces to the spherical model (of Berlin and Kac, 1952) with a *uniform* spherical field—for references and a recent review of this topic in disordered $O(n)$ systems at large n, which involve a more complicated nonuniform spherical field, see Khorunzhy *et al.*[15] What is not so well known is that Stanley's technique for $n \to \infty$ can be applied *exactly* to the same *fully finite* system,[17,21] in which the integration defined for the bulk is replaced by a discrete sum over the eigenvalues, without requiring the thermodynamic limit (of infinite size). Again, a uniform spherical field is sufficient to describe physical properties of the finite system, irrespective of whether the boundary conditions are periodic (PBC) or antiperiodic (APBC), provided that the (translationally invariant) interactions are not in any way affected. This simplifies the problem and distinguishes the mechanisms of broken translational invariance due to nonperiodic boundary conditions from that of the interactions requiring (under APBC) a mere shift in the eigenvalues of the system. It can then be proven that the fully finite (microcanonical) spherical model[21] under PBC or APBC in the *absence* of an external field is precisely equivalent to the corresponding *mean* (or canonical) spherical model.[17]

One aspect applicable to bulk $O(n)$ models with $n > 4$ is that the singular part of the specific heat $c^{(s)} = -T\partial^2 f^{(s)}/\partial T^2$ is irrelevant [e.g., the critical exponent for $\varepsilon = 4 - d \ll 1$ is $\alpha = -\varepsilon(n-4)/2(nb+8) < 0$], and hence the free energy $f^{(s)}$ in the absence of an external (magnetic) field gives *no* local linear response. However, relevant local features in the magnetic susceptibily $\chi = -\partial^2 f^{(s)}/\partial H^2|_{H\to 0}$ are expected to persist for general n (i.e., the critical exponent $\gamma > 0$ for any n). An explicit derivation of $\chi(\mathbf{r})$ has indeed been shown to confirm this prediction for the ferromagnetic $O(\infty)$ model (of *uniform* spherical field) confined to a domain $\Omega = L^{d-d'} \times \infty^{d'}$ ($d' \geqslant 2$) under APBC.[11] In that study, the non-uniform susceptibility is brought about by the appearance of a defect (or inhomogeneity), which in turn is due to the initial presence of a uniform external field $H > 0$ as spins on either side of the interface are coupled to the field in opposite senses (relative to their preferred local alignment). Equivalently, $\chi(\mathbf{r})$ can be derived from the correlation function [20] through the fluctuation-response theorem— without the necessity of applying an external field at any point in the calculation. For nonsingular finite systems ($d' \leqslant 2$) there is no sharp phase transition ($L < \infty$) at $T > 0$, therefore the two approaches, using either the microcanonical or mean spherical model, are expected give identical results.[15]

In this paper I extend the work in refs. 11, 19, and 20 in order to analyze the local susceptibility $\chi(\mathbf{r})$ of a (hypercubic) spherical model ferromagnet confined to geometry $\Omega = L^{d-d'} \times \infty^{d'}$ under a more general class of nonperiodic boundary conditions known as *twisted* boundary condition (TBC), defined through a continuously varying parameter $\underline{\tau}$ (with components $\tau_1, \ldots, \tau_d$), of which PBC ($\tau_j = 0$) and APBC ($\tau_j = 1/2$) are two extremes. The TBC employed here are essentially the same as the ones used recently by Chakravarty[22] and Brézin *et al.*,[23] and again, as with PBC and APBC for the $O(\infty)$ model, a *uniform* (or mean) spherical field is sufficient to describe the properties of the system.[11,19,20] This work compliments recent results[14] based on methods developed by Abraham and Robert[13] to determine phase separation for the same model under the influence of boundary conditions involving a nonuniform external field $H(\mathbf{r})$.

In Section 2 the susceptibility is derived from the (nonuniform) magnetization in the presence of a *uniform* external field, results of which are compared to the corresponding fluctuation-response theorem at $H = 0$. As expected, there is complete agreement between the two approaches. Comparison to the correlation length[18,19] $\xi(T; \Omega)$ [i.e., $\chi(\mathbf{r})/\xi^2$] reveals a nontrivial variation of amplitude near the bulk transition temperature T_c. In Section 3, I derive a closed-form expression for the susceptibility confined to geometry $\Omega = L \times \infty^2$ in the vicinity of the interface ($|\mathbf{r}| \ll L$ for APBC). Under TBC ($0 < \tau_j < 1/2$) one finds that the interface is not only in a different position than under APBC, but its location may also depend on the temperature of the system, contrasting with APBC, where saturation occurs.[11,20] The limiting case $|\underline{\tau}| \to 0$ of $\chi(\mathbf{r})$ is examined in detail revealing a smoothly varying large-scale structural phase transition at a temperature

$T_0 < T_c$, which has no analog in the bulk limit $L \to \infty$, unless $H > 0$.[13,14] Section 4 is a summary of concluding remarks about the previous sections, including a discussion on the nature of the new phase transition observed in this work.

2. LOCAL SUSCEPTIBILITY UNDER TWISTED BOUNDARY CONDITIONS

We extend the methods developed by Barber and Fisher,[17] as well as by Singh *et al.*,[11] to evaluate the magnetization in the presence of a *uniform* external field for a fully finite spherical model ferromagnet ($\Omega = \prod_{j=1}^{d} L_j$) under TBC, i.e.,

$$\sigma(r_j + L_j) = e^{2\pi i \tau_j} \sigma(r_j) \qquad (j = 1, ..., d) \tag{1}$$

where $\underline{\tau}$ is a vector whose components $\tau_1, ..., \tau_d$ lie in the interval $(0, 1/2)$. For this problem the local (to be distinguished from the *mean* or overall) susceptibility is defined as

$$\chi(\mathbf{r}, T; \Omega) = \left.\frac{\langle \sigma(\mathbf{r}) \rangle}{H}\right|_{H \to 0}, \qquad \tau = |\underline{\tau}| > 0 \tag{2}$$

where $\langle \cdots \rangle$ denotes the (mean spherical) canonical ensemble average. Since translationally invariant (nearest neighbor) interactions J considered here are not affected by the imposed TBC, the problem is diagonalizable in terms of the plane wave modes, $e^{i\mathbf{k}\cdot\mathbf{r}}$, just as in the PBC case[17]; furthermore, by the principle of local and overall spin equivalence, $\langle |\sigma(\mathbf{r})|^2 \rangle = 1$, which implies translational invariance of the correlation function $G(\mathbf{R}; \Omega)$ [see Eqs. (13) and (43)], a uniform spherical field λ is sufficient to describe the physical quantities of the system.[20] After some algebra, we arrive at the exact formula

$$\chi(\mathbf{r}) = \frac{1}{2J} \sum_{\{n_j\}} \frac{\varepsilon_{\mathbf{k}}^{\mathbf{r}}}{\phi + 2\sum_{j=1}^{d} (1 - \cos k_j a)} \tag{3}$$

with

$$k_j = \frac{2\pi(n_j + \tau_j)}{L_j}, \qquad n_j = 0, 1, ..., N_j - 1, \qquad N_j = \frac{L_j}{a}, \qquad N = \prod_{j=1}^{d} N_j \tag{4}$$

where a is the lattice cutoff and $\phi = \lambda/J - 2d$ is a thermodynamic variable expressible in terms of temperature T (and field H) through an elimination of λ with the spherical constraint [Eq. (43)]. Here $\varepsilon_{\mathbf{k}}^{\mathbf{r}} = N^{-1/2} e^{i\mathbf{k}\cdot\mathbf{r}} \varepsilon_{\mathbf{k}}$, where $\varepsilon_{\mathbf{k}}$ are the usual distribution coefficients[17]

$$\varepsilon_{\mathbf{k}} = N^{-1/2} \sum_{\mathbf{r}'} e^{-ik\cdot\mathbf{r}'} = \prod_{j=1}^{d} \left[e^{-i(k_j/2)(L_j+a)} \frac{\sin(k_j L_j/2)}{\sin(k_j a/2)} N_j^{-1/2} \right] \tag{5}$$

In Eq. (3) it is implied that only the *real* part of $\chi(\mathbf{r})$ shall contribute to the physics and, by symmetry, each component j ($\in d$) of the phase factor in $\varepsilon_{\mathbf{k}}^{\mathbf{r}}$ may effectively be replaced by a cosine.

These coefficients have the properties

$$\sum_{\mathbf{r}} \varepsilon_{\mathbf{k}}^{\mathbf{r}} = |\varepsilon_{\mathbf{k}}|^2 = \prod_{j=1}^{d} \left[\frac{\sin^2(k_j L_j/2)}{\sin^2(k_j a/2)} N_j^{-1} \right] \tag{6}$$

and

$$\lim_{\{r_j \to (L_j + a)/2\}} \varepsilon_{\mathbf{k}}^{\mathbf{r}} = N^{-1/2} |\varepsilon_{\mathbf{k}}| \tag{7}$$

which reproduce the overall $\bar{\chi} = N^{-1} \sum_{\mathbf{r}} \chi(\mathbf{r})$ and "long-distance" ($\chi_{>}$) susceptibilities, respectively. The results derived here are in perfect agreement with those obtained under the more familiar PBC and APBC[17]; for instance,

$$\lim_{\{\tau_j \to 0\}} \varepsilon_{\mathbf{k}} = N^{-1/2} \delta_{\mathbf{k},0} \tag{8}$$

and

$$\lim_{\{\tau_j \to 1/2\}} \varepsilon_{\mathbf{k}} = \prod_{j=1}^{d} \{ e^{i\psi_j} N_j^{-1/2} \csc[\pi(n_j + \tfrac{1}{2})/N_j] \} \tag{9}$$

Consider the same system confined to a more general geometry $\Omega = \prod_j^{d^*} L_j \times \prod_{i=1}^{d'} L_i$, and then let $L_i \to \infty$ in the d' dimensions. The result is again Eq. (3), but with d replaced by d^* in the summation as well as distribution coefficients [see also Eqs. (15)–(18)]. The only implicit (bulk) d-dimensional dependence that remains unchanged is the variable ϕ. The $d^* = 1$ case ($\Omega = L \times \infty^{d'}$) for general $d' \leqslant 2$ can be expressed in closed form (see Appendix of ref. 11)

$$\chi(r) = \frac{1}{2J} \cdot \frac{\omega}{(\omega - 1)^2} \left\{ 1 - \frac{(1 - e^{2\pi i \tau})(\omega^{N+1-r} + \omega^r)}{(\omega + 1)(\omega^N - e^{2\pi i \tau})} \right\} \tag{10}$$

where the Hermitian variable ω is given by

$$\omega = 1 + \frac{\phi}{2} + \frac{[\phi(4+\phi)]^{1/2}}{2} \tag{11}$$

Again this agrees with results for APBC ($\tau \to 1/2$)[11] and PBC ($\tau \to 0$). For TBC physical results are recovered by taking the real part of Eq. (10).

2.1. Relationship to Correlation Function

One expects the above results for the local susceptibility, derived from Eq. (2), to be precisely reproduced from the exact zero-field ($H=0$) correlation function[20] $G(\mathbf{R}) = \langle \sigma(\mathbf{r})\, \sigma(\mathbf{r}') \rangle = \langle \sigma(\mathbf{0})\, \sigma(\mathbf{R}) \rangle$ (with $\mathbf{R} = \mathbf{r} - \mathbf{r}'$) for a system confined to a domain $\Omega = \prod_{j=1}^{d^*} L_j \times \infty^{d'}$ through the fluctuation-response theorem:

$$k_B T \chi(\mathbf{r}) = \sum_{\{R_j\}} \sum_{\{R_i\}} G(\mathbf{R}) \tag{12}$$

with $R_j = a - r_j, ..., L_j - r_j$ runs over the crystal in the finite directions ($j \in d^*$) while $R_i = -\infty, ..., \infty$ is unbounded in the infinite directions ($i \in d'$).

The exact correlation function for a fully finite $O(\infty)$ model ferromagnet ($d'=0$) of *uniform* field ϕ under TBC possessing translationally invariant (nearest neighbor) interactions has recently been determined[20,21] (see also Joyce[24] and Henkel and Weston[18])

$$G(\mathbf{R}; \Omega) = \frac{k_B T}{2JN} \sum_{\{n_j\}} \frac{\prod_{j=1}^{d} \cos(k_j R_j)}{\phi + 2 \sum_{j=1}^{d} (1 - \cos k_j a)} \tag{13}$$

Using the Poisson summation formula (PSF)

$$\sum_{q=-\infty}^{\infty} \cos(2\pi\tau q)\, I_{Nq+R/a}(x) = \frac{1}{N} \sum_{n=0}^{N-1} \cos\left[2\pi(n+\tau)\frac{R}{Na}\right] e^{x\cos[2\pi(n+\tau)/N]} \tag{14}$$

in which $I_\mu(x)$ is the modified Bessel function of integer order, along with the integral representation $\phi^{-1} = \int_0^\infty e^{-\phi x/2}\, dx/2$ in Eq. (13), and keeping L_j finite (for all $j \in d^*$) while letting $L_i \to \infty$ (for all $i \in d'$), produces a correlation function for a finite system confined to a (more general) geometry $\Omega=\prod_{j=1}^{d^*} L_j \times \infty^{d'}$, viz.

$$G(\mathbf{R};\Omega)=\frac{k_B T}{4J}\int_0^\infty e^{-\phi x/2}\prod_{j=1}^{d^*}\left[\sum_{q_j=-\infty}^{\infty}\cos(2\pi\tau_j q_j)\, e^{-x} I_{(q_j L_j+R_j)/a}(x)\right] \times \prod_{i=1}^{d'}\left[e^{-x} I_{R_i/a}(x)\right] dx \tag{15}$$

Up to this point no approximation has been made. Applying the (infinite) d'-dimensional sum in Eq. (12) to Eq. (15), with aid of the well-known identity

$$\sum_{\mu=-\infty}^{\infty} I_\mu(x)=e^x \tag{16}$$

effectively removes any structural dependence of $G(\mathbf{R};\Omega)$ on d' and (of course) R_i, where $i\in d'$. Summing over the remaining d^* (finite) dimensions, by again using Eq. (14), gives precisely the results derived from $\langle\sigma(\mathbf{r})\rangle$ in Eq. (2) confined to general geometry

$$\chi(\mathbf{r})=\frac{1}{2J}\sum_{\{n_j\}}\frac{\varepsilon_{\mathbf{k}}^{\mathbf{r}}}{\phi+2\sum_{j=1}^{d^*}(1-\cos k_j a)} \tag{17}$$

with an effective *real* contribution to the distribution coefficients

$$\varepsilon_{\mathbf{k}}^{\mathbf{r}}=\prod_{j=1}^{d^*}\left[\cos[(k_j/2)(2r_j-a-L_j)]\,\frac{\sin(k_j L_j/2)}{\sin(k_j a/2)}\,\frac{a}{L_j}\right] \tag{18}$$

Using this approach, no consideration has been given to an external field at any point in the calculation ($H=0$).

It turns out that the exact expressions for $G(\mathbf{R})$ and $\chi(\mathbf{r})$ provide more information than is required to describe their relevant scaling behavior. To see this, I shall apply a continuum version of the fluctuation-response formula to the *scaled* correlation function under TBC confined to geometry $\Omega=L^{d^*}\times\infty^{d'}$, i.e., Eq. (12) is replaced by

$$k_B T^{\chi}(\underline{\eta})\approx\left(\frac{L}{a}\right)^d \prod_{j=1}^{d^*}\int_{-\eta_j}^{1-\eta_j} d(\varepsilon_\perp)_j \prod_{i=1}^{d'}\int_{-\infty}^{\infty} d(\varepsilon_{\|})_i\, G(\underline{\varepsilon};\Omega) \tag{19}$$

where, to leading order in $|\mathbf{R}|$, $L\gg a$,[20]

$$G(\underline{\varepsilon};\Omega)\approx\frac{k_B T}{4\pi^{d/2}J}\left(\frac{a}{L}\right)^{d-2}\sum_{\mathbf{q}(d^*)}\prod_{j=1}^{d^*}\cos(2\pi\tau_j q_j) \times\left(\frac{y}{(|\mathbf{q}+\underline{\varepsilon}_\perp|^2+\varepsilon_{\|}^2)^{1/2}}\right)^{(d-2)/2} K_{(d-2)/2}(2y(|\mathbf{q}+\underline{\varepsilon}_\perp|^2+\varepsilon_{\|}^2)^{1/2}) \tag{20}$$

with scaled parameters

$$y = (L/2a)\sqrt{\phi}, \qquad \underline{\varepsilon}_\perp = \mathbf{R}_\perp/L, \qquad \underline{\varepsilon}_{||} = \mathbf{R}_{||}/L, \qquad \underline{\eta} = \mathbf{r}/L \tag{21}$$

This sum over all $\mathbf{q}$ in d^* dimensions now involves the other modified Bessel functions, $K_\nu(x)$. Integration of G over the d' dimensions is isotropic and can be reduced to a one-dimensional integral

$$\prod_{i=1}^{d'} \int_{-\infty}^{\infty} d(\varepsilon_{||})_i = \frac{2\pi^{d'/2}}{\Gamma(d'/2)} \int_0^\infty d\varepsilon_{||} \varepsilon_{||}^{d'-1}, \qquad \varepsilon_{||} = \left[\sum_{i=1}^{d'} (\varepsilon_{||})_i^2 \right]^{1/2} \tag{22}$$

the result of which is tabulated.[25] The local susceptibility in this approximation becomes

$$\chi(\underline{\eta}) \approx \frac{1}{4\pi^{d^*/2}J} \left(\frac{L}{a}\right)^2 \sum_{\mathbf{q}(d^*)} \prod_{j=1}^{d^*} \cos(2\pi\tau_j q_j) \int_{-\eta_j}^{1-\eta_j} d(\varepsilon_\perp)_j \times \left(\frac{y}{|\mathbf{q} + \underline{\varepsilon}_\perp|}\right)^{(d^*-2)/2} K_{(d^*-2)/2}(2y\,|\mathbf{q} + \underline{\varepsilon}_\perp|) \tag{23}$$

proving that the integration of Eq. (20) over $\underline{\varepsilon}_{||}$ in d' dimensions effectively removes any structural dependence of $\chi(\underline{\eta})$ on d' and (of course) $\underline{\varepsilon}_{||}$, as it applies explicitly to the parameter y (which itself may implicitly depend on d' through the spherical constraint equation[19]). This is precisely the (universal) behavior observed in the exact calculation.

Application of the PSF to Eq. (23) replaces the unbounded $\mathbf{R}_\perp$-space lattice sum by a reciprocal ($\mathbf{k}_\perp$-space) sum, thereby reducing the problem from a d^*-dimensional integral (over complicated arguments of Bessel functions) to a decoupled product of simple one-dimensional integrals contained within the distribution coefficients, whence

$$\chi(\underline{\eta}) \approx \frac{1}{8J} \left(\frac{L}{a}\right)^2 \sum_{\mathbf{n}(d^*)} \frac{\varepsilon^{\eta}_{\mathbf{n}+\underline{\tau}}}{y^2 + \pi^2\,|\mathbf{n} + \underline{\tau}|^2} \tag{24}$$

This result is valid at any temperature $T > 0$ and $L \gg a$, provided $\underline{\eta}$ is sufficiently far from the interface. The physical contribution to the scaled distribution coefficients is now given by

$$\varepsilon^{\eta}_{\mathbf{n}+\underline{\tau}} = \prod_{j=1}^{d^*} \left\{ \cos\left[2\pi(n_j + \tau_j)\left(\eta_j - \frac{1}{2}\right)\right] \cdot \frac{\sin \pi(n_j + \tau_j)}{\pi(n_j + \tau_j)} \right\} \tag{25}$$

a result which follows from Eqs. (17) and (18) directly through lowest-order infrared replacements (i.e., $k_j^{\ll a^{-1}}$) and a subsequent extension of the d^*-dimensional sum over $\mathbf{n}$ to infinity in all directions. All other contributions are irrelevant to the properties inherent in Eqs. (24) and (25).

2.2. Relationship to Correlation Length

In the region of first-order phase transition ($T < T_c$) the local susceptibility provided by Eq. (24) is asymptotically determined by those terms of the sum over $\mathbf{n}(d^*)$ for which $|\mathbf{n} + \underline{\tau}| = \tau$, with the result

$$\chi(\underline{\eta}) = g_{\underline{\tau}} \frac{1}{8J} \left(\frac{L}{a}\right)^2 \frac{\varepsilon_{\underline{\tau}}^{\underline{\eta}}}{y^2 + \pi^2 \tau^2}, \qquad y^2 \to -\pi^2 \tau^2 \tag{26}$$

Here, $g_{\underline{\tau}}$ denotes the multiplicity of terms making a dominant contribution to the expression for $\chi(\underline{\eta})$; in general, $g_{\underline{\tau}} = 2^m$, where m ($\leqslant d^*$) is the number of components, τ_j of $\underline{\tau}$ that equal 1/2—for each of these components, *two* terms (with $n_j = 0$ or -1) contribute equally toward the sum. Equation (26) reveals a close relationship between the susceptibility and the correlation length ξ as a function of boundary conditions. Under TBC this quantity is known to be[18,19]

$$\xi(T; \Omega) \approx \frac{L}{2(y^2 + \pi^2 \tau^2)^{1/2}}, \qquad 0 \leqslant \tau \leqslant (d^*)^{1/2}/2 \tag{27}$$

and upon substitution into Eq. (26) can be related to the simpler PBC ($\tau = 0$)

$$\left(\frac{\chi(\underline{\eta})}{\xi^2}\right)_{\mathrm{TBC}} \approx g_{\underline{\tau}} \varepsilon_{\underline{\tau}}^{\underline{\eta}} \left(\frac{\chi}{\xi^2}\right)_{\mathrm{PBC}}, \qquad T < T_c \tag{28}$$

Specializing to APBC and considering the overall $[\bar{\chi} \approx \prod_{j=1}^{d^*} \int_0^1 d\eta_j \, \chi(\underline{\eta})]$ and "long-distance" ($\chi_> = \chi\{\eta_j \to 1/2\}$) susceptibilities, one gets

$$\left(\frac{\bar{\chi}}{\xi^2}\right)_{\mathrm{APBC}} \approx \left(\frac{2}{\pi}\right)^{d^*} \left(\frac{\chi_>}{\xi^2}\right)_{\mathrm{APBC}} \approx \left(\frac{8}{\pi^2}\right)^{d^*} \left(\frac{\chi}{\xi^2}\right)_{\mathrm{PBC}} \tag{29}$$

which may indeed apply generally to corresponding $O(n)$ models. One observes that $\bar{\chi}/\xi^2$ is reduced below the PBC result, $1/2Ja^2$, while $\chi_>/\xi^2$ is enhanced for all relevant temperatures. At $T > T_c (y \gg 1)$, leading bulk behavior is realized $[\xi \cong \xi_B \approx L/2y \sim (T - T_c)^{-1/(d-2)}]$ with negative $O(\xi_B/L)$ finite-size corrections for $\bar{\chi}/\xi^2$ and positive $O(e^{-L/\xi_B})$ corrections for $\chi_>/\xi^2$.

In between these temperature regimes, particularly near T_c, there appears a significant variation of χ/ξ^2 [for either $\bar{\chi}$ or $\chi(\underline{\eta})$] involving the critical amplitudes.[26] If $L \to \infty$, this variation becomes cusplike. As far as exponents are concerned, the spherical model is special in that the bulk critical exponent η governing fluctuations in the order parameter is zero; hence, there is no singular temperature dependence near T_c, even in the hyperscaling regime ($d < d_> = 4$). However, for $2 \leqslant n \leqslant \infty$, the exponent η (not to be confused with the reduced distance parameter $\underline{\eta} = r/L$) is in general a small, positive number, and indeed we find by matching of first-order scaling forms in the region of second-order phase transition[27,28] the following *bulk* behavior:

$$\frac{\chi}{\xi^2} \sim \begin{cases} \dfrac{m_0^2(T)}{\Upsilon(T)} \sim (T_c - T)^{\eta\nu} & (T < T_c) \qquad (30a) \\ (T - T_c)^{\eta\nu} & (T > T_c) \qquad (30b) \end{cases}$$

where $m_0(T)$ is the spontaneous magnetization density, $\Upsilon(T)$ is the helicity modulus,[29] and ν is a critical exponent pertaining to the bulk correlation length ξ_B. We expect from finite-size scaling that there is a minimum somewhere in the core regime, where $|T - T_c|\, L^{1/\nu} = O(1)$, giving a measure of the critical rounding for $d' \leqslant 2$. It is here where the response of the system to the application of different boundary conditions is most sensitive, affecting the nature of the scaling behavior in a very significant way—for a discussion of this effect for the correlation length of the spherical model, see ref. 19.

3. INTERFACE LOCATION AS A FUNCTION OF TEMPERATURE

It is fortunate that for $d^* = 1$ ($\Omega = L \times \infty^{d'}$), $\chi(\eta)$ can be expressed in closed form, since asymptotic results for a wide range of spatial orientations at various temperatures are easily evaluated. From Eq. (23), and after some algebraic manipulation of certain one-dimensional sums, one finds

$$\chi(\eta, T; L \times \infty^{d'}) \approx \frac{1}{8J} \left(\frac{L}{ay}\right)^2 \left\{1 - \frac{\cosh[2y(\eta - 1/2)] \sin \pi\tau}{i \sinh(y - i\pi\tau)}\right\} \tag{31}$$

where, as before, the real part must be taken to get the proper physics. This result can be checked with the exact version from Eqs. (10) and (11) by considering the asymptotic replacements $\omega^N \approx e^{2y}$ and $\omega^r \approx e^{2y\eta}$, when $|\phi| \ll 1$ and $L \gg a$ at constant y. From Eqs. (10) and (31), one finds that under APBC

$$\sum_{R_\perp = r}^{L - r} G(R_\perp, R_{||}) = 0 \approx L \int_\eta^{1-\eta} d\varepsilon_\perp\, G(\varepsilon_\perp, \varepsilon_{||}) \tag{32}$$

even in the scaled (or continuum) limit, as is also true for each component of j ($\in d^* > 1$) through a direct examination of the distribution coefficients in Eqs. (18) and (25). This reveals the presence of an interface[6] in the system, resulting in a strongly uneven reduction of $\chi(\eta)$, which happens to lie at (or very near) to the origin ($\eta \sim a/L$) for all T. Under the more general TBC ($0 < \tau < 1/2$) the interface defect separating ferromagnetic $[\chi(\eta) > 0]$ from diamagnetic $[\chi(\eta) < 0]$ domains in the crystal is necessarily *outside* the range initially prescribed in calculating the extensive quantities of the system: $0 < \eta = r/L < 1$. The volume of this domain is artificially imposed and merely represents a measure or scale of the system size. The true physical domain $\Omega_{\text{phys}} = D^{d^*} \times \infty^{d'}$ is actually larger ($D > L$) and its volume (at least in the finite dimensions) can at times depend strongly on the temperature, as we shall see.

The position of the interface(s) relative to the origin ($\eta = 0$) is predetermined by the quantum number shift parameter $\underline{\tau}$, and for a system with $d^* = 1$ its position is found asymptotically from the zero(s) of Eq. (31), viz.

$$\eta = \eta_0 \approx \frac{1}{2} \pm \frac{1}{2y} \cosh^{-1}\left(\frac{1}{p^2 \cosh y}\right) \tag{33}$$

where

$$p = \left(\frac{\sinh^2 y}{\sin^2 \pi\tau} + 1\right)^{-1/2} = \prod_{n=-\infty}^{\infty} \left[1 + \frac{y^2}{\pi^2 (n+\tau)^2}\right]^{-1/2} \tag{34}$$

Equation (33) allows us to determine the behavior of $\chi(\eta)$ at any T in the vicinity of the chosen interface, i.e.,

$$\chi_<(\eta) \approx J^{-1} \left(\frac{L}{2a}\right)^2 y^{-1} (\eta - \eta_0)(1 - p^2)^{1/2} (1 + p^2 \cos^2 \pi\tau)^{1/2} \tag{35}$$

with $a/L \ll \eta - \eta_0 \ll 1$ and $0 < p < \infty$. In this interpretation $\underline{\tau}$ may be regarded as a measure of the "geometry-dependent doping level" of interfacial impurities in the extended system that severely reduce magnetic fluctuations close to an interface. It is shown here that PBC ($\tau \to 0$) represent the dilute limit where virtually no impurities exist except at infinity (i.e., $\eta_0 \to \infty$) and hence *no* pinning or infrared cutoff[19,20] occurs in the system, whereas APBC ($\tau \to 1/2$) represent saturation in which all available impurity states of the system are filled—i.e., no defects can occur inside Ω. In this sense, these position states appear as fermionic in nature.

[6] The interfacial free energy for $O(n)$ models with continuous symmetry ($n \geq 2$) is proportional to the helicity modulus[29] and should be distinguished from Ising-type systems, whose corresponding interfacial free energy is proportional to the surface tension.[10]

At $T<T_c$, $y^2 \to -\pi^2\tau^2$ and from Eq. (34)

$$p^2 \approx \begin{cases} \dfrac{\pi\tau \tan \pi\tau}{y^2+\pi^2\tau^2}, & \tau<\dfrac{1}{2} \quad (36a) \\ \left(\dfrac{\pi}{y^2+(\pi/2)^2}\right)^2, & \tau=\dfrac{1}{2} \quad (36b) \end{cases}$$

From this the short-distance susceptibility (35) becomes

$$\chi_<(\eta) \approx J^{-1}\left(\frac{L}{2a}\right)^2 (\eta-\eta_0) \begin{cases} \dfrac{\sin \pi\tau}{y^2+\pi^2\tau^2}, & \tau<\dfrac{1}{2} \quad (37a) \\ \dfrac{2}{y^2+(\pi/2)^2}, & \tau=\dfrac{1}{2} \quad (37b) \end{cases}$$

revealing the smooth variation of the factor g_τ as $\tau \to 1/2$ [see also Eq. (28)]. In the region of first-order phase transition the interface location (nearest to the origin) is independent of temperature, viz.

$$\eta_0 \approx \frac{1}{2}-\frac{1}{4\tau}, \qquad T<T_c \tag{38}$$

At the bulk critical temperature for $d=3$ we find that $y=\cosh^{-1} x$, where $x=(\frac{5}{4}-\sin^2 \pi\tau)^{1/2}$ and $p=2\sin \pi\tau$, while the seam is now in a different position:

$$\eta_0 \approx \frac{1}{2}-\frac{\cosh^{-1}[x^{-1}(5-4x^2)^{-1}]}{2\cosh^{-1} x}, \qquad T=T_c \tag{39}$$

At the temperature $T=T_0 \equiv (T)_{y\to 0}$, the interface has a location

$$\eta_0 \approx \tfrac{1}{2}-\tfrac{1}{2}(2\csc^2 \pi\tau-1)^{1/2} \tag{40}$$

which coincides with (39) when setting $\tau=1/6$ [see also Eq. (44)]. In the paramagnetic phase ($T>T_c$, $y \gg 1$), we find that $p \approx 2e^{-y}\sin \pi\tau \ll 1$ and the domain boundary is now situated at

$$\eta_0 \approx \frac{1}{2y}\ln(\sin^2 \pi\tau) \tag{41}$$

which, relative to L, for $\tau=O(1)$ is very close to (and on the negative side of) the origin. In this (paramagnetic) phase, the short-distance susceptibility has *no* L dependence, whereby

$$\chi_<(r) \approx \frac{1}{2J}\frac{\xi_B \bar{r}}{a^2}, \qquad a \ll \bar{r}=r-\xi_B \ln(\sin^2 \pi\tau) \ll \xi_B \tag{42}$$

If $\tau = 1/2$, the two interfaces are in closest proximity as $\eta_0 \approx 0, 1$ for all temperature. If $\tau < 1/2$, η_0 is outside the range Ω for all T and is farthest away at lower temperatures. When τ tends to zero, the interfaces spread out more until they reach infinity.

In order to determine y (or ϕ) as a function of size and temperature of the system one has to examine the constraint equation [for $H = 0$; see Eq. (13)]

$$G(\mathbf{R} = 0, T; L^d) = 1 = \frac{k_B T}{2JN} \sum_{\{n_j\}} \frac{1}{\phi + 2\sum_{j=1}^{d} (1 - \cos k_j a)} \tag{43}$$

which in scaled form, for a system confined to geometry $\Omega = L \times \infty^2$ at $T = T_0$ (i.e., $y = 0$), becomes[19,30]

$$\frac{1}{T_0} - \frac{1}{T_c} \approx -\frac{k_B a}{4JL} \ln(2 \sin \pi\tau), \qquad L \gg a \tag{44}$$

It is apparent from this that as τ gets very small $O(e^{-JL/k_B T a})$ the temperature T_0 slips out of the critical region and firmly into the region of first-order phase transition ($T < T_c$). Specifically, by setting $T = T_0 = (l+1)^{-1} T_c$ in Eq. (44) where $l > 0$, we find that the correlation length (27) for a system confined to the ferromagnetic domain $\Omega_{\text{phys}} = D \times \infty^2$ of width $D \approx \sqrt{2}\, L/\pi\tau$ becomes

$$\left.\frac{\xi}{L}\right|_{T = T_0} \approx \frac{1}{2\pi\tau} \approx e^{4\pi J l L/k_B T_c} = e^{2\pi[\Upsilon(T_0)/k_B T_0] L} \tag{45}$$

where $\Upsilon(T) = 2Ja^5 m_0^2(T) = (2J/a)(1 - T/T_c)$ is the helicity modulus of the spherical model.[29] This is precisely the scaling behavior observed for ξ under PBC in the region $T < T_c$ ($d' = 2$, $d = 3$).[28] In this limit of very small τ, the temperature $T_0 < T_c$, separating real and imaginary y, appears to be where a type of large-scale structural phase transition occurs (while bulk quentities remain unaffected). To illustrate how this phase transition appears, we examine the (short) long-range order of the correlation function[20]

$$a^{-2d} G(R \ll \xi, T < T_c; \Omega_{\text{phys}}) \approx \begin{cases} m_0^2(T) \cos(2\pi\tau R_\perp/L), & T < T_0 \quad (46a) \\ m_0^2(T), & T > T_0 \quad (46b) \end{cases}$$

When $\tau R_\perp/L = O(1)$ and $L \ll R = O(\xi_{T=T_0}) \ll \xi$ we must have $T < T_0$— only then is the cosine factor in Eq. (46a) relevant. Otherwise if $T > T_0$, it is necessary that $\tau R/L \ll 1$ in order for $R \ll \xi_{T>T_0} \ll \xi_{T=T_0}$ to contribute to the (short) long-range order in $G(\mathbf{R})$. Therefore, at temperatures above T_0 the parameter τ (in this case governing the twist in the order parameter field) is *irrelevant* for $G(R \ll \xi, T > T_0)$, while below T_0 it may play a dominant role, even for τ exponentially small.

Finally, it is instructive to determine the characteristic domain length D as a function of temperature for very small τ:

(i) At $T \geqslant T_c > T_0$,

$$D \approx \frac{L}{y} \ln\left(\frac{1}{\tau^2}\right) \gg \xi \cong \xi_B \tag{47}$$

where $y = \ln[(1+\sqrt{5})/2]$ for $T = T_c$ and $y \approx L/2\xi_B \gg 1$ for $T > T_c$.

(ii) At $T_0 \leqslant T < T_c$ we find that $0 \leqslant y \sim \tau \ll 1$, and thus

$$D \approx \frac{L}{y} \cosh^{-1}\left(1 + \frac{y^2}{\pi^2\tau^2}\right) \sim \frac{L}{y} > \xi \tag{48}$$

(iii) At $T < T_0$, $y^2 \to -\pi^2\tau^2$ and

$$D \approx L/2\tau \ll \xi \tag{49}$$

One interesting feature here is that, although domain walls are farther apart at lower T (relative to a or L), their separation relative to ξ is indeed much narrower (or more correlated) than at higher temperatures. In region (iii) an *extended* striped ($d^* = 1$) or checkerboard ($d^* = 2, 3, \ldots$) superlattice of ferrodiamagnetic domains exists within the range of correlation ($D \ll \xi$); moreover the interfaces are frozen independently of temperature for any $T < T_0$ (see also ref. 14). This effect should not be confused with the temperature-independent saturation for systems under APBC at all $T > 0$. In regions (i) and (ii), interface location shows a dependence on temperature through the (thermogeometric) parameter $y(T; \Omega)$ and one finds that $\chi(\eta)$, for η significantly outside the domain containing the origin ($D > \xi$), gives unphysical results.

4. CONCLUDING REMARKS

The results reported in this paper provide a significant extension to an earlier calculation of the local susceptibility $\chi(\mathbf{r}, T; \Omega)$ of a finite-sized spherical model ferromagnet ($\Omega = L^{d-d'} \times \infty^{d'}$, $d' \leqslant 2$) under antiperiodic boundary conditions.[11] Essentially, I repeat the analysis for the same system subject to a more general set of *twisted* boundary conditions, defined through a continuously varying parameter $\underline{\tau}(d-d')$, with components τ_j such that $0 \leqslant \tau_j \leqslant 1/2$ [see Eq. (1)]; this generalizes the concept of boundary conditions from the extreme case of PBC on the one hand to APBC on the other. It is appealing to leave $\underline{\tau}$ as an adjustable parameter, as it controls the collective-mode behavior of the system leading to a host of characteristic finite-size effects. These effects, in the case of the correlation function[20] and correlation length,[19] have been investigated recently and have shown a nontrivial dependence on τ at various regimes of temperature. Similarly, in this study the finite-size scaling behavior of $\chi(\mathbf{r})$ and the relative position of interfaces are also greatly influenced by this effect. By including the whole range of TBC in the analysis, new physical information is observed not evident for systems under PBC or even APBC.

To begin with, I have shown that under all TBC the local susceptibility, as derived from the magnetization $\langle \sigma(\mathbf{r}) \rangle$ in the presence of a uniform external field ($H > 0$), is precisely the same as that derived from the zero-field ($H = 0$) correlation function $G(\mathbf{R}) \equiv \langle \sigma(\mathbf{r})\, \sigma(\mathbf{r}') \rangle = \langle \sigma(0)\, \sigma(\mathbf{R}) \rangle$ through the fluctuation-response theorem. Furthermore, it is remarkable that *all* relevant features of $\chi(\mathbf{r})$ are retained if we replace the exact correlation function of Eq. (13) or (15) with its asymptotic version (valid for $R, L \gg a$) in Eq. (20), and then apply an *integration* [Eq. (19)] instead of a *summation* [Eq. (12)] over the "initial" domain $\Omega = L^{d-d'} \times \infty^{d'}$. A possible *universal* feature observed in this work that may apply to more general systems under the same conditions is the apparent shift in dimensionality of the system [$d \to d^*$, cf. Eq. (20) $\to$ Eq. (23)] upon integrating (or summing) the correlation function over $\varepsilon_{\|} = R_{\|}/L$ in the d' (infinite) dimensions.

Next, a closed-form description of the local susceptibility is used to provide information on the interface location(s) (or domain length D defining $\Omega_{\text{phys}} = D \times \infty^2$) from the zero(s) of $\chi(\eta)$. Then the behavior of $\chi(\eta)$ in the vicinity of the seam is found in terms of $y(T; \Omega)$ for general $T > 0$. As τ becomes exponentially small, a type of structural phase transition appears at T_0 ($< T_c$, where $T_0 = 0$ at $\tau = 0$), very similar in form to the "second transition" observed for the spherical model under *external* boundary conditions.[14] Although there can be no well-defined bulk analog to this phenomenon without applying an external field, similar properties exist between the two phase transitions. For instance, a *ground-state* condensation takes place for $T < T_0$ (i.e., the magnetization profile freezes), while a generalized condensation of a possible infinite number of low-lying energy levels occurs for $T_0 < T < T_c$ (i.e., there is a temperature dependence in the profile)—for details and further references, see Patrick.[14] When $T < T_0$ we find that $L \ll D \ll \xi$ ($y^2 < 0$), whereas if $T > T_0$, $L \ll \xi < D$ ($y^2 > 0$). This is reminiscent of a commensurate–incommensurate (CI) transition,[16,31] in that there is a periodic superstructure of domains commensurate with the ground-state spin-wave mode $\mathbf{k}_0 = 2\pi\underline{\tau}/L$ at $T < T_0$. In the incommensurate phase ($T > T_0$), this periodicity is irrelevant, as the location of domain walls now depends continuously on temperature, while results significantly outside the domain Ω_{phys} are essentially uncorrelated. The main difference is that a CI transition is customarily investigated for models with competing short-range interactions providing a *microscopic* modulation in the system $[D \leqslant O(\xi_B) \ll L]$, whereas here the competition is between ferromagnetic nearest neighbor interactions and the imposed (internal) nonperiodic boundary conditions $(0 < \tau \leqslant 1/2)$, varying over much larger length scales $[\xi \gg D \geqslant O(L)]$, thereby causing a much weaker (yet influencial) *macroscopic* modulation in the system.

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