

Finite-size effects in the spherical model of ferromagnetism: Antiperiodic boundary conditions

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Explicit expressions are derived for the free energy, the specific heat, and the magnetic susceptibility of a spherical model of spins on a d -dimensional hypercubical lattice, of size $L_1 \times L_2 \times \cdots \times L_d$, under antiperiodic boundary conditions. The relevant scaling functions that govern the critical behavior of the system are obtained and, with the use of the asymptotic properties of these functions, various predictions of the Privman-Fisher hypothesis [Phys. Rev. B **30**, 322 (1984)] on the hyperuniversality of finite systems are verified. Approach towards standard critical behavior, both for $T < T_c(\infty)$ and $T > T_c(\infty)$, is examined. In the former case, the approach generally takes place through a power law; only in some special situations does one obtain an exponential law instead. In the latter case, the approach is generally exponential, except for the susceptibility of the system which (somewhat surprisingly) displays a finite-size effect dominantly determined by the surface-to-volume ratio of the lattice.

I. INTRODUCTION

In a recent paper¹ (hereafter referred to as I) we derived explicit expressions for various thermodynamic functions of a field-free spherical model of spins on a hypercubical lattice, of size $L_1 \times L_2 \times \cdots \times L_d$, under periodic boundary conditions. The expressions thus obtained were found to be in full conformity with the hypothesis recently put forward by Privman and Fisher,² according to which the "singular" part of the free-energy density of a finite system (of volume $L \times L \times \cdots \times L = L^d$, d being less than the upper critical dimension, $d_>$, of the system), near the bulk critical point $T = T_c(\infty)$, may be expressed in the form

$$f^{(s)}(t, h; L) \equiv \frac{F^{(s)}}{V k_B T} \approx L^{-d} Y(C_1 t L^{1/\nu}, C_2 h L^{\Delta/\nu}), \quad (1)$$

where t and h are the (reduced) temperature and field variables,

$$t = [T - T_c(\infty)]/T_c(\infty), \quad h = \mu_{\text{eff}} H / k_B T, \quad (2)$$

$x_1 (= C_1 t L^{1/\nu})$ and $x_2 (= C_2 h L^{\Delta/\nu})$ are the appropriate scaled variables, ν and Δ being the familiar bulk indices, while C_1 and C_2 are certain *nonuniversal*, system-dependent scale factors. The function $Y(x_1, x_2)$ is then a *universal* function, common to all systems in the same universality class as the given system. Of course, the precise nature of this function would vary significantly as we move from one geometry to another; the same would be true if we alter the set of boundary conditions to which the system is subjected. This variation may, in turn, affect the mathematical character of the finite-size effects expected in the system and, hence, the manner in which

the various thermodynamic quantities pertaining to the system approach their standard bulk behavior as $L \rightarrow \infty$. To elucidate these questions for a spherical model system subjected to *antiperiodic* boundary conditions, rather than *periodic* ones, constitutes the main purpose of this paper.

Of pivotal importance in expression (1) are the scale factors, C_1 and C_2 , which can be determined from a study of the corresponding *bulk* system.^{3,4} As shown in I, the scale factors appropriate to the spherical model are

$$C_1 = K_c a^{-(d-2)}, \quad C_2 = K_c^{-1/2} a^{-(d+2)/2}, \quad (3)$$

where $K_c [= J/k_B T_c(\infty)]$ stands for the interaction parameter of the system, a denotes the lattice constant, while d is restricted by the inequality $2 < d < 4$. The formal structure of the Privman-Fisher hypothesis for a *finite* spherical model is thereby laid.

To test the foregoing hypothesis and its varied consequences, as summarized in Sec. II, for the finite-sized spherical model in d dimensions; we derive explicit expressions for the relevant thermodynamic functions of the field-free system, $x_2 = 0$, of spins on a hypercubical lattice (of size $L_1 \times L_2 \times \cdots \times L_d$) under antiperiodic boundary conditions; see Sec. III. While the scale factors C_1 and C_2 , and certain asymptotic forms of the scaling function $Y(x_1, x_2)$ and some of its derivatives, could be determined from the appropriate bulk results, our analysis of the finite system enables us to derive complete mathematical form of these functions valid for *all* values of x_1 . In view of the fact that these functions are characteristic of the geometry of the lattice (which may, for convenience, be designated as $L^{d^*} \times \infty^{d'}$, where $d^* + d' = d$), finite-size effects in various thermodynamic properties of the system are also geometry dependent. Although most of the re-

sults derived here pertain to $2 < d < 4$, special cases arising from the most relevant dimension $d=3$, viz., a cube ($d^*=3$), a cylinder ($d^*=2$) and a film ($d^*=1$) are given special consideration. In all cases, the analytical results obtained here are found to be in complete agreement with the ones following from the Privman-Fisher hypothesis; see Sec. IV.

We have also examined at length the approach of the various physical properties of the system towards standard bulk behavior as $L \rightarrow \infty$. For $T < T_c(\infty)$, the approach turns out to be formally the same as in the case of periodic boundary conditions, in that it generally takes place through a power law; only in the special case $d'=2$ (of which a film in three dimensions is a good example) does one obtain an exponential law instead. One distinguishing feature of the present boundary conditions is the appearance of an L^{-2} term in the free-energy density of the system; this entails a helicity modulus $\Upsilon(T)$ which, for models with $O(n)$ symmetry ($n \rightarrow \infty$), can be related to the order parameter, $\mathcal{M}_0(T)$, of the corresponding bulk system.⁵ For $T > T_c(\infty)$, on the other hand, the approach is generally exponential in nature, except for the surprising behavior of the susceptibility of the system which shows a finite-size effect dominantly determined by the surface-to-volume ratio of the lattice; see Sec. V. The source of this unexpected effect is identified in Sec. VI.

II. FORMULATION OF THE PROBLEM

In accordance with (1), the singular part of the specific heat per unit volume of the system is given by

$$c^{(s)}(t, h; L) \approx C_1^2 L^{\alpha/\nu} Y_{(1)}(C_1 t L^{1/\nu}, C_2 h L^{\Delta/\nu}) \quad (4)$$

and that of the magnetic susceptibility by

$$\chi^{(s)}(t, h; L) \approx C_2^2 L^{\gamma/\nu} Y_{(2)}(C_1 t L^{1/\nu}, C_2 h L^{\Delta/\nu}), \quad (5)$$

where $Y_{(1)}$ and $Y_{(2)}$ are appropriate derivatives of the original function $Y(x_1, x_2)$, while use has been made of the relationships

$$d\nu = 2 - \alpha, \quad \Delta = \beta + \gamma, \quad \alpha + 2\beta + \gamma = 2. \quad (6)$$

In the following we shall confine ourselves to the field-free situation ($h=0$); in view of this, the variable x_2 may not be displayed explicitly in the subsequent expressions.

Starting with the free-energy density $f^{(s)}(t; L)$, as given by Eq. (1) with $h=0$, we may write

$$f^{(s)}(t; L) \approx F_+ t^{2-\alpha} \quad (t > 0, L \rightarrow \infty). \quad (7)$$

This requires that the scaling function

$$Y(x_1) \rightarrow Y_+ x_1^{2-\alpha} \quad (x_1 \rightarrow +\infty), \quad (8)$$

with the universal coefficient

$$Y_+ = F_+ / C_1^{2-\alpha}. \quad (9)$$

This leads to the expected behavior of the specific heat of the system, viz.

$$c^{(s)}(t; L) \approx -F_+ (2-\alpha)(1-\alpha)t^{-\alpha} \quad (t > 0, L \rightarrow \infty). \quad (10)$$

For $t < 0$ and $L \rightarrow \infty$, there are two possibilities of interest here:

$$(i) \quad Y(x_1) \rightarrow Y_- |x_1|^{\nu(d-\epsilon)} \quad (x_1 \rightarrow -\infty), \quad (11)$$

so that

$$f^{(s)}(t; L) \approx Y_- C_1^{\nu(d-\epsilon)} |t|^{\nu(d-\epsilon)} L^{-\epsilon}, \quad (11')$$

the index ϵ is as yet undetermined but may be geometry dependent. Secondly,

$$(ii) \quad Y(x_1) \rightarrow Y_-^* (\ln |x_1| + \text{const}) \quad (x_1 \rightarrow -\infty), \quad (12)$$

so that

$$f^{(s)}(t; L) \approx Y_-^* \left[\ln C_1 + \ln |t| + \frac{1}{\nu} \ln L + \text{const} \right] L^{-d}. \quad (12')$$

In each case, the coefficient Y_- or Y_-^* is universal. The repercussion of this on the specific heat of the system is that, for $\epsilon \neq d$ or 2,

$$c^{(s)}(t; L) \propto |t|^{-(\alpha+\nu\epsilon)} L^{-\epsilon} \quad (t < 0, L \rightarrow \infty). \quad (13)$$

The special case $\epsilon \rightarrow d$ corresponds to possibility (12), for which $c^{(s)}(t; L)$ is still given by (13), i.e.,

$$c^{(s)}(t; L) \propto |t|^{-2} L^{-d} \quad (t < 0, L \rightarrow \infty). \quad (13')$$

For $\epsilon = d$ the leading term in $f^{(s)}(t; L)$ would be independent of t , while for $\epsilon = 2$ it would be proportional to t ; in either case, this term would not contribute toward $c^{(s)}(t; L)$. In passing we observe that the extreme case $\epsilon \rightarrow \infty$ would entail a function that vanishes exponentially fast with L .

Regarding the (zero-field) susceptibility of the system, the leading behavior for $t > 0$ and $L \rightarrow \infty$ would be the standard one, viz.

$$\chi_0^{(s)}(t; L) \approx C_+ t^{-\gamma} \quad (t > 0, L \rightarrow \infty), \quad (14)$$

which requires that

$$Y_{(2)}(x_1) \rightarrow G_+ x_1^{-\gamma} \quad (x_1 \rightarrow +\infty), \quad (15)$$

with the universal coefficient

$$G_+ = C_+ C_1^\gamma / C_2^2. \quad (16)$$

For $t < 0$ and $L \rightarrow \infty$, we may assume that $\chi_0^{(s)}(t; L)$ diverges as L^ξ . The function $Y_{(2)}(x_1)$ must then behave as

$$Y_{(2)}(x_1) \rightarrow G_- |x_1|^{\xi-\gamma} \quad (x_1 \rightarrow -\infty), \quad (17)$$

with the result that

$$\chi_0^{(s)}(t; L) \approx G_- C_1^{\xi-\gamma} C_2^2 |t|^{\xi-\gamma} L^\xi, \quad (18)$$

with G_- being universal. Note that the extreme case $\xi \rightarrow \infty$ would now entail a function that diverges exponentially fast with L . This completes the set of predictions, based on the Privman-Fisher hypothesis, which we propose to test at length in the sections ahead.

III. THERMODYNAMICS OF THE SPHERICAL MODEL ON A FINITE LATTICE

We consider a system of N spins, s_i , located at sites $\mathbf{r}_i (= \mathbf{n}_i a)$ of a hypercubical lattice [of size $N_1 a$

$\times N_2 a \times \cdots \times N_d a (= Na^d)$ interacting through the Hamiltonian

$$\mathcal{H} = -J \sum_{NN} s_i s_j - \mu_{\text{eff}} H \sum_{i=1}^N s_i + \lambda \sum_{i=1}^N s_i^2, \quad (19)$$

where the various symbols have their usual meanings. The spherical field λ , which is conjugate to the quantity $-\sum_i s_i^2$, is introduced so as to satisfy the constraint

$$\sum_{i=1}^N \langle s_i^2 \rangle \equiv \mathcal{S}^2 = N. \quad (20)$$

Under *antiperiodic* boundary conditions, the free energy per spin is given by⁴

$$F(\beta, H, \lambda) = \frac{1}{2N\beta} \sum_q \ln[\beta(\lambda - \mu_q)] - \frac{\mu_{\text{eff}}^2 H^2}{4N} \sum_q \frac{|\epsilon_q|^2}{\lambda - \mu_q}, \quad (21)$$

where $\beta = 1/k_B T$, q is a collective symbol for the set of numbers $\{n_j; j=1, 2, \dots, d\}$, while the eigenvalues μ_q and the distribution coefficients ϵ_q are given by

$$\begin{aligned} \mu_q &= 2J \sum_j \cos[2\pi(n_j + \frac{1}{2})/N_j], \\ \epsilon_q &= \prod_j e^{i\psi} N_j^{-1/2} \csc[\pi(n_j + \frac{1}{2})/N_j] \\ & \quad [n_j = 0, 1, \dots, (N_j - 1)], \end{aligned} \quad (22)$$

with $\psi [= \psi(n_j, N_j)]$ real. The magnetization per spin is then given by

$$\mathcal{M}(\beta, H) = \frac{\mu_{\text{eff}} H}{2N} \sum_q \frac{|\epsilon_q|^2}{\lambda - \mu_q}, \quad (23)$$

from which the *initial* (zero-field) susceptibility follows as

$$\chi_0(\beta, H) = \frac{\mu_{\text{eff}}^2}{2N} \sum_q \frac{|\epsilon_q|^2}{\lambda - \mu_q}. \quad (24)$$

In zero field, Eq. (21) reduces to

$$F(\beta, \lambda) = \frac{1}{2N\beta} \sum_{\{n_j\}} \ln \left\{ \beta \left[\lambda - 2J \sum_{j=1}^d \cos \left[\frac{2\pi(n_j + \frac{1}{2})}{N_j} \right] \right] \right\}, \quad (25)$$

while the constraint (20) assumes the form

$$2K = \frac{1}{N} \sum_{\{n_j\}} \left[\frac{\lambda}{J} - 2 \sum_{j=1}^d \cos \left[\frac{2\pi(n_j + \frac{1}{2})}{N_j} \right] \right]^{-1}, \quad (26)$$

where $K = \beta J$.

For the evaluation of the summations appearing in Eqs. (25) and (26), we adopt the procedure developed in I, with the (important) difference that in the present case we use the identity

$$\begin{aligned} \sum_{n_j=0}^{N_j-1} \exp \left[x \cos \left[\frac{2\pi(n_j + \tau)}{N_j} \right] \right] \\ = N_j \sum_{q_j=-\infty}^{\infty} \cos(2\pi\tau q_j) I_{N_j q_j}(x) \end{aligned} \quad (27)$$

with $\tau = \frac{1}{2}$, rather than with $\tau = 0$; as before, $I_\nu(x)$ denotes a modified Bessel function. We thus obtain

$$F(\beta, \phi) = F_B(\beta, \phi) - \frac{1}{2\beta} \sum_{\{q_j\}}' (-1)^{\sum_j q_j} \int_0^\infty e^{-\phi x/2} \prod_{j=1}^d [e^{-x} I_{N_j q_j}(x)] x^{-1} dx, \quad (28)$$

where $F_B(\beta, \phi)$ denotes the bulk free energy per spin,

$$F_B(\beta, \phi) = \frac{\ln K}{2\beta} + \frac{1}{2\beta} \int_0^\infty \{e^{-x/2} - e^{-\phi x/2} [e^{-x} I_0(x)]^d\} x^{-1} dx, \quad (29)$$

the variable ϕ being given by the usual expression

$$\phi = (\lambda/J) - 2d. \quad (30)$$

The equilibrium value of ϕ is determined by the constraint equation which now reads

$$2K = W_d(\phi) + \frac{1}{2} \sum_{\{q_j\}}' (-1)^{\sum_j q_j} \int_0^\infty e^{-\phi x/2} \prod_{j=1}^d [e^{-x} I_{N_j q_j}(x)] dx, \quad (31)$$

where

$$W_d(\phi) = \frac{1}{2} \int_0^\infty e^{-\phi x/2} [e^{-x} I_0(x)]^d dx. \quad (32)$$

It will be noted that the primed summations in Eqs. (28) and (31) imply that terms with $\mathbf{q} = \mathbf{0}$ are excluded. The foregoing expressions are quite general in respect of the actual values of the numbers N_j . For concreteness, however, we may specify the geometry of the system to be $L^{d^*} \times \infty^{d'}$, where $d^* = 1, 2$, or 3 while $d' = d - d^*$.

As for the evaluation of the integrals appearing in Eqs. (28) and (31), we make use of the asymptotic expansion¹

$$\begin{aligned} I_\nu(x) = \frac{e^{x-\nu^2/2x}}{\sqrt{2\pi x}} \left\{ 1 + \frac{1}{8x} + \frac{9-32\nu^2}{2!(8x)^2} \right. \\ \left. + \frac{225-928\nu^2+128\nu^4}{3!(8x)^3} + \cdots \right\} \end{aligned}$$

[which is Eq. (56) of I] and the integral⁶

$$\int_0^\infty x^{v-1} e^{-\alpha x - \beta/x} dx = 2(\beta/\alpha)^{v/2} K_v(2\sqrt{\alpha\beta}), \quad (33)$$

where $K_\nu(z)$ denotes the other modified Bessel function. At the same time we employ standard expansions^{3,4} of the bulk terms (29) and (32) for $2 < d < 4$ and $\phi \ll 1$. We thus obtain, to the desired order in a/L ,

$$F(\beta, \phi) = F_B(\beta, 0) + \frac{4K_c}{\beta} \left[\frac{ya}{L} \right]^2 - \frac{1}{\beta\pi^{d/2}} \left[\frac{ya}{L} \right]^d \left[\left| \Gamma \left[\frac{2-d}{2} \right] \right| + 2\overline{\mathcal{H}} \left[\frac{d}{2} \middle| d^*; y \right] \right] \quad (34)$$

and

$$K_c - K = \frac{1}{8\pi^{d/2}} \left[\frac{ya}{L} \right]^{d-2} \left[\left| \Gamma \left[\frac{2-d}{2} \right] \right| - 2\overline{\mathcal{H}} \left[\frac{d-2}{2} \middle| d^*; y \right] \right], \quad (35)$$

where $K_c [= \frac{1}{2} W_d(0)]$ is the value of K at the bulk critical temperature $T_c(\infty)$, y is the *thermogeometric parameter*^{1,7} appropriate to the given system,

$$y = \frac{1}{2} (L/a)\phi^{1/2}, \quad (36)$$

while

$$\overline{\mathcal{H}}(n | d^*; y) = \sum'_{q(d^*)} (-1)^{(\sum_j q_j)} \frac{K_n(2yq)}{(yq)^n} [q = (q_1^2 + q_2^2 + \dots + q_{d^*}^2)^{1/2} > 0]. \quad (37)$$

Equation (34) gives us free energy at constant λ (or ϕ); the one at constant \mathcal{S} can be obtained from it through the Legendre transformation

$$A(\beta, \mathcal{S}) = F(\beta, \phi) - \frac{\lambda\mathcal{S}^2}{N} = F(\beta, \phi) - 2Jd - 4J \left[\frac{ya}{L} \right]^2. \quad (38)$$

Combining Eqs. (34), (35), and (38), we obtain

$$A(\beta, \mathcal{S}) = F_B(\beta, 0) - 2Jd + \frac{1}{\beta\pi^{d/2}} \left[\frac{ya}{L} \right]^d \times \left[\left[\left| \frac{1}{2} - \frac{1}{d} \right| \right] \left| \Gamma \left[\frac{2-d}{2} \right] \right| - \overline{\mathcal{H}} \left[\frac{d-2}{2} \middle| d^*; y \right] - \overline{\mathcal{H}} \left[\frac{d}{2} \middle| d^*; y \right] \right]. \quad (39)$$

The *singular part of the reduced free energy per unit volume* is then given by

$$f^{(s)}(\beta; L) = \frac{A^{(s)}(\beta, \mathcal{S})}{k_B T a^d} = L^{-d} \left[\frac{y}{\sqrt{\pi}} \right]^d \left[\frac{1}{d} \Gamma \left[\frac{4-d}{2} \right] - \overline{\mathcal{H}} \left[\frac{d-2}{2} \middle| d^*; y \right] - \overline{\mathcal{H}} \left[\frac{d}{2} \middle| d^*; y \right] \right]. \quad (40)$$

To the same order in a/L , the *singular part of the reduced specific heat per unit volume* turns out to be

$$c^{(s)}(\beta; L) = -\frac{32\pi^{d/2} K^2}{a^d} \times \frac{(ya/L)^{4-d}}{\Gamma \left[\frac{4-d}{2} \right] + 2\overline{\mathcal{H}} \left[\frac{d-4}{2} \middle| d^*; y \right]}. \quad (41)$$

We shall now verify some of the predictions made in Sec. II.

IV. VERIFICATION OF THE SCALING PREDICTIONS

Introducing the scale factor C_1 , as given by Eq. (3), into the constraint equation (35), we obtain

$$C_1 L^{d-2} \left[1 - \frac{K}{K_c} \right] = \frac{y^{d-2}}{8\pi^{d/2}} \left[\left| \Gamma \left[\frac{2-d}{2} \right] \right| - 2\overline{\mathcal{H}} \left[\frac{d-2}{2} \middle| d^*; y \right] \right]. \quad (42)$$

The expression on the left-hand side of (42) is a generalization⁸ of the scaled variable x_1 of the Privman-Fisher hypothesis (1), with t replaced by

$$\tilde{t} = (K_c - K)/K_c = [T - T_c(\infty)]/T. \quad (43)$$

Note that the variable \tilde{t} reduces to t as $T \rightarrow T_c(\infty)$; in its present form, however, \tilde{t} will enable us to extend the validity of the hypothesis down to 0 K. Expression (40) for the free-energy density of the system is now seen to be manifestly in conformity with the Privman-Fisher hypothesis, with scaling function $Y(x_1)$ given by the parametric equations

$$Y(y) = \left[\frac{y}{\sqrt{\pi}} \right]^d \left[\frac{1}{d} \Gamma \left[\frac{4-d}{2} \right] - \overline{\mathcal{H}} \left[\frac{d-2}{2} \middle| d^*; y \right] - \overline{\mathcal{H}} \left[\frac{d}{2} \middle| d^*; y \right] \right], \quad (44)$$

$$x_1(y) = \frac{y^{d-2}}{8\pi^{d/2}} \left[\left| \Gamma \left[\frac{2-d}{2} \right] \right| - 2\overline{\mathcal{X}} \left[\frac{d-2}{2} \mid d^*; y \right] \right], \quad (45)$$

among which y is supposed to be eliminated. At the same time, expression (41) for the specific heat is in conformity with the corresponding generalization of the scaling formula (4), with

$$Y_{(1)}(y) = - \frac{32\pi^{d/2} y^{4-d}}{\Gamma((4-d)/2) + 2\overline{\mathcal{X}}((d-4)/2 \mid d^*; y)}, \quad (46)$$

see Eq. (6) of Ref. 8.

We shall now examine the limiting behavior of the scaling functions Y and $Y_{(1)}$ in different regimes of $\tilde{\tau}$ and L , and for different geometries of the lattice.

(a) $\tilde{\tau} > 0$, $L \rightarrow \infty$. In this regime, $x_1 \rightarrow +\infty$, with the result that y diverges while the functions $\overline{\mathcal{X}}(y)$ vanish exponentially. Equations (44) and (45) then give

$$Y(x_1) \simeq \frac{\Gamma((4-d)/2)}{d} \left[\frac{8\pi x_1}{|\Gamma((2-d)/2)|} \right]^{d/(d-2)}, \quad (47)$$

which confirms to requirement (8), with $\alpha = (d-4)/(d-2)$ and Y_+ is universal. The function $Y_{(1)}$ in turn behaves as

$$Y_{(1)}(x_1) \simeq - \frac{32\pi^2}{\Gamma((4-d)/2)} \left[\frac{8\pi x_1}{|\Gamma((2-d)/2)|} \right]^{(4-d)/(d-2)}. \quad (48)$$

Substituting (48) into (4), we get conformity with requirement (10). The situation in this regime is, therefore, qualitatively the same as in the case of periodic boundary conditions—insofar as the field-free quantities $f^{(s)}$ and $c^{(s)}$ are concerned; as will be seen in Sec. V, the quantity $\chi^{(s)}$ behaves quite differently under the two sets of boundary conditions.

(b) $\tilde{\tau} < 0$, $L \rightarrow \infty$. Here $x_1 \rightarrow -\infty$, while y^2 tends to the limiting value $-d^*\pi^2/4$; this arises from the fact that while the spherical field λ tends, as usual, to the lowest eigenvalue μ_0 of the system, the latter under antiperiodic boundary conditions is given by the expression, see Eq. (22),

$$\begin{aligned} \mu_0 &= 2J \sum_j \cos \left[\frac{\pi}{N_j} \right] = 2Jd - 4Jd^* \sin^2 \left[\frac{\pi a}{2L} \right] \\ &\simeq 2Jd - Jd^* \frac{\pi^2 a^2}{L^2}, \end{aligned} \quad (49)$$

so that

$$y^2 = \frac{1}{4} \left[\frac{L}{a} \right]^2 \phi = \frac{1}{4} \left[\frac{L}{a} \right]^2 \frac{\lambda - 2Jd}{J} \rightarrow -d^* \frac{\pi^2}{4}. \quad (50)$$

The asymptotic behavior of the functions $\overline{\mathcal{X}}(y)$ in this regime can be ascertained through analytic continuation, from positive to negative values of y^2 , with the result that

$$y^{2n} \overline{\mathcal{X}}(n \mid d^*; y) \rightarrow \begin{cases} 2^{d^*-1} \pi^{d^*/2} \Gamma \left[\frac{d^*}{2} - n \right] \left[y^2 + d^* \frac{\pi^2}{4} \right]^{-(d^*/2-n)}, & n < \frac{d^*}{2} \\ 2^{d^*-1} \pi^{d^*/2} \left[\ln \left[y^2 + d^* \frac{\pi^2}{4} \right]^{-1} + \text{const} \right], & n = \frac{d^*}{2} \\ C(n \mid d^*), & n > \frac{d^*}{2}, \end{cases} \quad \begin{aligned} &(51a) \\ &(51b) \\ &(51c) \end{aligned}$$

where C is a constant whose precise value depends on the parameters n and d^* . Equation (45) then gives

$$y^2 + d^* \frac{\pi^2}{4} \simeq \begin{cases} \left[\frac{\Gamma((2-d')/2)}{2^{3-d'} \pi^{d'/2} |x_1|} \right]^{2/(2-d')}, & d' < 2 \\ \text{const} \times \exp(-2^{3-d'} \pi |x_1|), & d' = 2. \end{cases} \quad \begin{aligned} &(52a) \\ &(52b) \end{aligned}$$

For $d' > 2$, we encounter a crossover to the new critical point, $T = T_c(L)$, a study of which would require a somewhat closer examination of the functions $\overline{\mathcal{X}}(y)$ for $n > d^*/2$; we hope to return to this aspect of the problem in a subsequent investigation.

Going back to Eqs. (44) and (45), we now find that the

functions $Y(y)$ and $x_1(y)$ are given predominantly by terms involving $\overline{\mathcal{X}}[(d-2)/2 \mid d^*; y]$; consequently, for $d' \leq 2$,

$$Y(x_1) \simeq d^* \pi^2 |x_1| = d^* \pi^2 C_1 L^{d-2} \left[\frac{K}{K_c} - 1 \right], \quad (53)$$

whence, using Eqs. (1) and (3),

$$f^{(s)}(\tilde{\tau}; L) \simeq d^* \pi^2 \frac{K - K_c}{a^{d-2} L^2}. \quad (54)$$

Equation (54) represents the most dominant finite-size effect in the free energy of the system in this regime. The L dependence of this effect is characteristic of the boundary

conditions employed here; a corresponding calculation under periodic boundary conditions¹ leads instead to a term of order $L^{-\epsilon}$, with $\epsilon=2(d-d')/(2-d')$ which is at least equal to d and hence greater than 2. One can readily show that expression (54) entails the *helicity modulus*^{5,9}

$$\Upsilon(T) = 2k_B T \frac{K - K_c}{a^{d-2}} = \frac{2J}{a^{d-2}} \left[1 - \frac{T}{T_c(\infty)} \right], \quad (55)$$

which in the present case can be related to the order parameter, $\mathcal{M}_0(T)$, of the corresponding bulk system. In passing we note that each of the d^* directions, in which

$$Y_{(1)}(x_1) \simeq \begin{cases} -\frac{8}{(2-d')} \left[\frac{\Gamma\left[\frac{2-d'}{2}\right]}{2^{3-d^*} \pi^{d'/2}} \right]^{2/(2-d')} |x_1|^{-(4-d')/(2-d')}, & d' < 2 \\ -\text{const} \times \exp(-2^{5-d} \pi |x_1|), & d' = 2. \end{cases} \quad (56a)$$

Substituting these results into (4), we find that prediction (13) is confirmed for $d' < 2$, with

$$\epsilon = \left[\frac{4-d'}{2-d'} - \frac{d-4}{d-2} \right] / \left[\frac{1}{d-2} \right] = 2 \left[\frac{d-d'}{2-d'} \right]. \quad (57)$$

Passage of the given system towards bulk behavior is, therefore, governed by a power law whose exponent is determined jointly by d and d' . For the special case $d'=2$, the function $c^{(s)}(\tilde{r}; L)$ would vanish exponentially as $L^{d-4} \exp(-2^{5-d} \pi C_1 L^{d-2} |\tilde{r}|)$. In these respects, the behavior of the system under antiperiodic boundary conditions is qualitatively the same as under periodic boundary conditions; quantitatively, however, the two cases are marked by a difference in amplitudes for their respective scaling functions.

Before closing this section we would like to point out that in the case of a film in three dimensions ($d=3$, $d^*=1$), which belongs to the special category $d'=2$, the final results can be obtained in a closed form and the exponential behavior seen more explicitly. We have in this case

$$\overline{\mathcal{H}}\left(\frac{1}{2} \mid 1; y\right) = -\frac{\pi^{1/2}}{y} \ln(1 + e^{-2y}), \quad (58)$$

$$\overline{\mathcal{H}}\left(-\frac{1}{2} \mid 1; y\right) = -\frac{\pi^{1/2}}{e^{2y} + 1},$$

with the result that

$$Y_{(1)}(y) = -32\pi y \coth y, \quad (59)$$

while

$$Y(x_1) = \cosh^{-1}\left(\frac{1}{2} e^{4\pi x_1}\right). \quad (60)$$

As $x_1 \rightarrow -\infty$, $y \rightarrow i\pi/2$, in accordance with the limiting relationship

$$\left[y^2 + \frac{\pi^2}{4} \right] \simeq \frac{\pi}{2} e^{-4\pi |x_1|}, \quad (61)$$

the system is finite and subject to antiperiodic boundary conditions, contributes equally to expression (54) for $f^{(s)}(\tilde{r}; L)$. More generally, we would have here the sum $\sum_{j=1}^{d^*} L_j^{-2}$ instead of the factor $d^* L^{-2}$; this would, nevertheless, correspond to the same expression for $\Upsilon(T)$ as given in Eq. (55).

It is not difficult to see that the leading term (54) in $f^{(s)}(\tilde{r}; L)$ does not contribute to the specific-heat function $c^{(s)}(\tilde{r}; L)$. To study that function one has to go beyond the level of approximation registered in (54). It is simpler, however, to turn to the scaling function (46) which now reduces to

whence one obtains

$$Y_{(1)}(x_1) \simeq -8\pi^2 e^{-4\pi |x_1|}. \quad (62)$$

It follows that the function $c^{(s)}(\tilde{r}; L)$ in this case vanishes as $L^{-1} \exp(-4\pi C_1 L |\tilde{r}|)$.

V. MAGNETIC SUSCEPTIBILITY

We shall now analyze the initial susceptibility of the system, as given by Eqs. (22) and (24). For simplicity of treatment, we apply antiperiodic boundary conditions in the directions in which L_j 's are finite and periodic boundary conditions in the directions in which L_j 's tend to infinity; this should not affect the nature of the final results of our calculation, for the choice of boundary conditions in the latter directions cannot be of any material consequence. The formal expression for χ_0 , per unit volume, now becomes

$$\chi_0 = \frac{\mu_{\text{eff}}^2}{2Ja^d \prod_{j=1}^{d^*} N_j^2} \sum_{n(d^*)} \frac{\prod_{j=1}^{d^*} \csc^2[\pi(n_j + \frac{1}{2})/N_j]}{\phi + 4 \sum_{j=1}^{d^*} \sin^2[\pi(n_j + \frac{1}{2})/N_j]}. \quad (63)$$

Comparing (63) with the corresponding expression under periodic boundary conditions, namely,

$$\chi_0^{(P)} = \frac{\mu_{\text{eff}}^2}{2Ja^d \phi(P)}, \quad (64)$$

we have every reason to expect some significant differences between the two cases.

Using the representation

$$\frac{1}{z} = \frac{1}{2} \int_0^\infty e^{-zx/2} dx, \quad (65)$$

the sum in (63) can be written as

$$\begin{aligned} \Sigma_{(d^*)} &= \frac{1}{2} \sum_{n(d^*)} \left[\prod_{j=1}^{d^*} \csc^2 \left[\frac{\pi(n_j + \frac{1}{2})}{N_j} \right] \right] \int_0^\infty \exp \left[-\frac{1}{2} \phi x - 2x \sum_{j=1}^{d^*} \sin^2[\pi(n_j + \frac{1}{2})/N_j] \right] dx \\ &= \frac{1}{2} \int_0^\infty e^{-\phi x/2} \left[\prod_{j=1}^{d^*} S_j(x) \right] dx, \end{aligned} \tag{66}$$

where

$$S_j(x) = \sum_{n_j=0}^{N_j-1} \csc^2 \left[\frac{\pi(n_j + \frac{1}{2})}{N_j} \right] e^{-2x \sin^2[\pi(n_j + 1/2)/N_j]}. \tag{67}$$

Writing identity (27) in the form

$$\sum_{n_j=0}^{N_j-1} \exp \left[-2x \sin^2 \left[\frac{\pi(n_j + \frac{1}{2})}{N_j} \right] \right] = N_j \sum_{q_j=-\infty}^{\infty} (-1)^{q_j} [e^{-x I_{N_j q_j}}(x)]$$

and carrying out integration over x , we get

$$S_j(x) = N_j^2 - 2N_j \sum_{q_j=-\infty}^{\infty} (-1)^{q_j} \int_0^x e^{-t I_{N_j q_j}}(t) dt, \tag{68}$$

where use has been made of the fact that^{4,10}

$$S_j(0) = N_j^2. \tag{69}$$

It then follows that

$$\Sigma_{(d^*)} = \frac{\prod_{j=1}^{d^*} N_j^2}{2} \int_0^\infty e^{-\phi x/2} \prod_{j=1}^{d^*} \left[1 - \frac{2}{N_j} \sum_{q_j=-\infty}^{\infty} (-1)^{q_j} \int_0^x e^{-t I_{N_j q_j}}(t) dt \right] dx. \tag{70}$$

The evaluation of $\Sigma_{(1)}$ is straightforward; see the Appendix. We obtain, for $\phi \ll 1$,

$$\Sigma_{(1)} = \frac{N_1^4}{4y^2} \left[1 - \frac{\tanh y}{y} \right], \tag{71}$$

where $y (= \frac{1}{2} N_1 \phi^{1/2})$ is the same thermogeometric parameter as defined in Eq. (36). The susceptibility χ_0 for geometry $L^1 \times \infty^{d-1}$ thus turns out to be

$$\chi_0 = \frac{\mu_{\text{eff}}^2 L^2}{8Ja^{d+2}y^2} \left[1 - \frac{\tanh y}{y} \right]. \tag{72}$$

This leads to the reduced susceptibility

$$\chi_0^{(s)}(\beta; L) = \frac{\chi_0 k_B T}{\mu_{\text{eff}}^2} = \frac{L^2}{8Ka^{d+2}y^2} \left[1 - \frac{\tanh y}{y} \right], \tag{73}$$

which conforms to the scaling formula (5), with

$$\tilde{C}_2 = K^{-1/2} a^{-(d+2)/2}, \quad Y_{(2)}(y) = \frac{y - \tanh y}{8y^3}. \tag{74}$$

Note that the nonuniversal scale factor \tilde{C}_2 appearing here is a generalization of the scale factor C_2 of Eq. (3), to which it reduces as $T \rightarrow T_c(\infty)$; see also Eq. (7) of Ref. 8.

To examine the limiting behavior of the function $Y_{(2)}(x_1)$ in the two regimes of interest, we first observe that, for $\tilde{\tau} > 0$ and $L \rightarrow \infty$,

$$\begin{aligned} Y_{(2)}(x_1) &= \frac{1}{8y^2} - \frac{1}{8y^3} [1 - O(e^{-2y})] \\ &= \frac{1}{8} \left[\frac{|\Gamma((2-d)/2)|}{8\pi^{d/2}x_1} \right]^{2/(d-2)} \\ &\quad - \frac{1}{8} \left[\frac{|\Gamma((2-d)/2)|}{8\pi^{d/2}x_1} \right]^{3/(d-2)} + \dots, \end{aligned} \tag{75}$$

where the ellipsis represents exponentially small terms. The main term in (75) is consistent with requirement (15), with $\gamma = 2/(d-2)$ and G_+ universal; obviously, it will comply with the standard bulk behavior of χ_0 as displayed in Eq. (14). It is surprising, however, that the leading correction term in this case is algebraic, rather than the conventionally expected exponential, in character; one can readily see that this term entails a finite-size effect in χ_0 which varies as $L^{-1} \tilde{\tau}^{-(\gamma+\nu)}$ —apparently a “surface effect.” For $\tilde{\tau} < 0$ and $L \rightarrow \infty$, on the other hand,

$$Y_{(2)}(x_1) \simeq \frac{1}{\pi^2} \left[y^2 + \frac{\pi^2}{4} \right]^{-1} \propto \begin{cases} |x_1|^{2/(3-d)}, & d < 3 \\ \exp[4\pi|x_1|], & d = 3. \end{cases} \tag{76a}$$

$$\tag{76b}$$

Expression (76a) confirms the power-law prediction (17), with

$$\zeta = \left[\frac{2}{3-d} + \frac{2}{d-2} \right] / \left[\frac{1}{d-2} \right] = \frac{2}{3-d}, \quad d < 3. \quad (77)$$

Only for $d=3$, which belongs to the special category $d'=2$, is the approach of the system towards standard

$$\Sigma_{(3)} = \frac{N_1^2 N_2^2 N_3^2}{2} \int_0^\infty e^{-\phi x/2} \{ 1 - 2[P_1(x) + P_2(x) + P_3(x)] + 4[P_1(x)P_2(x) + P_1(x)P_3(x) + P_2(x)P_3(x)] - 8P_1(x)P_2(x)P_3(x) \} dx, \quad (78)$$

where

$$P_j(x) = \frac{1}{N_j} \sum_{q_j=-\infty}^{\infty} (-1)^{q_j} \int_0^x e^{-t} I_{N_j q_j}(t) dt. \quad (79)$$

Our experience with the case $d^*=1$ now tells us that, for $\tilde{t} > 0$ and $L_j \rightarrow \infty$, algebraic corrections to χ_0 would arise only from the term with $q_j=0$ in (79), while terms with $q_j \neq 0$ would give rise to exponential corrections. Concentrating on the former, we obtain

$$P_j(x) = \frac{1}{N_j} \left[\frac{2x}{\pi} \right]^{1/2} + \dots, \quad (80)$$

whence, for $\phi \ll 1$,

$$\int_0^\infty e^{-\phi x/2} P_j(x) dx \simeq \frac{2}{N_j \phi^{3/2}}, \quad (81a)$$

$$\int_0^\infty e^{-\phi x/2} P_j(x) P_k(x) dx \simeq \frac{8}{N_j N_k \pi \phi^2}, \quad (81b)$$

and

$$\int_0^\infty e^{-\phi x/2} P_1(x) P_2(x) P_3(x) dx \simeq \frac{12}{N_1 N_2 N_3 \pi \phi^{5/2}}. \quad (81c)$$

Substituting these results into (78) and introducing individual parameters

$$y_j = \frac{1}{2} N_j \phi^{1/2}, \quad j=1,2,3, \quad (82)$$

we obtain

$$\Sigma_{(3)} = \frac{N_1^2 N_2^2 N_3^2}{\phi} \left[1 - \left[\frac{1}{y_1} + \frac{1}{y_2} + \frac{1}{y_3} \right] + \frac{4}{\pi} \left[\frac{1}{y_1 y_2} + \frac{1}{y_1 y_3} + \frac{1}{y_2 y_3} \right] - \frac{6}{\pi} \frac{1}{y_1 y_2 y_3} + \dots \right], \quad (83)$$

where the ellipsis represents exponentially small terms. In view of the fact that y_j 's in this regime are proportional to L_j 's, we are clearly face to face with finite-size effects explicitly recognizable as "surface effects," "edge effects," and "corner effects." From (83), we readily obtain scaling functions for the susceptibility of a cube, a cylinder and a film:

bulk behavior exponential.

Going back to the general geometry, we consider the sum $\Sigma_{(3)}$, from which $\Sigma_{(2)}$ can also be obtained by a suitable operation letting $N_3 \rightarrow \infty$. Carrying out the product over j in (70), we obtain

$$[Y_{(2)}(y)]_{d^*=3} = \frac{1}{8y^2} \left[1 - \frac{3}{y} + \frac{12}{\pi y^2} - \frac{6}{\pi y^3} + \dots \right], \quad (84)$$

$$[Y_{(2)}(y)]_{d^*=2} = \frac{1}{8y^2} \left[1 - \frac{2}{y} + \frac{4}{\pi y^2} + \dots \right], \quad (85)$$

$$[Y_{(2)}(y)]_{d^*=1} = \frac{1}{8y^2} \left[1 - \frac{1}{y} + \dots \right], \quad (86)$$

subject only to errors exponential in y .

To study the problem in the other regime, viz. for $\tilde{t} < 0$ and $L \rightarrow \infty$, we go back to expression (79) for $P_j(x)$, introduce the asymptotic approximation¹

$$I_\nu(t) \simeq \frac{e^{t-\nu^2/2t}}{\sqrt{2\pi t}}, \quad (87)$$

which is sufficient to derive leading behavior of the various functions involved, and apply the Poisson identity¹¹

$$\sum_{q_j=-\infty}^{\infty} (-1)^{q_j} e^{-N_j^2 q_j^2 / 2t} = \frac{\sqrt{2\pi t}}{N_j} \sum_{n_j=-\infty}^{\infty} \exp[-2\pi^2 t (n_j + \frac{1}{2})^2 / N_j^2], \quad (88)$$

with the result that

$$P_j(x) \simeq \frac{1}{2} - \frac{1}{2\pi^2} \sum_{n_j=-\infty}^{\infty} \frac{\exp[-2\pi^2 x (n_j + \frac{1}{2})^2 / N_j^2]}{(n_j + \frac{1}{2})^2}. \quad (89)$$

This readily yields, see Eq. (68),

$$S_j(x) \simeq \frac{N_j^2}{\pi^2} \sum_{n_j=-\infty}^{\infty} \frac{\exp[-2\pi^2 x (n_j + \frac{1}{2})^2 / N_j^2]}{(n_j + \frac{1}{2})^2}. \quad (90)$$

Equation (66) now leads to the following results: (1) For $d^*=1$,

$$\Sigma_{(1)} \simeq \frac{N_1^2}{\pi^2} \sum_{n_1=-\infty}^{\infty} (n_1 + \frac{1}{2})^{-2} \left[\phi + \frac{4\pi^2 (n_1 + \frac{1}{2})^2}{N_1^2} \right]^{-1} = \frac{N_1^2}{\phi} \left[1 - \frac{\tanh(\frac{1}{2} N_1 \phi^{1/2})}{(\frac{1}{2} N_1 \phi^{1/2})} \right], \quad (91)$$

in agreement with (71) and hence with the same consequences as outlined above. (2) For $d^*=2$,

$$\Sigma_{(2)} \simeq \frac{N_1^2 N_2^2}{\pi^4} \sum_{n_{1,2}=-\infty}^{\infty} (n_1 + \frac{1}{2})^{-2} (n_2 + \frac{1}{2})^{-2} \left[\phi + \frac{4\pi^2(n_1 + \frac{1}{2})^2}{N_1^2} + \frac{4\pi^2(n_2 + \frac{1}{2})^2}{N_2^2} \right]^{-1}. \quad (92)$$

As ϕ approaches its limiting value $-(\pi^2/N_1^2 + \pi^2/N_2^2)$, the dominant behavior of this function is determined by terms with $n_{1,2}=0$ and -1 , with the result that, for $N_1=N_2$,

$$Y_{(2)} \rightarrow \frac{8}{\pi^4} \left[y^2 + \frac{\pi^2}{2} \right]^{-1} \propto |x_1|^{2/(4-d)}. \quad (93)$$

(3) For $d^*=3$,

$$\Sigma_{(3)} \simeq \frac{N_1^2 N_2^2 N_3^2}{\pi^6} \sum_{n_{1,2,3}=-\infty}^{\infty} (n_1 + \frac{1}{2})^{-2} (n_2 + \frac{1}{2})^{-2} (n_3 + \frac{1}{2})^{-2} \left[\phi + \frac{4\pi^2(n_1 + \frac{1}{2})^2}{N_1^2} + \frac{4\pi^2(n_2 + \frac{1}{2})^2}{N_2^2} + \frac{4\pi^2(n_3 + \frac{1}{2})^2}{N_3^2} \right]^{-1}, \quad (94)$$

whence, for $N_1=N_2=N_3$,

$$Y_{(2)} \rightarrow \frac{64}{\pi^6} \left[y^2 + \frac{3\pi^2}{4} \right]^{-1} \propto |x_1|^{2/(5-d)}. \quad (95)$$

Combining Eqs. (76a), (93), and (95), we conclude that, for general d^* , the scaling function for $\chi_0^{(s)}$ in the regime under consideration is of the asymptotic form

$$Y_{(2)} \simeq \frac{8^{d^*-1}}{\pi^{2d^*}} \left[y^2 + d^* \frac{\pi^2}{4} \right]^{-1} \propto |x_1|^{2/(2+d^*-d)}. \quad (96)$$

This confirms our prediction (17), with exponent ξ given by

$$\xi = \left[\frac{2}{2-d'} + \frac{2}{d-2} \right] / \left[\frac{1}{d-2} \right] = 2 \left[\frac{d-d'}{2-d'} \right], \quad (97)$$

which is exactly the same as obtained in the case of periodic boundary conditions; see Eq. (89) of I. A comparison of Eq. (97) with (57) reveals another important fact, namely, that for the system under study, exponents ξ and ϵ are identically equal.

VI. CONCLUDING REMARKS

We have evaluated analytically the zero-field free energy, the specific heat and the magnetic susceptibility of a spherical model of spins on a finite lattice in d dimensions under *antiperiodic* boundary conditions. Specializing to the geometry $L^{d^*} \times \infty^{d'}$, where $d^* + d' = d$, we have verified several predictions of the Privman-Fisher hypothesis on the hyperuniversality of finite systems. Relevant scaling functions have been derived and a detailed examination of the asymptotic behavior of these functions has been carried out in two regimes: for (a) $T > T_c(\infty)$ and $L \rightarrow \infty$, and for (b) $T < T_c(\infty)$ and $L \rightarrow \infty$. In the former regime, we find that finite-size corrections to standard bulk results are, in general, exponential in nature. In the case of susceptibility, however, we obtain the unexpected result that finite-size effects are algebraic instead and can be recognized explicitly as surface effects, edge effects,

and corner effects. The origin of these effects can be traced back to the distribution coefficients ϵ_q which appear explicitly in the expression for susceptibility; see Eqs. (22) and (24). This does not, however, tell us why the resulting effects should have the kind of character found here, which is generally regarded as foreign to both periodic and antiperiodic boundary conditions.^{12,13} Customarily, the kind of effects displayed in Eqs. (83)–(86) are expected only in the case of *free* boundary conditions (that correspond to the case $\tau=1$ in the Barber-Fisher notation⁴). In view of the present findings, we tend to think that finite-size effects in the latter case may turn out to be even more involved than one is normally accustomed to; a detailed study of the finite-sized spherical model under free boundary conditions is currently under way.

There is no new surprise in the second regime—just that the findings reported in I are further corroborated by the present study. Once again we find that, as $L \rightarrow \infty$, the given system approaches standard bulk behavior generally through a power law, with a well-defined exponent, which seems to be the rule rather than exception. The only exception within the premises of our calculation is provided by the case $d'=2$, of which a film in three dimensions ($d=3$, $d^*=1$) is a well-known example, in that it is marked by an exponential approach instead. At this point it seems important to add that, for the system under study, the results obtained in this regime apply all the way down to 0 K. To achieve this, we simply had to introduce an appropriate generalization of the parameters t and C_2 of the Privman-Fisher hypothesis; see Eqs. (43) and (74) in relation to Eqs. (2) and (3). A detailed account of this generalization, and the consequences thereof, are being reported separately.⁸

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APPENDIX

To evaluate $\Sigma_{(1)}$, as defined in Eq. (70), we interchange the order of integration over t and x , with the result that

$$\Sigma_{(1)} = \frac{N_1^2}{\phi} \left[1 - \frac{2}{N_1} \sum_{q_1=-\infty}^{\infty} (-1)^{q_1} \int_0^{\infty} e^{-(1+\phi/2)t} I_{N_1 q_1}(t) dt \right]. \quad (\text{A1})$$

We now use the integral⁶

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

to obtain

$$\Sigma_{(1)} = \frac{N_1^2}{\phi} \left[1 - \frac{4}{N_1 [\phi(4+\phi)]^{1/2}} \sum_{q_1=-\infty}^{\infty} (-1)^{q_1} \omega^{-|N_1 q_1|} \right], \quad (\text{A2})$$

$$\Sigma_{(1)} = \frac{N_1^2}{\phi} \left[1 - \frac{4}{N_1 [\phi(4+\phi)]^{1/2}} \frac{\omega^{N_1-1}}{\omega^{N_1+1}} \right], \quad (\text{A3})$$

where

$$\omega = (1 + \frac{1}{2}\phi) + \frac{1}{2}[\phi(4+\phi)]^{1/2}. \quad (\text{A4})$$

Equation (A3) gives $\Sigma_{(1)}$ exactly.

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

$$\Sigma_{(1)} = \frac{N_1^4}{4y^2} \left[1 - \frac{\tanh y}{y} \right], \quad (\text{A5})$$

as quoted in the text. It is important to observe that, for $y \gg 1$, $\Sigma_{(1)}$ reduces to the asymptotic expression

$$\Sigma_{(1)} \simeq \frac{N_1^4}{4y^2} \left[1 - \frac{1}{y} \right], \quad (\text{A6})$$

which follows directly from (A2) by retaining the term with $q_1=0$ only.

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