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Finite-size effects in the spherical model of ferromagnetism: Zero-field susceptibility under antiperiodic boundary conditions

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The overall zero-field susceptibility $\bar{\chi}$ of a finite-sized spherical model of spins under various *anti*periodic boundary conditions is reexamined with a view to explaining the finite-size effects of an algebraic nature found recently by Singh and Pathria. The cause of this "unexpected" behavior at temperatures above the bulk critical temperature $T_c(\infty)$ is seen to lie in the spatial variation of the local susceptibility which, on averaging over the system, leads precisely to the effects found previously. Below $T_c(\infty)$, the influence of antiperiodic conditions is even more severe, in that not only are the finite-size amplitudes for $\bar{\chi}$ modified but, for the local susceptibility, new exponents also appear.

I. INTRODUCTION

In recent papers,[1,2] hereafter referred to as I and II, Singh and Pathria have derived explicit expressions for various thermodynamic functions of a spherical model of spins on a hypercubical lattice, of size $L_1 \times \cdots \times L_d$ with $2<d<4$, under both periodic and antiperiodic boundary conditions. The expressions thus obtained were found to be in full conformity with the Privman-Fisher hypothesis[3] on a finite system, of volume L^d, near the bulk critical temperature $T_c(\infty)$. Subsequently it was shown[4] that for a system in general geometry $L^{d^*} \times \infty^{d'}$, where $d^*+d'=d$ and $d' \le 2$, these expressions conformed equally well to a generalized form of the aforementioned hypothesis which extended its validity to all temperatures below $T_c(\infty)$.

An integral part of these investigations was to study the limiting behavior of the scaling functions governing the various quantities of interest in different regimes of the temperature variable $\tilde{t}$ $(=[T-T_c(\infty)]/T)$ and thereby deduce the precise nature of the finite-size effects appearing in the system or the manner in which the actual physical quantities pertaining to the system approach their standard bulk behavior as $L\to\infty$. For $\tilde{t}<0$, the approach turned out to be through power laws if d' was less than 2; for $d'=2$, however, exponential behavior was found instead. For $\tilde{t}>0$, on the other hand, the approach was generally exponential, except for the surprising behavior of the zero-field susceptibility of the system under *anti*periodic boundary conditions which displayed a finite-size effect determined mainly by the surface-to-volume ratio of the lattice. To be precise, the overall susceptibility (per spin) of a system with $d^*=3$ under these conditions turned out to be[2]

$$\bar{\chi}(L_j;T)=\frac{1}{2J\phi}\left[1-\left[\frac{1}{y_1}+\frac{1}{y_2}+\frac{1}{y_3}\right]+\frac{4}{\pi}\left[\frac{1}{y_1y_2}+\frac{1}{y_1y_3}+\frac{1}{y_2y_3}\right]-\frac{6}{\pi}\frac{1}{y_1y_2y_3}+\mathscr{E}(L_1,L_2,L_3)\right], \quad (1)$$

where y_j's are the *thermogeometric* or *scaled length parameters* of the system,

$$y_j=\tfrac{1}{2}N_j\sqrt{\phi}=\tfrac{1}{2}L_j/\xi^* \quad (N_j=L_j/a;\ j=1,2,3)\ ; \quad (2)$$

here, $\xi^*(=a/\sqrt{\phi})$ is a measure of the *correlation length* in the given system,[5] $\mathscr{E}(L_1,L_2,L_3)$ denotes terms decaying exponentially with the L_j, while other symbols have their usual meanings. In view of the fact that, for $\tilde{t}>0$ and $L_j\to\infty$, the y_j are directly proportional to the L_j, this result portrays the existence not only of "surface" effects but of "edge" effects and "corner" effects as well. Customarily, such effects are regarded as foreign to both periodic and antiperiodic boundary conditions and are expected to appear only in the case of free (i.e., Dirichlet) boundary conditions.[6] To discern the true cause of this "anomaly" and to examine its consequences for the general problem of susceptibility in a finite system under *anti*periodic boundary conditions constitute the main purposes of the present communication.

The basic point to emphasize here is that, while in *zero* field the system is translationally invariant under both periodic and antiperiodic boundary conditions, in *nonzero* field this invariance is retained only for periodic boundary conditions and is *broken* for antiperiodic ones; this makes the *local* susceptibility in the latter case a function of the space coordinates $\mathbf{r}$. It can then be argued that, while the difference between the local susceptibility $\chi(\mathbf{r};L_j)$ and the corresponding bulk limit $\chi(\mathbf{r};\infty)$ would be exponentially small (at least for $\tilde{t}>0$), the difference between the *overall* susceptibility

$$\bar{\chi}(L_j)=\frac{1}{N_1N_2N_3}\sum_{r_1=1}^{N_1}\sum_{r_2=1}^{N_2}\sum_{r_3=1}^{N_3}\chi(\mathbf{r},L_j)\ , \tag{3}$$

and the corresponding bulk limit $\bar{\chi}(\infty)$ may well be algebraic in nature. To see this more clearly, we may refer to Fig. 1 which shows a one-dimensional situation in an ensemble environment, with the antiperiodic boundary condition

$$s(i+N_1)=-s(i) \tag{4}$$

imposed on the spins of the system. The zero-field local susceptibility $\chi(r_1;L_1)$ may then be derived from the standard formula

$$\chi(r_1;L_1)\equiv\left.\frac{\partial}{\partial H}\langle s(r_1)\rangle\right|_{H=0}=\frac{1}{k_BT}\sum_{r_1'=1}^{N_1}\langle s(r_1)s(r_1')\rangle\ , \tag{5}$$

where H is the magnetic field which acts uniformly on all spins. Now, in view of condition (4), the correlation function $\langle s(r_1)s(r_1')\rangle$ must satisfy the relations

$$\langle s(r_1)s(N_1+r_1-k)\rangle=-\langle s(r_1)s(r_1-k)\rangle=-G(|k|) \tag{6}$$

provided $1\le r_1\le\frac{1}{2}(N_1+1)$ and $r_1\le|k|\le\frac{1}{2}(N_1+1)$, whereas, under the same restrictions,

$$\langle s(r_1)s(r_1+k)\rangle=+G(|k|)\ . \tag{7}$$

Physically these relations reflect the fact that although the "antiferromagnetic seam" introduced into the lattice at $r_1=N_1$ by the condition (4) has *no local effects* in a *strictly zero* magnetic field—indeed, the "seam" may be moved to any other position in the lattice, merely by changing the sign convention on the spins $s_1,s_2,\ldots,s_l$, with no effect on the zero-field free energy of the system—the application of an external field H converts the "seam" into a *local inhomogeneity* in the lattice since spins on opposite sides of the seam are, in effect, coupled to the field in opposite senses (relative to their preferred local alignment). It now follows from relations (6) and (7) that a number of terms in sum (5) cancel in pairs and, apart from a minor end effect arising as $k\to\frac{1}{2}(N_1+1)$, we are left with the expression

$$\chi(r_1;L_1)=\frac{1}{k_BT}\sum_{k=-r_1+1}^{r_1-1}\langle s(r_1)s(r_1+k)\rangle$$
$$=\frac{1}{k_BT}\left[G(0)+2\sum_{k=1}^{r_1-1}G(k)\right]\ ; \tag{8}$$

thus, $\chi(r_1;L_1)$ turns out to be a monotonically increasing function of r_1 for $1\le r_1\le\frac{1}{2}(N_1+1)$. For the special case $r_1=1$, which corresponds to a "corner" of the lattice just at the antiferromagnetic seam, we have the simple result

$$\chi(1;L_1)=\frac{G(0)}{k_BT}=\frac{\langle s^2(1)\rangle}{k_BT}=\frac{1}{k_BT}\ , \tag{9}$$

which is independent of the interaction parameter J. Next, in view of the symmetry of the lattice, we must have

$$\chi(r_1;L_1)=\chi(N_1+1-r_1;L_1)\ , \tag{10}$$

so that, for $r_1>\frac{1}{2}(N_1+1)$, χ steadily decreases (as a mirror-image of the first half) until we reach the other "corner" of the lattice, $r_1=N_1$, where χ has exactly the same value as at $r_1=1$.

We now observe that, since the correlation function $G(k)$ is significant only for k less than (or of order) ξ, the correlation length in the system, the susceptibility function $\chi(r_1;L_1)$ varies significantly with r_1 only so long as r_1 is less than (or of order) ξ. For $r_1\gg\xi$, χ essentially levels off to a limiting, "long-distance" value, $\chi_>(L_1)$, which may differ from the corresponding bulk limit only

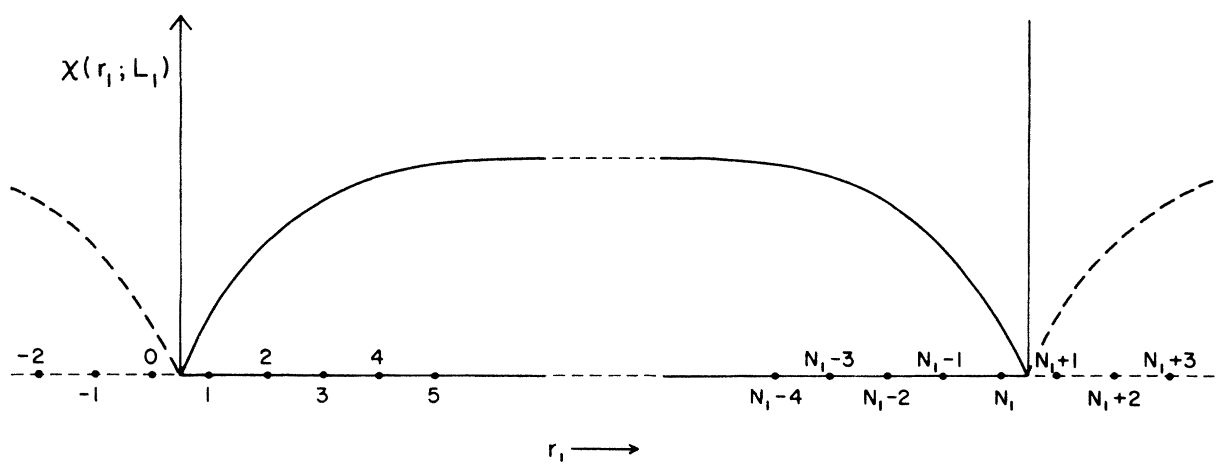

FIG. 1. Schematic diagram showing the *local* susceptibility $\chi(r_1;L_1)$ in a one-dimensional chain as a function of r_1 under antiperiodic boundary conditions.

by exponentially small terms. The space dependence of χ, however, will lead to an overall result of the form

$$\bar{\chi}(L_1)=\chi_>(L_1)[1-O(\xi/L_1)] =\chi_{\text{bulk}}[1-O(\xi/L_1)+\mathscr{E}(L_1)] . \quad (11)$$

It is now very plausible that an extension of the foregoing argument to three dimensions will lead to a result of the form (1). Clearly, no such effects are expected in the case of periodic boundary conditions where, in place of (4), one has $s(i+N_1)=+s(i)$.

In Sec. II we present an exact formulation of the quantity $\chi(\mathbf{r};L_j)$ for a spherical model of spins under antiperiodic boundary conditions and examine the one-dimensional situation, $L_1\times\infty^{d-1}$, in complete detail. The general geometry, $L^{d^*}\times\infty^{d'}$, is considered in Secs. III and IV. It turns out that, while for $\tilde{t}>0$ the physical nature of the space-dependent function $\chi(\mathbf{r};L_j)$, and hence of the overall function $\bar{\chi}(L_j)$, is precisely the same as outlined above, the corresponding results for $\tilde{t}<0$ are affected even more seriously. This is essentially due to the fact that the correlation length ξ in the latter regime assumes a macroscopic value; as a consequence, the effects explained above now prevail throughout the system, are no longer a simple correction to the corresponding bulk results, and affect not only the amplitudes of $\chi(\mathbf{r};L_j)$ and $\bar{\chi}(L_j)$ but, for $r \ll L_j$, the various exponents as well.

II. LOCAL SUSCEPTIBILITY $\chi(\mathbf{r};L_j)$ UNDER ANTIPERIODIC BOUNDARY CONDITIONS

Using the framework of Barber and Fisher,[7] we can readily show that for a partially infinite system, with periodic boundary conditions imposed in the directions in which the system is infinite and antiperiodic boundary conditions in the directions in which it is finite, the *local* susceptibility $\chi(\mathbf{r};L_j)$ $[\equiv\partial\langle s(\mathbf{r})\rangle/\partial H]$ in the limit of zero field is given by

$$\chi(\mathbf{r};L_j)=\frac{1}{2J\prod_{j=1}^{d^*}N_j}\sum_{\{n_j\}}\frac{\prod_{j=1}^{d^*}\sin[\pi(n_j+\frac{1}{2})(2r_j-1)/N_j]/\sin[\pi(n_j+\frac{1}{2})/N_j]}{\phi+4\sum_{j=1}^{d^*}\sin^2[\pi(n_j+\frac{1}{2})/N_j]}\quad [n_j=0,1,\ldots,(N_j-1)] , \quad (12)$$

where $\mathbf{r}=(r_1,\ldots,r_{d^*})$, while other quantities have their usual meanings; in the sequel, the lattice constant a will be set equal to unity, so that $N_j=L_j$. The parameter ϕ, a measure of the correlation length in the system,[5] is defined by the relation

$$\phi=(\lambda/J)-2d , \quad (13)$$

where λ is the usual spherical field, and is determined by the constraint equation of the system; see, for instance, Eq. (26) of II. For obtaining the *overall* susceptibility, $\bar{\chi}(L_j)$, from Eq. (12), we make use of the formula

$$\sum_{r_j=1}^{N_j}\sin[\alpha_j(2r_j-1)]=\sin^2(\alpha_jN_j)/\sin\alpha_j , \quad (14)$$

with the result

$$\bar{\chi}(L_j)=\frac{1}{2J\prod_{j=1}^{d^*}N_j^2}\sum_{\{n_j\}}\frac{\prod_{j=1}^{d^*}\operatorname{cosec}^2[\pi(n_j+\frac{1}{2})/N_j]}{\phi+4\sum_{j=1}^{d^*}\sin^2[\pi(n_j+\frac{1}{2})/N_j]} , \quad (15)$$

as in Eq. (63) of II.

To render Eq. (12) into a more tractable form, we follow the procedure developed in earlier work,[1,2] supplementing it with the formula

$$\sum_{k=-r+1}^{r-1}\cos(2xk)=\sin[(2r-1)x]/\sin x \quad (r=1,2,3,\ldots) . \quad (16)$$

We thus obtain

$$\chi(\mathbf{r},L_j)=\frac{1}{4J}\int_0^\infty e^{-(1/2)\phi x}\prod_{j=1}^{d^*}\left[\sum_{q_j=-\infty}^{\infty}(-1)^{q_j}\left[\sum_{k_j=-r_j+1}^{r_j-1}[e^{-x}I_{\nu_j}(x)]\right]\right]dx , \quad (17)$$

where $\nu_j=N_jq_j+k_j$ and $I_\nu(z)$ is the modified Bessel function. The special case $d^*=1$ can be handled straightforwardly; see the Appendix. For $\phi \ll 1$, the resulting expression can be written in the *scaled* form

$$\chi(r_1;L_1)\approx\frac{N_1^2}{8Jy_1^2}\left[1-\frac{\cosh(y_1-z_1)}{\cosh y_1}\right] \quad \text{for } r_1,\ N_1 \gg 1 , \quad (18)$$

where, as before,

$$y_1 = \tfrac{1}{2} N_1 \sqrt{\phi} = \tfrac{1}{2} L_1/\xi^*, \quad z_1 = r_1 \sqrt{\phi} = r_1/\xi^* . \tag{19}$$

In the limit as $z_1 \to y_1$ (i.e., $r_1 \to \frac{1}{2}N_1$), the local susceptibility (18) approaches the "long-distance" value (indicated by a subscript $>$), viz.,

$$\chi_>(L_1) \approx \frac{N_1^2}{8Jy_1^2}(1-\operatorname{sech} y_1) = \frac{1}{2J\phi(L_1)}(1-\operatorname{sech} y_1) , \tag{20}$$

which may be compared with the standard bulk result

$$\chi(\infty) = \frac{1}{2J\phi(\infty)} . \tag{21}$$

For small z_1, on the other hand, the local susceptibility approaches the asymptotic "short-distance" form (indicated by a subscript $<$) given by

$$\chi_<(r_1;L_1) \approx \frac{N_1^2}{8Jy_1^2} z_1 \tanh y_1 = \frac{r_1}{2J[\phi(L_1)]^{1/2}} \tanh y_1 , \tag{22}$$

which applies close to the antiferromagnetic seam where $r_1 \ll N_1$. Note that the ratio of the short-distance to the long-distance local susceptibilities is

$$\chi_<(r_1;L_1)/\chi_>(L_1) \approx z_1 \coth(\tfrac{1}{2}y_1) . \tag{23}$$

The overall susceptibility, $\bar{\chi}(L_1)$, can now be obtained straightforwardly from Eq. (18) as

$$\bar{\chi}(L_1) \approx \frac{1}{y_1}\int_0^{y_1} \chi(z_1;y_1)\,dz_1 = \frac{N_1^2}{8Jy_1^2}\left[1-\frac{\tanh y_1}{y_1}\right] , \tag{24}$$

in agreement with Eq. (72) of II.

We shall now examine these results in different regimes of interest.

(i) $\tilde{t} > 0$, $L_1 \to \infty$. Here y_1 is of order N_1 and hence is much greater than unity. We then obtain

$$\chi(r_1;L_1) \approx \frac{N_1^2}{8Jy_1^2}(1-e^{-z_1}), \quad \chi_>(L_1) \approx \frac{N_1^2}{8Jy_1^2} \tag{25}$$

and

$$\chi_<(r_1;L_1) \approx \frac{N_1^2 z_1}{8Jy_1^2} \quad (z_1 \ll 1) ; \tag{26}$$

deviations from the corresponding bulk results are in this case exponentially small, as indeed one expects under antiperiodic boundary conditions. The overall susceptibility, however, turns out to be

$$\bar{\chi}(L_1) \approx \frac{N_1^2}{8Jy_1^2}\left[1-\frac{1}{y_1}\right] ; \tag{27}$$

the deviation from the corresponding bulk result is, evidently, now algebraic. The reason for this, hitherto "unexpected," behavior is now clear—it arises from the fact that the local susceptibility $\chi(r_1;L_1)$ is significantly less than the long-distance value $\chi_>(L_1)$ unless $z_1 \gg 1$. On averaging over the lattice, this leads to an overall reduction, in $\bar{\chi}$, of order $(1/y_1)$. The cause of the "anomaly," at least for $d^* = 1$, is thereby explained.

In passing we observe that, while $\chi_>$, the long-distance local susceptibility, is proportional to ϕ^{-1} and hence to $\tilde{t}^{-\gamma}$, the short-distance local susceptibility diverges as

$$\chi_< \sim \tilde{t}^{-\gamma_<} \quad (r_1 \text{ fixed}) , \tag{28}$$

where $\gamma_< = \gamma - \nu$; in writing this result we have made use of the fact that the variable z_1 in this regime is simply r_1/ξ and is therefore proportional to $\tilde{t}^{\nu}$. Thus, the short-distance local susceptibility $\chi_<(r_1;L_1)$ is not only much smaller in value than the long-distance local susceptibility $\chi_>(L_1)$, but is also less singular.

(ii) $\tilde{t} < 0$, $L_1 \to \infty$. Here $y_1^2 \simeq -\pi^2/4$, with the result that

$$\chi(r_1;L_1) \approx \frac{N_1^2}{2\pi^2 J\epsilon} \sin z_1', \quad \chi_>(L_1) \approx \frac{N_1^2}{2\pi^2 J\epsilon} , \tag{29}$$

and

$$\chi_<(r_1;L_1) \approx \frac{N_1^2 z_1'}{2\pi^2 J\epsilon} \quad (z_1' \ll 1) , \tag{30}$$

where

$$z_1' = r_1\sqrt{|\phi|} = \frac{r_1}{\frac{1}{2}N_1}[(-y_1^2)]^{1/2} \simeq \frac{\pi r_1}{N_1} , \tag{31}$$

while (for $L_j = L$)

$$\epsilon = \frac{1}{\pi}\left[y^2 + \frac{\pi^2}{4}\right] \simeq \begin{cases} \left[\dfrac{\Gamma[(3-d)/2]}{4\pi|x_1|}\right]^{2/(3-d)} & (d<3) , \\ \tfrac{1}{2}\exp(-4\pi|x_1|) & (d=3) , \end{cases} \tag{32}$$

in which $x_1 = C_1 L^{d-2}\tilde{t}$—a generalization[4] of the finite-size scaled variable, proportional to $L^{1/\nu}t$, introduced by Privman and Fisher.[3] The overall susceptibility is now given by

$$\bar{\chi}(L_1) \approx \frac{N_1^2}{\pi^3 J\epsilon} \approx \frac{2}{\pi}\chi_>(L_1) , \tag{33}$$

which implies a significant reduction below the limiting value $\chi_>$. Once again, we observe that the short-distance local susceptibility $\chi_<$ is not only much smaller than the long-distance value $\chi_>$, but is less singular as well; thus, while $\chi_>$ diverges as L^{ζ} (when $L \to \infty$), with $\zeta = 2/(3-d)$, one finds

$$\chi_< \sim L^{\zeta_<}, \quad \text{with } \zeta_< = \zeta - 1 \quad (r_1 \text{ fixed}) . \tag{34}$$

(iii) In between regimes (i) and (ii) lies the "core" region where $|x_1| = O(1)$. The value of y_1 in this region has generally to be determined numerically. For $d=3$, however, the constraint equation is sufficiently simple to yield an explicit expression for y_1 in terms of x_1, namely

$$y_1(x_1) = \cosh^{-1}(\tfrac{1}{2}e^{4\pi x_1}) ; \tag{35}$$

see, for instance, Eq. (60) of II. This enables us to evaluate the quantities listed in Eqs. (18), (20), (22), and (24) as explicit functions of L_1 and $\tilde{t}$ over all regimes of interest, including the "core" region. Thus, at the erstwhile critical point ($\tilde{t}=0$), we obtain

$$\chi(r_1;L_1)\approx\frac{9N_1^2}{8\pi^2 J}\left[2\cos\left[\frac{\pi}{3}-(z_1')_c\right]-1\right],$$

$$\chi_>(L_1)\approx\frac{9N_1^2}{8\pi^2 J} \tag{36}$$

and

$$\chi_<(r_1;L_1)\approx\frac{9\sqrt{3}N_1^2(z_1')_c}{8\pi^2 J}\quad[(z_1')_c\ll 1], \tag{37}$$

where

$$(z_1')_c=\frac{r_1}{\frac{1}{2}N_1}[(-y_1^2)_c]^{1/2}=\frac{2\pi r_1}{3N_1}. \tag{38}$$

The overall susceptibility is now given by

$$\bar{\chi}(L_1)\approx\frac{9N_1^2}{8\pi^3 J}(3\sqrt{3}-\pi)\approx\frac{3\sqrt{3}-\pi}{\pi}\chi_>(L_1), \tag{39}$$

which again represents a significant reduction below the bulk value. We also observe that, while the long-distance susceptibility $\chi_>$ in this region varies as L^2, the short-distance susceptibility $\chi_<$ (for fixed r_1) diverges only as L^1. We now proceed to examine the situation in a general geometry where d^* may exceed unity.

III. LOCAL SUSCEPTIBILITY IN A GENERAL GEOMETRY FOR $\tilde{t}>0$

We start with Eq. (17) and, on the basis of our experience with the case $d^*=1$, observe that for $\tilde{t}>0$ and $L_j\to\infty$ terms with $q_j\neq 0$ give rise to exponential corrections only; terms with $q_j=0$, on the other hand, lead to corrections which may in the end turn out to be algebraic instead. Concentrating on the latter, we write

$$\chi(\mathbf{r};L_j)=\frac{1}{4J}\int_0^\infty e^{-(1/2)\phi x}\prod_{j=1}^{d^*}\left[\sum_{k_j=-r_j+1}^{r_j-1}[e^{-x}I_{k_j}(x)]\right]dx. \tag{40}$$

Now, making use of the asymptotic results

$$I_\nu(x)\simeq\frac{e^{x-\nu^2/2x}}{\sqrt{2\pi x}} \tag{41}$$

and

$$\sum_{k=-r+1}^{r-1}e^{-k^2/2x}\simeq\sqrt{2\pi x}\,\mathrm{erf}\left[\frac{r}{\sqrt{2x}}\right], \tag{42}$$

where erf$z$ is the well-known error function, we obtain

$$\chi(\mathbf{r};L_j)=\frac{1}{4J}\int_0^\infty e^{-(1/2)\phi x}\prod_{j=1}^{d^*}\mathrm{erf}\left[\frac{r_j}{\sqrt{2x}}\right]dx \tag{43}$$

or, in *scaled* form,

$$2J\phi(L_j)\chi(\mathbf{r};L_j)=F(z_j)$$
$$=\int_0^\infty e^{-u}\prod_{j=1}^{d^*}\mathrm{erf}\left[\frac{z_j}{2\sqrt{u}}\right]du$$
$$\le 1\quad(z_j=r_j[\phi(L_j)]^{1/2}), \tag{44}$$

which may be compared with the corresponding bulk result, viz.,

$$2J\phi(\infty)\chi(\infty)=1. \tag{45}$$

In view of the fact that in this regime (where $y_j\gg 1$) the difference between the quantities $\phi(L_j)$ and $\phi(\infty)$ is exponentially small,[8] the influence of antiperiodic boundary conditions on the susceptibility of the system is mainly determined by the function $F(z_j)$. For $z_j\gg 1$, i.e., for $r_j\gg\xi$, the function $F(z_j)$ approaches unity, which means that the local susceptibility $\chi(\mathbf{r};L_j)$ is essentially equal to its limiting value $\chi_>(L_j)$ which, in turn, is practically the same as the bulk value $\chi(\infty)$. If, however, one or more of the z_j happen to be less than (or of order) unity, the corresponding factors in the integrand will reduce the value of $F(z_j)$ below unity. For instance, points near the "surface" of the lattice, where only one of the r_j (say, r_1) is less than (or of order) ξ, will lead to an overall diminution in χ of order $\xi/L_1\sim 1/y_1$. Those near the "edges" of the lattice, where two of the r_j (say, r_1 and r_2) are less than (or of order) ξ, will lead to an overall effect of order $\xi^2/L_1L_2\sim 1/y_1y_2$. And, finally, for those near the "corners" of the lattice, where all three r_j play a decisive role, the effect will be of order $\xi^3/L_1L_2L_3\sim 1/y_1y_2y_3$. Accordingly, the overall susceptibility $\bar{\chi}(L_j)$ of the lattice will indeed be of the form shown in (1). For a quantitative assessment of this effect, we may average over $\mathbf{r}$ right away and obtain[9]

$$\left\langle\mathrm{erf}\left[\frac{z_j}{2\sqrt{u}}\right]\right\rangle_{\mathrm{av}}\equiv\frac{1}{y_j}\int_0^{y_j}\mathrm{erf}\left[\frac{z_j}{2\sqrt{u}}\right]dz_j$$
$$=\frac{2\sqrt{u}}{y_j}\int_0^{y_j/2\sqrt{u}}(1-\mathrm{erfc}t)dt$$
$$\approx 1-\frac{2\sqrt{(u/\pi)}}{y_j}\quad(y_j\gg 1). \tag{46}$$

Substituting this result into (44), we get

$$2J\phi(L_j)\bar{\chi}(L_j)=\int_0^\infty e^{-u}\prod_{j=1}^{d^*}\left[1-\frac{2\sqrt{(u/\pi)}}{y_j}\right]du, \tag{47}$$

which, for $d^*=3$, leads precisely to Eq. (1). Algebraic effects in the overall susceptibility of the system, which appeared as "surface" effects, "edge" effects and "corner" effects in the lattice,[2] are thus fully accounted for.

For an analysis of the short-distance local susceptibility, $\chi_<(\mathbf{r};L_j)$, for $z_j\ll 1$, we make use of the relation

$$\mathrm{erf}t\equiv\frac{2}{\sqrt{\pi}}\int_0^t e^{-u^2}du\simeq\frac{2}{\sqrt{\pi}}te^{-\alpha t^2}\quad(0<\alpha<1), \tag{48}$$

and the integral[10]

$$\int_0^\infty x^{\nu-1}e^{-tx-s/x}dx=2\left[\frac{s}{t}\right]^{\nu/2}K_\nu(2\sqrt{st}\,)\ , \quad (49)$$

where $K_\nu(z)$ denotes the second modified Bessel function, to obtain

$$2J\phi(L_j)\mathcal{X}_<(\mathbf{r};L_j)\simeq\begin{cases} z_1 \quad (d^*=1)\ , & (50)\\ \dfrac{z_1z_2}{\pi}\left[\ln\left[\dfrac{1}{z_1^2+z_2^2}\right]+c_2\right] \quad (d^*=2)\ , & (51)\\ c_3z_1z_2z_3/(z_1^2+z_2^2+z_3^2)^{1/2} \quad (d^*=3)\ , & (52)\end{cases}$$

where c_2 and c_3 are constants. One may at this stage examine the $\tilde{t}$ dependence of $\mathcal{X}_<$ which enters through the parameter ϕ. On invoking a critical exponent $\gamma_<$, as in (28), we find from (50) that $\mathcal{X}_<$ varies as $\phi^{-1}\xi^{-1}\sim\tilde{t}^{-\gamma+\nu}\sim\tilde{t}^{-(1/2)\gamma}$ for $d^*=1$ but, from (51), as

$$\phi^{-1}\xi^{-2}\ln\xi\sim\tilde{t}^{-\gamma+2\nu}\ln(1/\tilde{t})\sim\ln(1/\tilde{t})$$

for $d^*=2$, so that one is tempted to conclude generally that

$$\gamma_<=\gamma-d^*\nu=\frac{2-d^*}{2}\gamma \quad (d^*<d)\ . \quad (53)$$

For $d^*=3$, this would lead to an expected dependence of the form $\phi^{-1}\xi^{-3}$ whereas the actual result shown in (52) is of the form $\phi^{-1}\xi^{-2}$ which, in the present model, is $\tilde{t}$ independent! The resolution of this dilemma lies in the fact that the term appearing in (52) belongs to the nonsingular part of $\mathcal{X}_<$ while the singular part is determined by the next higher-order term in ϕ: a short calculation yields

$$\mathcal{X}_<^{(\text{sing})}(\mathbf{r};L_j)=-\frac{z_1z_2z_3}{J\pi\phi} \quad (3<d)\ , \quad (54)$$

which indeed conforms to the relationship (53).

The case $d^*=d$ is, however, special. While Eq. (53) now seems to suggest $\gamma_<=-2\beta=-1$, a detailed examination of the case $d^*=d=3$ shows that the leading singular term in $\mathcal{X}_<$ is not of the form $\tilde{t}^{\,1}$ but is rather of the form $\tilde{t}^{\,2}$. This may be understood in terms of the arguments presented in the Introduction, according to which the leading singular term in $\mathcal{X}_<$ for $d^*=d$ should, in view of the role played by the correlations $G(\mathbf{r},\mathbf{r}')$, be of the form $\tilde{t}^{\,1-\alpha}$, i.e., $\tilde{t}^{\,2}$.

The "corner" site ($r_j=1$, all j) presents a rather exceptional situation: Eq. (12) yields

$$\mathcal{X}(1;L_j)=\frac{1}{2J\prod_{j=1}^{d^*}N_j}\sum_{\{n_j\}}\frac{1}{\phi+4\sum_{j=1}^{d^*}\sin^2[\pi(n_j+\frac{1}{2})/N_j]}\ . \quad (55)$$

For $d^*=d$, the sum appearing on the right-hand side of (55) is exactly the same as the one appearing in the constraint equation of the system: see Eq. (26) of II. This fact leads to

$$[\mathcal{X}(1;L_j)]_{d^*=d}=\frac{K}{J}=\frac{1}{k_BT}\ , \quad (56)$$

in perfect agreement with (9). The specific influence of $G(\mathbf{r},\mathbf{r}')$ shows up as soon as any of the r_j's exceeds unity, and the temperature dependence of $\mathcal{X}(\mathbf{r};L_j)$ then changes qualitatively.

IV. LOCAL SUSCEPTIBILITY IN A GENERAL GEOMETRY FOR $\tilde{t}<0$

For a study of the situation with $\tilde{t}<0$ and $L_j\to\infty$, we go back to Eq. (17) and employ the asymptotic expression (41) and the Poisson identity

$$\sum_{q_j=-\infty}^{\infty}(-1)^{q_j}e^{-N_j^2(q_j+\epsilon_j)^2/2x}=\frac{\sqrt{2\pi x}}{N_j}\sum_{n_j=-\infty}^{\infty}\cos[2\pi(n_j+\tfrac{1}{2})\epsilon_j]e^{-2\pi^2x[n_j+(1/2)]^2/N_j^2}\ , \quad (57)$$

to obtain

$$\mathcal{X}(\mathbf{r};L_j)=\frac{1}{4J}\int_0^\infty e^{-(1/2)\phi x}\prod_{j=1}^{d^*}\left[\frac{1}{N_j}\sum_{n_j=-\infty}^{\infty}\left[e^{-2\pi^2x[n_j+(1/2)]^2/N_j^2}\sum_{k_j=-r_j+1}^{r_j-1}\cos[2\pi(n_j+\tfrac{1}{2})k_j/N_j]\right]\right]dx\ . \quad (58)$$

The summation over k_j and the integration over x can be readily carried out, with the result

$$\mathcal{X}(\mathbf{r};L_j)=\frac{1}{2J\prod_{j=1}^{d^*}N_j}\sum_{n_j=-\infty}^{\infty}\frac{\prod_{j=1}^{d^*}\sin[\pi(n_j+\frac{1}{2})(2r_j-1)/N_j]/\sin[\pi(n_j+\frac{1}{2})/N_j]}{\phi+4\pi^2\sum_{j=1}^{d^*}(n_j+\frac{1}{2})^2/N_j^2}\ . \quad (59)$$

Since ϕ in this regime is very close to its minimum value $-\pi^2\sum_j(1/N_j^2)$, the leading behavior of $\chi(\mathbf{r};L_j)$ is determined by the most dominant terms in the sum, viz., the ones with $n_j=0$ or -1. We thus obtain, for $r_j \gg 1$,

$$\chi(\mathbf{r};L_j)\approx\frac{1}{2J}\left[\frac{4}{\pi}\right]^{d^*}\frac{\prod_{j=1}^{d^*}\sin z_j'}{\phi+\pi^2\sum_{j=1}^{d^*}(1/N_j^2)}, \tag{60}$$

where

$$z_j'=\pi r_j/N_j \quad (j=1,\ldots,d^*) . \tag{61}$$

This now leads to the following results.

(i) For $d^*=1$, the previous expression (29) is precisely recaptured, thus confirming the derivation presented in Sec. II.

(ii) For $d^*=2$ (and $N_1=N_2$), one obtains

$$\chi(r_1,r_2)\approx\frac{2N_1^2\sin z_1'\sin z_2'}{J\pi^2(y^2+\pi^2/2)}, \tag{62}$$

which, in terms of the scaled variable x_1, reads

$$\chi(r_1,r_2)\approx\frac{2N_1^2\sin z_1'\sin z_2'}{J\pi^3}\left[2\pi|x_1|/\Gamma\left[\frac{4-d}{2}\right]\right]^{2/(4-d)} . \tag{63}$$

(iii) For $d^*=3$ (and $N_1=N_2=N_3$), one finds

$$\chi(r_1,r_2,r_3)\approx\frac{8N_1^2\sin z_1'\sin z_2'\sin z_3'}{J\pi^3(y^2+3\pi^2/4)}\approx\frac{8N_1^2\sin z_1'\sin z_2'\sin z_3'}{J\pi^4}\times\left[\pi|x_1|/\Gamma\left[\frac{5-d}{2}\right]\right]^{2/(5-d)} . \tag{64}$$

With each $\sin z_j'$ replaced by its average value $2/\pi$, Eqs. (63) and (64) yield expressions for $\bar{\chi}$ which are in complete agreement with Eqs. (93) and (95) of II. It is now straightforward to see that for $z_j'=O(1)$ one has $\chi(\mathbf{r})\sim L^{\zeta}$, with $\zeta=2(d-d')/(2-d')$, but for $z_j'\ll 1$, one obtains

$$\chi_<(\mathbf{r})\sim L^{\zeta_<}, \text{ with } \zeta_<=\zeta-d^* \quad (r_j \text{ fixed}) . \tag{65}$$

In the special case $d^*=d$, the leading behavior of the short-distance susceptibility $\chi_<(\mathbf{r})$ is seen to be L-independent. It is then probable that terms with $n_j=0$ and -1 are no longer dominant, in which case $\chi_<$ cannot be determined from Eq. (60) as such. One must then go back to Eq. (59) and assess the contribution of terms with $n_j\neq 0, -1$ as well. This would entail an even more complex analysis of the problem than presented here.

V. CONCLUDING REMARKS

The main purpose of the present investigation has been to demonstrate how finite-size effects of an algebraic nature arise in the susceptibility of a finite-sized spherical model under antiperiodic boundary conditions at temperatures above $T_c(\infty)$. To achieve this end, we have carried out a detailed study of the *local* susceptibility $\chi(\mathbf{r};L_j)$ of the system whose variation in space is seen to be responsible for the algebraic corrections in the *overall* susceptibility $\bar{\chi}(L_j)$. For $T>T_c(\infty)$, this variation is significant only over short distances, of order ξ, from the antiferromagnetic "seams" in the system; accordingly, the main effect in $\bar{\chi}$ turns out to be a correction behaving as ξ/L_j, which is clearly algebraic in nature. For $T<T_c(\infty)$, however, the influence of antiperiodic boundary conditions turns out to be more severe because the spatial variation of $\chi(\mathbf{r};L_j)$ now extends throughout the system. A qualitative difference nevertheless exists between "long-distance" regions with $r_j=O(L_j)$ and those with $r_j \ll L_j$, i.e., close to the seams. While in the former the manner in which χ approaches its standard bulk behavior, as $L_j\to\infty$, remains the same as under periodic boundary conditions, viz., as L^{ζ}, with $\zeta=2(d-d')/(2-d')$, and only its amplitude is modified, in the latter the manner of approach is also modified: $\chi(\mathbf{r},L)$, at fixed $\mathbf{r}$, diverges only as $L^{\zeta_<}$, with $\zeta_<=\zeta-d^*$.

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APPENDIX

To evaluate $\chi(r_1;L_1)$ from Eq. (17) in the special case $d^*=1$, we first integrate over x, using the formula[10]

$$\int_0^\infty e^{-\alpha x}I_\nu(\beta x)dx=\frac{\beta^\nu}{(\alpha^2-\beta^2)^{1/2}[\alpha+(\alpha^2-\beta^2)^{1/2}]^\nu} \quad (\alpha>\beta,\ \nu>-1) ,$$

and obtain

$$\chi(r_1;L_1)=\frac{\omega}{2J(\omega^2-1)}\times\sum_{q_1=-\infty}^{\infty}(-1)^{q_1}\left[\sum_{k_1=-r_1+1}^{r_1-1}\omega^{-|N_1q_1+k_1|}\right], \tag{A1}$$

where

$$\omega=(1+\tfrac{1}{2}\phi)+\tfrac{1}{2}\sqrt{\phi(4+\phi)} . \tag{A2}$$

Carrying out the summations over k_1 and q_1, we obtain the *exact* result

$$\chi(r_1;L_1)=\frac{\omega}{2J(\omega-1)^2}\left[1-\frac{2(\omega^{N_1-r_1+1}+\omega^{r_1})}{(\omega+1)(\omega^{N_1}+1)}\right] . \tag{A3}$$

As expected, $\chi(r_1;L_1)$ is symmetric about the point $\frac{1}{2}(N_1+1)$.

For $\phi \ll 1$, we have $\omega \simeq 1+\sqrt{\phi}$, whence $\omega^{N_1} \simeq e^{2y_1}$ and $\omega^{r_1} \simeq e^{z_1}$, where $y_1 = \frac{1}{2}N_1\sqrt{\phi}$ and $z_1 = r_1\sqrt{\phi}$. Equation (A3) then assumes the *scaled* form

$$\chi(r_1;L_1) \approx \frac{N_1^2}{8Jy_1^2}\left[1-\frac{\cosh(y_1-z_1)}{\cosh y_1}\right] \quad (r_1,N_1 \gg 1) . \tag{A4}$$

It is important to note that, for $y_1 \gg 1$, this reduces to

$$\chi(r_1;L_1) \approx \frac{N_1^2}{8Jy_1^2}(1-e^{-z_1}) , \tag{A5}$$

which follows directly from (A1) by retaining only the term with $q_1 = 0$.

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[1]S. Singh and R. K. Pathria, Phys. Rev. B 31, 4483 (1985); herein referred to as I.

[2]S. Singh and R. K. Pathria, Phys. Rev. B 32, 4618 (1985); herein referred to as II.

[3]V. Privman and M. E. Fisher, Phys. Rev. B 30, 322 (1984).

[4]S. Singh and R. K. Pathria, Phys. Rev. Lett. 55, 347 (1985).

[5]Under periodic boundary conditions, ξ^* $(=a\phi^{-1/2})$ represents the true correlation length, $\xi(L_j;T)$, of the finite system; see, for instance, S. Singh and R. K. Pathria, Phys. Rev. B 33, 672 (1986). Under antiperiodic conditions, however, the relationship between ξ^* and $\xi(L_j;T)$ is not so straightforward. While for $T > T_c(\infty)$ (where ϕ is positive and only weakly dependent on L_j), ξ^* is expected to be essentially equivalent to the true ξ, the same cannot be said of other regimes where ϕ assumes negative values, making ξ^* unreal. In view of the fact that, as the temperature of the system is reduced below $T_c(\infty)$, ϕ creeps toward the limiting value $-\pi^2\sum_j N_j^{-2}$, see Eq. (60) of the text, the true correlation length $\xi(L_j;T)$ may possibly be determined by an expression of the form $a(\phi+\pi^2\sum_j N_j^{-2})^{-1/2}$. Clearly, this question needs to be explored further.

[6]See, for instance, M. N. Barber, in *Phase Transitions and Critical Phenomena,* edited by C. Domb and J. L. Lebowitz (Academic, New York, 1983), Vol. 8, pp. 145–266.

[7]M. N. Barber and M. E. Fisher, Ann. Phys. (N.Y.) 77, 1 (1973).

[8]To see this, we refer to the constraint equation of the system, which is given by Eq. (45) of II, and note that, for $y \gg 1$, the function

$$\overline{\mathscr{K}}(\nu \mid d^*;y) \approx -2d^*K_\nu(2y)/y^\nu \approx -d^*\pi^{1/2}e^{-2y}/y^{\nu+1/2} \ll 1 .$$

A comparison of the given (finite) system with the corresponding bulk one, both at a common fixed temperature $T > T_c(\infty)$, then gives

$$[\phi(\infty)]^{(d-2)/2} \approx [\phi(L)]^{(d-2)/2}\left[1+\frac{2d^*\pi^{1/2}e^{-L/\xi(\infty)}}{\left|\Gamma\left(\frac{2-d}{2}\right)\right|[L/2\xi(\infty)]^{(d-1)/2}}\right] .$$

It follows that

$$\frac{\phi(L)-\phi(\infty)}{\phi(\infty)} \approx -\frac{2d^*\pi^{1/2}}{\Gamma\left(\frac{4-d}{2}\right)}\left[\frac{2\xi(\infty)}{L}\right]^{(d-1)/2} e^{-L/\xi(\infty)} ,$$

which is indeed exponentially small.

[9]M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Functions* (Dover, New York, 1970).

[10]I. S. Gradshteyn and I. M. Ryzhik, *Table of Integrals, Series and Products* (Academic, New York, 1980).