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Spin-spin correlations in a finite-sized spherical model under twisted boundary conditions

Scott Allen and R. K. Pathria
Department of Physics, University of Waterloo, Waterloo, Ontario, Canada N2L 3G1
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Finite-size effects in the correlation function $G(\mathbf{R},T;L)$ of a spherical-model ferromagnet, confined to geometry $L^{d-d'}\times\infty^{d'}$ $(2<d<4, d'\leq 2)$ and subjected to *twisted* boundary conditions, are analyzed. Focusing our attention on the region of first-order phase transition ($T<T_c$), we examine the influence of the twist parameter τ on the function $G(\mathbf{R},T;L)$ in different regimes of the distance parameter $\boldsymbol{\varepsilon}$ ($=\mathbf{R}/L$). We find that the functional dependence of the function G on the parameter $\boldsymbol{\varepsilon}$ is highly anisotropic, in that it depends very differently on the components, $\boldsymbol{\varepsilon}_\perp$ and $\boldsymbol{\varepsilon}_\parallel$, of $\boldsymbol{\varepsilon}$ pertaining to the finite and the infinite directions, respectively. While the long-range order in the direction of $\boldsymbol{\varepsilon}_\perp$ is significantly altered by the parameter τ, it is curtailed very seriously in the direction of $\boldsymbol{\varepsilon}_\parallel$. In fact, for $\varepsilon_\parallel \gg 1$, the qualitative features of the correlation function acquire characteristics of a d'-dimensional bulk system, though the correlation length ξ appearing therein still pertains to the actual, finite-sized system. The net result is that long-range order in the direction of $\mathbf{R}_\parallel$ persists only to distances small in comparison with ξ which, for $d'<2$, is known to be $O\{L(L/a)^{(d-2)/(2-d')}\}$, a being the lattice constant.

I. INTRODUCTION

In recent years considerable attention has been paid to the study of phase transitions in finite-sized systems with a view to examining the manner in which the various physical quantities pertaining to the system are influenced by the finiteness of the space to which it is confined and to determining the extent to which the predicted behavior of the system conforms to the dictates of the finite-size scaling theory; for an overview of these matters, see review articles by Barber[1] and Privman.[2] While studies along these lines have covered certain aspects of the problem with relative thoroughness—in that they have looked at $O(n)$ models with continuous ($n\geq 2$) as well as discrete ($n=1$) symmetry, models confined to a general geometry $L^{d-d'}\times\infty^{d'}$ (with different regimes of the parameters d and d'), models undergoing a first-order phase transition ($T<T_c$) as well as those undergoing a second-order phase transition ($T\simeq T_c$), etc.—an aspect that has not been so well covered is the one relating to the nature of the boundary conditions imposed on the system. Frequently, for reasons of simplicity (if nothing else), one employs periodic boundary conditions (PBC's) and hopes that the results so obtained reflect the reality of the situation under study. On occasion, one employs nonperiodic boundary conditions and obtains results significantly different from the ones following from PBC's, leading to the inference that the correct choice of the boundary conditions for any given situation is, in all likelihood, a nontrivial matter. Several instances of this have appeared in the literature and are recorded in the review articles cited above.

A specific instance of this type arose in the study of magnetic susceptibility, both local $\chi(\mathbf{r},T;L)$ and overall $\bar{\chi}(T;L)$, of a finite-sized spherical model confined to geometry $L^{d-d'}\times\infty^{d'}$ (with $2<d<4$ and $d'\leq 2$) and subjected to antiperiodic boundary conditions (APBC's).[3,4] The results obtained in that study differed radically from the ones pertaining to PBC's (Ref. 5) and, in turn, threw new light on the physics underlying that problem. In particular, we learned something about the role played by the "antiferromagnetic seams" introduced by the APBC's,

$$s(r_j+L_j)=-s(r_j)\quad (j=1,\ldots,d^*;\ d^*=d-d')\ , \tag{1}$$

at the points $r_j=L_j$ of the lattice. Although these interfacial seams appear to have no local effect on the free-energy density $f^{(s)}$ of the system in a strictly zero magnetic field, the application of a nonzero field converts them into local inhomogeneities in the lattice, for spins on either side of an interface are, in effect, coupled to the field in opposite senses (relative to their preferred local alignment). This led to a somewhat unexpected result for χ revealing a broken translational invariance more in line with systems under free boundary conditions,[6] and yet APBC's appear to be more akin to PBC's, since in both cases the excited states of the system can be decomposed into plane waves; of course, the isotropic interactions among nearest-neighbor spins are not in any way altered by the interfaces imposed through APBC's. We suspect that the presence of these seams would have a major influence on the spin-spin correlation function $G(\mathbf{R},T;L)$ as well, for the latter determines χ directly through the fluctuation-response theorem—without the necessity of applying an external field at any point in the calculation.[4] As far as we know, this influence has not been explored to any significant extent so far.

Another aspect of the foregoing results is that the problem is diagonalizable under the APBC's as well, requiring a mere shift in the eigenvalues of the system. In the absence of an external magnetic field, each spin in the system is equivalent; consequently, the correlation function at zero separation is independent of location—as is the case with PBC's—for the constraint equation $N^{-1}\sum_{\mathbf{r}}\langle s^2(\mathbf{r})\rangle=1$ turns out to be equivalent to the constraint $\langle s^2(\mathbf{r})\rangle=1$ at each site $\mathbf{r}$ under both PBC's and

APBC's. This ensures that a uniform spherical field[4,7] λ is sufficient to describe the function $G(\mathbf{R},T;L)$ as well as the local features of the quantity χ. Even if we do not assume spin equivalence to begin with and the spherical field in the original model is space dependent, the present model, as represented by Eq. (3), may be termed the "mean-spherical-field" model.

In this paper we analyze the correlation function of a finite-sized spherical model under nonperiodic boundary conditions and examine the characteristic influence of these boundary conditions in different regimes of the parameters $\boldsymbol{\varepsilon}$ $(=\mathbf{R}/L)$ and T. For generality, we employ the so-called twisted boundary conditions (TBC's), defined through a continuously varying parameter $\boldsymbol{\tau}$ (with components $\tau_1,\ldots,\tau_{d^*}$), of which PBC's $(\tau_j=0)$ and APBC's $(\tau_j=\frac{1}{2})$ are two extreme cases; the TBC's employed here are essentially the same as the ones used recently by Chakravarty[8] and by Brézin *et al.*[9] It is important to emphasize here that, just as in the case of APBC's, a uniform spherical field is quite appropriate to describe all relevant properties of the system under the *entire* set of TBC's, provided that a phase factor in the form of (2) is incorporated into the boundary conditions. For analysis, we follow the approach of an earlier paper by Singh and Pathria[10] (hereafter referred to as *I*), which tackled the same problem under PBC's; however, the situation with $\tau>0$ can at times be so different from the one with $\tau=0$ that both physical and mathematical aspects of the analysis have to be handled with special care. In Sec. II we establish the basic expressions for the correlation function $G(\mathbf{R},T;L)$ in three different forms, so that in different regimes of the parameters involved one may employ the form most suited for the occasion. In Sec. III we examine finite-size effects in the correlation function and analyze them in detail for different regimes of interest. Not surprisingly, the effect associated with the component $\mathbf{R}_{\parallel}$ of $\mathbf{R}$ (which pertains to directions in which the system is infinite) turns out to be very different in nature from the one associated with the component $\mathbf{R}_{\perp}$ (which pertains to directions in which the system is finite). The contrast between the two becomes most dramatic when one considers the propagation of long-range order in the system at temperatures below T_c over a wide range of distances. In fact, for $R_{\parallel} \gg L$, the mathematical form of the correlation function bears no resemblance to the one for a d-dimensional bulk system; it becomes characteristic of a d'-dimensional bulk system instead. In the process, it yields a much-needed expression for the correlation length, $\xi(T;L)$, of the system that is rather tricky to obtain otherwise.[11,12] At the same time, even the term representing long-range order in the system (that continues to govern correlations in the direction of $\mathbf{R}_{\perp}$) does not escape the (adverse) influence of the TBC's, which contrasts sharply with the case of PBC's that leave this term unaffected. Finally, in Sec. IV, we make some general remarks on the problem studied here.

II. CORRELATION FUNCTION OF A FINITE-SIZED SPHERICAL MODEL UNDER TWISTED BOUNDARY CONDITIONS

We consider a spherical-model system based on a simple hypercubic lattice of dimensions $L_1\times\cdots\times L_d$ and subjected to twisted boundary conditions

$$s(r_j+L_j)=e^{2\pi i\tau_j}s(r_j)\quad (j=1,\ldots,d)\,, \tag{2}$$

where $\boldsymbol{\tau}$ is a vector whose components $\tau_1,..,\tau_d$ lie in the interval $(0,\frac{1}{2})$. In view of the fact that the zero-field spin-spin correlation function of the system must be *even* in all components of $\mathbf{R}$, we have[11–14]

$$G(\mathbf{R},T;L)=\frac{T}{2N}\sum_{\{n_j\}}\frac{\prod_{j=1}^{d}\cos(k_jR_j)}{\lambda-2J\sum_{j=1}^{d}\cos(k_ja)}\,, \tag{3}$$

where

$$k_j=2\pi(n_j+\tau_j)/L_j\,,$$
$$n_j=0,1,\ldots,N_j-1\,, \tag{4}$$
$$N_j=L_j/a,\quad N=\prod_{j=1}^{d}N_j\,;$$

here λ denotes the uniform "spherical field" pertaining to the model, J is the nearest-neighbor interaction parameter, while a is the lattice constant. The field λ is determined by the constraint equation[3,14]

$$N=\frac{T}{2}\sum_{\{n_j\}}\frac{1}{\lambda-2J\sum_{j=1}^{d}\cos(k_ja)}\,. \tag{5}$$

Following the procedure developed in *I* and choosing our geometry to be $L^{d^*}\times\infty^{d'}$, where $d^*+d'=d>2$, we obtain (for R_j, $L\gg a$)

$$G(\mathbf{R},T;L)\approx\frac{T}{4\pi^{d/2}J}\left[\frac{a}{L}\right]^{d-2}\sum_{\mathbf{q}(d^*)}\prod_{j=1}^{d^*}\cos(2\pi\tau_jq_j)\left[\frac{y}{\sqrt{|\mathbf{q}+\boldsymbol{\varepsilon}_\perp|^2+\varepsilon_\parallel^2}}\right]^{(d-2)/2}K_{(d-2)/2}\left(2y\sqrt{|\mathbf{q}+\boldsymbol{\varepsilon}_\perp|^2+\varepsilon_\parallel^2}\right)\,, \tag{6}$$

where

$$\boldsymbol{\varepsilon}_\perp=\mathbf{R}_\perp/L,\quad \boldsymbol{\varepsilon}_\parallel=\mathbf{R}_\parallel/L\,; \tag{7}$$

here, $\mathbf{R}_\perp$ is the component of $\mathbf{R}$ in the d^*-dimensional subspace in which the system is finite in extent, while $\mathbf{R}_\parallel$ $(=\mathbf{R}-\mathbf{R}_\perp)$ is the corresponding component in the d'-dimensional subspace in which the system is infinite. The sum involving modified Bessel functions $K_\nu(x)$ goes over the entire $\mathbf{q}$ space in d^* dimensions, while the parameter y is a *scaled* variable, defined by the relation

$$y=\frac{1}{2}\frac{L}{a}\sqrt{\phi}\quad\left[\phi=\frac{\lambda}{J}-2d\right], \tag{8}$$

and is determined by the constraint equation (5), which takes the form[12]

$$\left[\frac{1}{T}-\frac{1}{T_c}\right]\approx\frac{1}{4\pi^{(4-d)/2}J}\left[\frac{a}{L}\right]^{d-2}Q_\tau\left[\frac{d-2}{2}\middle|d^*;y\right]\quad(2<d<4), \tag{9}$$

where

$$Q_\tau(\nu|d^*;y)=\left[\frac{y^2}{\pi^2}\right]^\nu\left[\sum_{\mathbf{q}(d^*)}{}'\prod_{j=1}^{d^*}\cos(2\pi\tau_j q_j)\frac{K_\nu(2yq)}{(yq)^\nu}+\frac{1}{2}\Gamma(-\nu)\right]; \tag{10}$$

note that the primed summation over $\mathbf{q}(d^*)$ appearing here excludes the term with $\mathbf{q}=\mathbf{0}$.

Now, since the minimum value of λ under the present boundary conditions, see Eqs. (3) and (4), is

$$\lambda_{\min}=2J\sum_{j=1}^{d}\cos(2\pi a\tau_j/L)\simeq 2Jd-\frac{4\pi^2Ja^2}{L^2}\sum_{j=1}^{d^*}\tau_j^2, \tag{11}$$

the minimum value of y^2, attainable at $T=0$ K, is $-\pi^2\tau^2$. As shown elsewhere,[15] the function Q_τ, defined in (10), is regular in y^2 for all $y^2>-\pi^2\tau^2$; accordingly, Eq. (9) determines y^2, as a function of T and L, for all $T>0$ K. In the same vein, we expect that expression (6) for $G(\mathbf{R},T;L)$ is also regular in y^2 for all $y^2>-\pi^2\tau^2$. To see this explicitly, we apply Poisson's summation formula to the sum in (6), with the result

$$G(\mathbf{R},T;L)\approx\frac{T}{4\pi^{d'/2}J}\left[\frac{a}{L}\right]^{d-2}\sum_{\mathbf{n}(d^*)}\prod_{j=1}^{d^*}\cos\{2\pi\varepsilon_j(n_j+\tau_j)\}\left[\frac{\varepsilon_\parallel}{\sqrt{y^2+\pi^2|\mathbf{n}+\boldsymbol{\tau}|^2}}\right]^{(2-d')/2}K_{(2-d')/2}(2\varepsilon_\parallel\sqrt{y^2+\pi^2|\mathbf{n}+\boldsymbol{\tau}|^2}). \tag{12}$$

Expression (12), without any problem, can be continued analytically into the region $y^2<0$—right up to, but excluding, the point $y^2=-\pi^2\tau^2$, where the true singularity of the problem lies. In terms of temperature, this expression is manifestly valid down to, but excluding, $T=0$ K.

In view of the fact that our expressions for $G(\mathbf{R},T;L)$ are regular for all $y^2>-\pi^2\tau^2$, we may obtain yet another form, which turns out to be very useful in the region of first-order phase transition ($T<T_c$). For $0>y^2>-\pi^2\tau^2$, which covers the entire region of the first-order phase transition as well as a part of the region of the second-order phase transition, we define a new variable $v=\sqrt{-y^2}$, so that $0<v<\pi\tau$. In terms of v, Eq. (6) takes the form (see Appendix A)

$$G(\mathbf{R},T;L)\approx\frac{T\,\mathrm{cosec}\{\pi(d-2)/2\}}{8\pi^{(d-2)/2}J}\left[\frac{a}{L}\right]^{d-2}\times\sum_{\mathbf{q}(d^*)}\prod_{j=1}^{d^*}\cos(2\pi\tau_j q_j)\left[\frac{v}{\sqrt{|\mathbf{q}+\boldsymbol{\varepsilon}_\perp|^2+\varepsilon_\parallel^2}}\right]^{(d-2)/2}J_{-(d-2)/2}(2v\sqrt{|\mathbf{q}+\boldsymbol{\varepsilon}_\perp|^2+\varepsilon_\parallel^2}), \tag{13}$$

where $J_{-\nu}(x)$ is an ordinary Bessel function. The parameter v, as a function of T and L, is determined by the corresponding version of Eq. (9), viz., the one with

$$Q_\tau(\nu|d^*;v)=\frac{\pi\,\mathrm{cosec}(\pi\nu)}{2}\left[\frac{v^2}{\pi^2}\right]^\nu\sum_{\mathbf{q}(d^*)}{}'\prod_{j=1}^{d^*}\cos(2\pi\tau_j q_j)\frac{J_{-\nu}(2vq)}{(vq)^\nu}, \tag{14}$$

that is,

$$\left[\frac{1}{T}-\frac{1}{T_c}\right]\approx\frac{\mathrm{cosec}\{\pi(d-2)/2\}}{8\pi^{(d-2)/2}J}\left[\frac{a}{L}\right]^{d-2}\sum_{\mathbf{q}(d^*)}{}'\prod_{j=1}^{d^*}\cos(2\pi\tau_j q_j)\left[\frac{v}{q}\right]^{(d-2)/2}J_{-(d-2)/2}(2vq). \tag{15}$$

Note that in the summands of Eqs. (10), (14), and (15) the factor $\prod_{j=1}^{d^*}\cos(2\pi\tau_j q_j)$ may be replaced by a better-looking factor, $\cos(2\pi\boldsymbol{\tau}\cdot\mathbf{q})$, for the additional terms so added vanish identically on summation over $\mathbf{q}(d^*)$. This completes the derivation of our basic expressions for the function $G(\mathbf{R},T;L)$.

III. FINITE-SIZE EFFECTS IN THE CORRELATION FUNCTION

We start with the regime $T\gtrsim T_c$ for which $y\gg1$. As seen earlier,[12] the parameter y and the *bulk* correlation length ξ_B in this regime are connected by a straightforward, τ-independent relationship, viz., $\xi_B=L/2y=O(a)$. In view of this relationship, Eq. (6) may be written as

$$G(\mathbf{R},T;L)\approx\frac{T}{2(2\pi)^{d/2}J}\sum_{\mathbf{q}(d^*)}\prod_{j=1}^{d^*}\cos(2\pi\tau_j q_j)\left[\frac{a^2}{\xi_B\sqrt{|\mathbf{q}L+\mathbf{R}_\perp|^2+R_\parallel^2}}\right]^{(d-2)/2}K_{(d-2)/2}(\sqrt{|\mathbf{q}L+\mathbf{R}_\perp|^2+R_\parallel^2}/\xi_B)\;. \tag{16}$$

Since L here is much greater than ξ_B, contributions from terms with $\mathbf{q}\neq\mathbf{0}$ toward the sum in (16) are exponentially small. The major contribution coming from the term with $\mathbf{q}=\mathbf{0}$, we recover the standard bulk result

$$G(\mathbf{R},T;\infty^d)=\frac{T}{2(2\pi)^{d/2}J}\left[\frac{a^2}{\xi_B R}\right]^{(d-2)/2}K_{(d-2)/2}(R/\xi_B) \tag{17a}$$

$$\approx\frac{Ta^{d-2}}{4J\xi_B^{(d-3)/2}(2\pi R)^{(d-1)/2}}e^{-R/\xi_B}\quad(R\gg\xi_B)\;. \tag{17b}$$

For $T<T_c$, we employ Eq. (13) instead, split the ($\mathbf{q}=\mathbf{0}$) term from the rest of the sum and combine the latter with Eq. (15). This gives

$$G(\mathbf{R},T;L)=\left[1-\frac{T}{T_c}\right]+\frac{T\operatorname{cosec}\{\pi(d-2)/2\}}{8\pi^{(d-2)/2}J}\left[\frac{a^2 v}{LR}\right]^{(d-2)/2}J_{-(d-2)/2}\left[\frac{2vR}{L}\right]+G^*(\mathbf{R},T;L)\quad(0<v<\pi\tau)\;, \tag{18}$$

where

$$G^*(\mathbf{R},T;L)=\frac{T\operatorname{cosec}\{\pi(d-2)/2\}}{8\pi^{(d-2)/2}J}\left[\frac{a}{L}\right]^{d-2}\sum_{\mathbf{q}(d^*)}{}'\prod_{j=1}^{d^*}\cos(2\pi\tau_j q_j)\left[\left[\frac{v}{\Lambda_\varepsilon(\mathbf{q})}\right]^{(d-2)/2}J_{-(d-2)/2}[2v\Lambda_\varepsilon(\mathbf{q})]-\left[\frac{v}{\Lambda_0(\mathbf{q})}\right]^{(d-2)/2}J_{-(d-2)/2}[2v\Lambda_0(\mathbf{q})]\right]\;, \tag{19}$$

while

$$\Lambda_\varepsilon(\mathbf{q})=\sqrt{|\mathbf{q}+\boldsymbol{\varepsilon}_\perp|^2+\varepsilon_\parallel^2},\quad \Lambda_0(\mathbf{q})=q\;. \tag{20}$$

For $vR\ll L$, we make use of the expansion[16]

$$J_{-\nu}(x)=\frac{\left[\frac{1}{2}x\right]^{-\nu}}{\Gamma(1-\nu)}-\frac{\left[\frac{1}{2}x\right]^{2-\nu}}{\Gamma(2-\nu)}+\cdots\quad(0<\nu<1,\ x\ll 1)\;, \tag{21}$$

along with the standard result

$$\sin(\pi\nu)=\frac{\pi}{\Gamma(\nu)\Gamma(1-\nu)}\;; \tag{22}$$

the middle term in (18) then gives

$$\frac{T}{8\pi^{d/2}J}\Gamma\left[\frac{d-2}{2}\right]\left[\frac{a}{R}\right]^{d-2}+\frac{T}{8\pi^{d/2}J}\Gamma\left[\frac{d-4}{2}\right]\frac{(\pi^2\tau^2)a^{d-2}R^{4-d}}{L^2}+\cdots\;. \tag{23}$$

One readily sees that the leading terms in Eqs. (18) and (23), together, reproduce the *bulk* correlation function for $T<T_c$, while the subsequent terms of (23), along with the function $G^*(\mathbf{R},T;L)$, determine finite-size effects.

In what follows we focus our attention on the region of first-order phase transition ($T<T_c$) and carry out an explicit study of finite-size effects in the function $G(\mathbf{R},T;L)$ for different regimes of the parameters $\boldsymbol{\varepsilon}_\perp$ and $\boldsymbol{\varepsilon}_\parallel$.

A. Case 1: $R\ll L$

Expression (19) in this case may be expanded as a power series in the variables $\varepsilon_\perp^2$ and $\varepsilon_\parallel^2$. Assuming, for simplicity, that $\tau_1=\cdots=\tau_{d^*}$ ($=\tau/\sqrt{d^*}$) and retaining only the leading terms of the series, we obtain for the function $G^*(\mathbf{R},T;L)$

$$\frac{Tv^d}{8\pi^{(d-2)/2}Jd^*}\left[\frac{a}{L}\right]^{d-2}\left[-2\mathcal{J}_\tau\left[\frac{d-2}{2}\middle|d^*;v\right]\varepsilon_\perp^2+\mathcal{J}_\tau\left[\frac{d}{2}\middle|d^*;v\right](d'\varepsilon_\perp^2-d^*\varepsilon_\parallel^2)\right]\;, \tag{24}$$

where

$$\mathcal{J}_\tau(\nu|d^*;v)=\operatorname{cosec}(\pi\nu)\sum_{\mathbf{q}(d^*)}{}' \cos(2\pi\boldsymbol{\tau}\cdot\mathbf{q})\frac{J_{-\nu}(2vq)}{(vq)^\nu} . \tag{25}$$

Now, the first term in (24) may be simplified with the help of Eq. (15), yielding

$$-\left[1-\frac{T}{T_c}\right]\frac{2v^2}{d^*}\varepsilon_\perp^2 \approx -\left[1-\frac{T}{T_c}\right]\frac{2\pi^2\tau^2}{d^*}\varepsilon_\perp^2 . \tag{26a}$$

The second term, on the other hand, reduces to

$$\frac{\pi^{d/2}T}{4Jd^*}N_\tau\left[\frac{d}{2}\middle|d^*\right]\left[\frac{a}{L}\right]^{d-2}(d'\varepsilon_\perp^2-d^*\varepsilon_\parallel^2) , \tag{26b}$$

where the constant $N_\tau(\nu|d^*)$ has been defined in Ref. 15. Equations (26), along with the L-dependent term in (23), determine the leading finite-size effects in this regime.

B. Case 2: $R=O(L)$

For this case we go back to the full correlation function $G(\mathbf{R},T;L)$, see Eq. (6), and write

$$G(\mathbf{R},T;L)\approx\frac{T}{4\pi^{(4-d)/2}J}\left[\frac{a}{L}\right]^{d-2}Q_\tau^\varepsilon\left[\frac{d-2}{2}\middle|d^*;y\right] , \tag{27}$$

where Q_τ^ε is a generalization of (10):

$$Q_\tau^\varepsilon(\nu|d^*;y)=\left[\frac{y^2}{\pi^2}\right]^\nu\sum_{\mathbf{q}(d^*)}\prod_{j=1}^{d^*}\cos(2\pi\tau_j q_j)\frac{K_\nu(2y\sqrt{|\mathbf{q}+\boldsymbol{\varepsilon}_\perp|^2+\varepsilon_\parallel^2})}{(y\sqrt{|\mathbf{q}+\boldsymbol{\varepsilon}_\perp|^2+\varepsilon_\parallel^2})^\nu} \quad (\varepsilon>0). \tag{28a}$$

Equivalently, we may write in terms of v

$$Q_\tau^\varepsilon(\nu|d^*;v)=\frac{\pi\operatorname{cosec}(\pi\nu)}{2}\left[\frac{v^2}{\pi^2}\right]^\nu\sum_{\mathbf{q}(d^*)}\prod_{j=1}^{d^*}\cos(2\pi\tau_j q_j)\frac{J_{-\nu}(2v\sqrt{|\mathbf{q}+\boldsymbol{\varepsilon}_\perp|^2+\varepsilon_\parallel^2})}{(v\sqrt{|\mathbf{q}+\boldsymbol{\varepsilon}_\perp|^2+\varepsilon_\parallel^2})^\nu} \quad (\varepsilon>0); \tag{28b}$$

cf. Eq. (14). A third version, which is most useful in determining the limiting behavior of the function Q_τ^ε as $y^2\to-\pi^2\tau^2$, or $v\to\pi\tau$, is obtained by applying Poisson's summation formula to Eq. (28a), with the result

$$Q_\tau^\varepsilon(\nu|d^*;y)=\pi^{d^*/2-2\nu}\sum_{\mathbf{n}(d^*)}\prod_{j=1}^{d^*}\cos\{2\pi\varepsilon_j(n_j+\tau_j)\}\left[\frac{\varepsilon_\parallel}{\sqrt{y^2+\pi^2|\mathbf{n}+\boldsymbol{\tau}|^2}}\right]^{d^*/2-\nu}K_{d^*/2-\nu}(2\varepsilon_\parallel\sqrt{y^2+\pi^2|\mathbf{n}+\boldsymbol{\tau}|^2}) , \tag{28c}$$

which, when substituted into (27), leads to Eq. (12), as expected.

It is not difficult to see that the functions Q_τ^ε satisfy the recurrence relation

$$\frac{\partial}{\partial\varepsilon_\parallel^2}[\pi^{2\nu}Q_\tau^\varepsilon(\nu|d^*;y)]=-\pi^{2(\nu+1)}Q_\tau^\varepsilon(\nu+1|d^*;y) . \tag{29}$$

Equation (27) may, therefore, be expanded as a power series in $\varepsilon_\parallel^2$:

$$G=\frac{T}{4\pi^{(4-d)/2}J}\left[\frac{a}{L}\right]^{d-2}\sum_{l=0}^{\infty}Q_\tau^{\varepsilon_\perp}\left[\frac{d}{2}-1+l\middle|d^*;y\right]\frac{(-\pi^2\varepsilon_\parallel^2)^l}{l!} , \tag{30}$$

where

$$Q_\tau^{\varepsilon_\perp}(\nu|d^*;y)=[Q_\tau^\varepsilon(\nu|d^*;y)]_{\varepsilon_\parallel=0} . \tag{31}$$

The limiting behavior of the function $Q_\tau^{\varepsilon_\perp}$, as $y^2\to-\pi^2\tau^2$, is examined in Appendix B.

Now, combining Eq. (30) with (9) and using asymptotic expressions for the functions $Q_\tau^{\varepsilon_\perp}$ and Q_τ, we obtain (for $T<T_c$ and $d'<2$) to leading order in a/L

$$G(\mathbf{R},T;L)\approx\left[1-\frac{T}{T_c}\right]\prod_{j=1}^{d^*}\cos(2\pi\tau_j\varepsilon_j)+\frac{T}{4\pi^{(4-d)/2}J}\left[\frac{a}{L}\right]^{d-2}\left\{L_\tau^{\varepsilon_\perp}\left[\frac{d-2}{2}\middle|d^*\right]-\prod_{j=1}^{d^*}\cos(2\pi\tau_j\varepsilon_j)L_\tau\left[\frac{d-2}{2}\middle|d^*\right]\right\}$$
$$+\frac{T}{4\pi^{(4-d)/2}J}\left[\frac{a}{L}\right]^{d-2}\sum_{l=1}^{\infty}N_\tau^{\varepsilon_\perp}\left[\frac{d}{2}-1+l\middle|d^*\right]\frac{(-\pi^2\varepsilon_\parallel^2)^l}{l!} ; \tag{32}$$

note that the last group of terms, which represents finite-size effects primarily due to the component $\varepsilon_{\parallel}$, is relevant only if $d'>0$. Equation (32) contains leading corrections, arising from both $\varepsilon_\perp$ and $\varepsilon_\parallel$, to the correlation function of the system.

It is instructive to see how the results of Sec. III A follow from Eq. (32). For this, we assume that $\tau_1=\cdots=\tau_{d^*}$ $(=\tau/\sqrt{d^*})$ and write

$$\prod_{j=1}^{d^*}\cos(2\pi\tau_j\varepsilon_j)\simeq 1-2\pi^2\sum_{j=1}^{d^*}\tau_j^2\varepsilon_j^2=1-2\pi^2(\tau^2/d^*)\varepsilon_\perp^2 . \tag{33}$$

Next, we use Eqs. (B3b) and (B7), along with their counterparts from Ref. 15, to write

$$\begin{aligned}L_\tau^{\varepsilon_\perp}(\nu|d^*)-\prod_{j=1}^{d^*}\cos(2\pi\tau_j\varepsilon_j)L_\tau(\nu|d^*)&\simeq\frac{1}{2\pi^{d^*/2}}\sum_{r=0}^{\infty}\frac{\tau^{2r}}{r!}\left\{D_\tau^{\varepsilon_\perp}(\nu-r|d^*)-\left[1-\frac{2\pi^2\tau^2}{d^*}\varepsilon_\perp^2\right]D_\tau(\nu-r|d^*)\right\}\\&\simeq\frac{1}{2\pi^{d^*/2}}\sum_{r=0}^{\infty}\frac{\tau^{2r}}{r!}\left\{\pi^{d^*/2-2\nu+2r}\Gamma(\nu-r)\varepsilon_\perp^{-2\nu+2r}+\frac{2\pi^2\tau^2}{d^*}D_\tau(\nu-r|d^*)\varepsilon_\perp^2\right.\\&\qquad\left.+\left[\frac{2(\nu-r+1)}{d^*}-1\right]\pi^2D_\tau(\nu-r+1|d^*)\varepsilon_\perp^2\right\} .\end{aligned}\tag{34}$$

The first term in (34) is precisely equal to

$$\frac{\pi}{2}\operatorname{cosec}(\pi\nu)\left[\frac{\tau}{\pi\varepsilon_\perp}\right]^{\nu}J_{-\nu}(2\pi\tau\varepsilon_\perp) ,\tag{35}$$

while the second and third terms, together, reduce to

$$\frac{1}{2\pi^{d^*/2}}\sum_{r=0}^{\infty}\frac{\tau^{2r}}{r!}\left[\frac{2(\nu+1)}{d^*}-1\right]\pi^2D_\tau(\nu-r+1|d^*)\varepsilon_\perp^2=\frac{2\pi^2}{d^*}(\nu+1-\tfrac{1}{2}d^*)N_\tau(\nu+1|d^*)\varepsilon_\perp^2 .\tag{36}$$

A similar operation on the last set of terms in (32) yields

$$\sum_{l=1}^{\infty}N_\tau^{\varepsilon_\perp}\left[\frac{d}{2}-1+l|d^*\right]\frac{(-\pi^2\varepsilon_\parallel^2)^l}{l!}\simeq\frac{\pi}{2}\operatorname{cosec}(\pi\nu)\sum_{l=1}^{\infty}\left[\frac{\tau}{\pi\varepsilon_\perp}\right]^{\nu+l}J_{-\nu-l}(2\pi\tau\varepsilon_\perp)\frac{(\pi^2\varepsilon_\parallel^2)^l}{l!}-\pi^2N_\tau\left[\frac{d}{2}\middle|d^*\right]\varepsilon_\parallel^2 .\tag{37}$$

Combining (35) and (37), we obtain

$$\frac{\pi}{2}\operatorname{cosec}(\pi\nu)\left[\frac{\tau}{\pi\varepsilon}\right]^{\nu}J_{-\nu}(2\pi\tau\varepsilon)-\pi^2N_\tau\left[\frac{d}{2}\middle|d^*\right]\varepsilon_\parallel^2 ,\tag{38}$$

where $\varepsilon=\sqrt{\varepsilon_\perp^2+\varepsilon_\parallel^2}$. Substituting (33), (36), and (38) into (32), and remembering that ν here is equal to $(d-2)/2$, we recover precisely the results of Sec. III A.

C. Case 3: $R_\perp=O(L)$, $R_\parallel\gg L$

For this case we employ Eq. (12) instead and observe that, for $\varepsilon_\parallel\gg 1$ and $y^2\simeq-\pi^2\tau^2$, only those terms, of the sum over $\mathbf{n}(d^*)$, for which $|n_j+\tau_j|=\tau_j$ make dominant contribution toward the function $G(\mathbf{R},T;L)$, with the result

$$G(\mathbf{R},T;L)\approx g_\tau\left[\frac{a}{L}\right]^{d^*}\prod_{j=1}^{d^*}\cos(2\pi\tau_j\varepsilon_j)\times\frac{T}{2(2\pi)^{d'/2}J}\left[\frac{\xi R_\parallel}{a^2}\right]^{(2-d')/2}\times K_{(2-d')/2}(R_\parallel/\xi) ,\tag{39}$$

where

$$\xi=L/2\sqrt{y^2+\pi^2\tau^2} .\tag{40}$$

Here, g_τ denotes the multiplicity of the terms making dominant contribution to the expression for G; in general, $g_\tau=2^r$, where r $(\le d^*)$ is the number of components τ_j of τ that equal $\frac{1}{2}$— for each of these components, *two* terms (with $n_j=0$ and -1) contribute equally toward the sum.

Clearly, the correlation function in this case splits into two factors— highlighting the fact that, while the decay of correlations in the direction of $\mathbf{R}_\perp$ is determined solely by the "twist parameter" τ, that in the direction of $\mathbf{R}_\parallel$ is determined by a (correlation) function pertaining in form to a d'-dimensional bulk system, cf. Eq. (17a), but scaled by a (correlation) length ξ pertaining to the actual system in geometry $L^{d^*}\times\infty^{d'}$ and *not* to the d'-dimensional bulk system (which would have nothing to do with L). The consequences of expression (40) for ξ have been studied at length in Ref. 12.

We note that, in the regime $L\ll R_\parallel\ll\xi$, Eq. (39), with the help of the formula[16]

$$K_\mu(x)\approx\frac{1}{2}\left[\Gamma(\mu)\left[\frac{1}{2}x\right]^{-\mu}+\Gamma(-\mu)\left[\frac{1}{2}x\right]^{\mu}\right]\quad(0<\mu<1,\ x\ll 1) ,\tag{41}$$

gives (for $0<d'<2$)

$$G(\mathbf{R},T;L)\approx g_\tau \left[\frac{a}{L}\right]^{d^*} \prod_{j=1}^{d^*} \cos(2\pi\tau_j\varepsilon_j) \frac{T}{4(2\pi)^{d'/2}J} \left\{ \Gamma\left[\frac{2-d'}{2}\right]\left[\frac{2\xi^2}{a^2}\right]^{(2-d')/2} + \Gamma\left[\frac{d'-2}{2}\right]\left[\frac{R_\parallel^2}{2a^2}\right]^{(2-d')/2} \right\} . \quad (42)$$

Substituting for $\xi(T;L)$ from Ref. 12, the first term in (42) reduces to

$$\left[1-\frac{T}{T_c}\right] \prod_{j=1}^{d^*} \cos(2\pi\tau_j\varepsilon_j) , \quad (43)$$

while the second may be written as

$$\tau_\tau \left[\frac{a}{L}\right]^{d^*} \prod_{j=1}^{d^*} \cos(2\pi\tau_j\varepsilon_j) \times \frac{T}{8\pi^{d'/2}J} \Gamma\left[\frac{d'-2}{2}\right]\left[\frac{a}{R_\parallel}\right]^{d'-2} . \quad (44)$$

Expressions (43) and (44) may be compared with the leading terms of Eqs. (32) and (23), respectively.

IV. CONCLUDING REMARKS

In this paper we have analyzed finite-size effects in the correlation function $G(\mathbf{R},T;L)$ of a spherical model confined to geometry $L^{d-d'}\times\infty^{d'}$ ($2<d<4$, $d'\leq 2$) and subjected to twisted boundary conditions (2). These boundary conditions are defined through a continuously varying parameter $\tau(d^*)$, with components τ_j such that $0\leq\tau_j\leq\frac{1}{2}$; this generalizes the concept of boundary conditions from the extreme case of PBC's on the one hand to that of APBC's on the other. The parameter τ modifies the collective-mode eigenenergies of the system, as shown in Eq. (4), which leads to a host of characteristic finite-size effects in the various properties of the system. These effects, in the case of the magnetic susceptibility χ (under APBC's) and the correlation length ξ (under TBC's), have been studied earlier;[3,4,11,12] in each of these cases, the effects arise essentially through the correlation function of the system, which itself had not been analyzed in any significant detail so far. It is hoped that the present investigation fills that gap in the literature.

In the preceding section we have examined the function $G(\mathbf{R},T;L)$ in different regimes of the parameters involved and in each case finite-size effects, which are now τ dependent, have been isolated. We have focussed our attention primarily on the region of first-order phase transition ($T<T_c$), where several important features are encountered. One of these relates to the long-range order in the system, which is significantly altered by the fact that the ground-state spin-wave vector is now "pinned" at the value $\mathbf{k}_0=2\pi\tau/L$. This leads to a twist in the order-parameter field, given by the factor $\prod_{j=1}^{d^*}\cos(2\pi\tau_j R_j/L)$, which goes with the conventional (bulk) term $M_0^2(T)$; see Eq. (32) or (43). In the short distance limit ($a\ll R\ll L$), the correlation function takes on the characteristics of a (d-dimensional) bulk system, which include the long-range term just described *plus* an isotropic term singular in $\varepsilon=\sqrt{\varepsilon_\perp^2+\varepsilon_\parallel^2}$; see Eq. (23). On the other hand, when $L\ll R\simeq R_\parallel\ll\xi$, the parameter d' alters the scene by providing a correction to the long-range term, which is analogous to the *bulk* isotropic term, except that now R is replaced by $R_\parallel$ and d by d'; see Eq. (44). The leading $\mathbf{R}_\perp$ dependence of G maintains its coherent form for all $R\gg a$ in the region of first-order phase transition, and yet when $R_\parallel\gg L$, the dependence of G on $R_\parallel$ becomes characteristic of a d'-dimensional bulk system—bearing no resemblance to the correlation function of a d-dimensional bulk system; see Eqs. (17a) and (39). These features throw some light on how the choice of boundary conditions affects the physical behavior of the given system.

Another interpretation of the parameter τ worth mentioning is that it may be regarded as a measure of the "geometry-dependent doping level of magnetic impurities" in the lattice that restricts the structure of the ground state, thus providing a basis for the energy expended in applying a twist to the order-parameter field. In this interpretation, the case $\tau\rightarrow 0$ would correspond to a clean, undoped system, whereas the other extreme ($\tau_j=\frac{1}{2}$) would imply saturation (in which case all available impurity states of the system are filled). In this sense, the impurity states appear as fermionic in nature.

In our analysis of the correlation function we have been concerned with static aspects alone, and yet the mathematics here is very similar to the one employed by Henkel and Weston[11] for a system in geometry $L^2\times\infty^1$, where *time* constitutes the infinite (Euclidean) subspace of dimension one. In our analysis there is no need to time-evolve the order parameter or to invoke time-ordered product of spins in defining the correlation function $G(\mathbf{R})$. Clearly, more work is needed to unravel the connection between these two approaches.

Finally, we would like to mention that an extension of the present study from dimensionality $2<d<4$ to $d\geq 4$ is currently in progress; so is the study of the magnetic susceptibility-both local, $\chi(\mathbf{r})$, and averaged, $\bar{\chi}$,—under conditions of general τ. The results of these studies will be reported subsequently.

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APPENDIX A

To render expression (6) into (13), we set $y=\pm iv$ and use the formula[16]

$$(\pm ix)^{\nu}K_{\nu}(\pm ix)=\frac{\pi x^{\nu}}{2\sin(\pi\nu)}\{J_{-\nu}(x)-e^{\pm i\pi\nu}J_{\nu}(x)\}\ , \tag{A1}$$

where $\nu=(d-2)/2$, and hence $0<\nu<1$. The resulting expression for G contains sums over $\mathbf{q}(d^*)$, with summands involving $J_{-\nu}(x)$ or $J_{\nu}(x)$. In view of the fact that the quantity under study is *real*, the latter sum must vanish identically—yielding the remarkable result

$$\sum_{\mathbf{q}(d^*)}\prod_{j=1}^{d^*}\cos(2\pi\tau_j q_j)\frac{J_{\nu}(2v\sqrt{|\mathbf{q}+\varepsilon_{\perp}|^2+\varepsilon_{\parallel}^2})}{(\sqrt{|\mathbf{q}+\varepsilon_{\perp}|^2+\varepsilon_{\parallel}^2})^{\nu}}=0$$
$$\{0\le\tau_j\le\tfrac{1}{2}(j=1,\ldots,d^*),\tau=|\tau(d^*)|>0,\ 0<v<\pi\tau\}\ . \tag{A2}$$

The remaining sum leads to Eq. (13).

The result embodied in Eq. (A2) constitutes a considerable generalization of the one given earlier,[17] which pertained to the special case $\varepsilon=0$. In that case, it seemed appropriate to split the $(q=0)$-term from the rest of the sum and write

$$\frac{v^{\nu}}{\Gamma(\nu+1)}+\sum_{\mathbf{q}(d^*)}{}'\cos(2\pi\tau\cdot\mathbf{q})\frac{J_{\nu}(2vq)}{q^{\nu}}=0\ . \tag{A3}$$

It turned out that Eq. (A3) was itself a generalization of the so-called Schlömilch series,[18] which is normally stated for $d^*=1$ and $\tau=\frac{1}{2}$ only. However, no special case of our new result (A2), with $\varepsilon\neq0$, has come to our attention so far.

In passing we observe that Eq. (A2), which has been established here for $0<\nu<1$, may in fact hold for all $\nu>-\frac{1}{2}$.

APPENDIX B

In this appendix we examine the limiting behavior of the functions $Q_{\tau}^{\varepsilon_{\perp}}(\nu|d^*;y)$ as $y^2\to-\pi^2\tau^2$. With $\varepsilon_{\parallel}\to0$, Eq. (28c) gives

$$Q_{\tau}^{\varepsilon_{\perp}}(\nu|d^*;y)=\tfrac{1}{2}\pi^{d^*/2-2\nu}\Gamma\left[\frac{d^*}{2}-\nu\right]\times\sum_{n(d^*)}\frac{\prod_{j=1}^{d^*}\cos\{2\pi\varepsilon_j(n_j+\tau_j)\}}{(y^2+\pi^2|\mathbf{n}+\tau|^2)^{d^*/2-\nu}}\ . \tag{B1}$$

Following the procedure of Ref. 15, we obtain in the desired limit

$$Q_{\tau}^{\varepsilon_{\perp}}(\nu|d^*;y)\approx\begin{cases}\tfrac{1}{2}g_{\tau}\pi^{d^*/2-2\nu}\Gamma\left[\frac{d^*}{2}-\nu\right]\prod_{j=1}^{d^*}\cos(2\pi\varepsilon_j\tau_j)\frac{1}{(y^2+\pi^2\tau^2)^{d^*/2-\nu}}+L_{\tau}^{\varepsilon_{\perp}}(\nu|d^*)\quad(\nu<\tfrac{1}{2}d^*)\ , & \text{(B2a)}\\ \tfrac{1}{2}g_{\tau}\pi^{-d^*/2}\prod_{j=1}^{d^*}\cos(2\pi\varepsilon_j\tau_j)\ln\left[\frac{1}{y^2+\pi^2\tau^2}\right]+M_{\tau}^{\varepsilon_{\perp}}(d^*)\quad(\nu=\tfrac{1}{2}d^*)\ , & \text{(B2b)}\\ N_{\tau}^{\varepsilon_{\perp}}(\nu|d^*)\quad(\nu>\tfrac{1}{2}d^*)\ , & \text{(B2c)}\end{cases}$$

where g_{τ} denotes the multiplicity of the terms, in the sum over $\mathbf{n}$ (d^*), for which $|\mathbf{n}+\tau|=\tau$; in general, $g_{\tau}=2^r$, where r $(\le d^*)$ is the number of components τ_j of τ that equal $\frac{1}{2}$—for each of these components, *two* terms (with $n_j=0$ and -1) contribute equally toward the sum. The constants L, M, and N appearing here can also be analyzed using the procedure of Ref. 15. To begin with, we get

$$L_{\tau}^{\varepsilon_{\perp}}(\nu|d^*)=\frac{1}{2\pi^{d^*/2}}\Gamma\left[\frac{d^*}{2}-\nu\right]\sum_{\mathbf{n}(d^*)}{}'\frac{\prod_{j=1}^{d^*}\cos\{2\pi\varepsilon_j(n_j+\tau_j)\}}{[|\mathbf{n}+\tau|^2-\tau^2]^{d^*/2-\nu}} \tag{B3a}$$

$$=\frac{1}{2\pi^{d^*/2}}\sum_{r=0}^{\infty}\frac{1}{r!}\left\{D_{\tau}^{\varepsilon_{\perp}}(\nu-r|d^*)\tau^{2r}-g_{\tau}\prod_{j=1}^{d^*}\cos(2\pi\varepsilon_j\tau_j)\frac{\Gamma\left[\frac{1}{2}d^*-\nu+r\right]}{\tau^{d^*-2\nu}}\right\}\ , \tag{B3b}$$

where

$$D_{\tau}^{\varepsilon_{\perp}}(\nu|d^*)=\begin{cases}\Gamma\left[\frac{d^*}{2}-\nu\right]\sum_{\mathbf{n}(d^*)}\frac{\prod_{j=1}^{d^*}\cos\{2\pi\varepsilon_j(n_j+\tau_j)\}}{|\mathbf{n}+\tau|^{d^*-2\nu}}\quad(\nu<\tfrac{1}{2}d^*) & \text{(B4a)}\\ \pi^{d^*/2-2\nu}\Gamma(\nu)\sum_{\mathbf{q}(d^*)}\frac{\prod_{j=1}^{d^*}\cos(2\pi\tau_j q_j)}{|\mathbf{q}+\varepsilon_{\perp}|^{2\nu}}\quad(\nu>0)\ . & \text{(B4b)}\end{cases}$$

The corresponding expression for $M_\tau^{\varepsilon_\perp}(d^*)$ can be written likewise; in particular, for $d^*=1$, we have

$$M_\tau^{\varepsilon_\perp}(1)=\frac{1}{2\pi^{1/2}}\left[D_\tau^{\varepsilon_\perp}(\tfrac{1}{2}|1)+g_\tau\cos(2\pi\varepsilon_\perp\tau)\ln(\pi^2\tau^2)+\sum_{r=1}^{\infty}\left\{D_\tau^{\varepsilon_\perp}(\tfrac{1}{2}-r|1)\frac{\tau^{2r}}{r!}-g_\tau\frac{\cos(2\pi\varepsilon_\perp\tau)}{r}\right\}\right]. \tag{B5}$$

Similarly,

$$N_\tau^{\varepsilon_\perp}(\nu|d^*)=\frac{1}{2\pi^{d^*/2}}\sum_{r=0}^{\infty}D_\tau^{\varepsilon_\perp}(\nu-r|d^*)\frac{\tau^{2r}}{r!}\ . \tag{B6}$$

Finally, we note that, for $\varepsilon_\perp \ll 1$ and $\tau_1=\cdots=\tau_{d^*}$, Eq. (B4b) yields the approximation

$$D_\tau^{\varepsilon_\perp}(\nu|d^*)\simeq\pi^{d^*/2-2\nu}\Gamma(\nu)\varepsilon_\perp^{-2\nu}+D_\tau(\nu|d^*)+\left\{\frac{2(\nu+1)}{d^*}-1\right\}\pi^2D_\tau(\nu+1|d^*)\varepsilon_\perp^2\ ; \tag{B7}$$

the constant $D_\tau(\nu|d^*)$ appearing here has been examined in detail in Ref. 15.

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