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On the Finite-Size Scalling Equation for the Spherical Model

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The mean spherical model with an arbitrary interaction potential, the Fourier transform of which has a long-wavelength exponent σ, $0<\sigma \leqslant 2$, is considered under periodic boundary conditions and fully finite geometry in d dimensions, when $\sigma < d < 2\sigma$. A new form of the finite-size scaling equation for the spherical field in the critical region is derived, which relates the temperature shift to Madelung-type lattice constants. The method of derivation makes use of the Poisson summation formula and a Laplace transformation of the momentum-space correlation function.

KEY WORDS: Finite-size scaling; spherical model; long-range interactions; Madelung lattice constants.

1. INTRODUCTION

The formulation of finite-size scaling ideas[1,2] at the beginning of the 1970s revived interest in the spherical model.[3-5] Due to the remarkable opportunity it offers for a rigorous study of finite-size effects at arbitrary dimensionality, this model became a touchstone for various scaling hypotheses and a source of new ideas in the general theory of finite-size scaling both in the critical region[6-12] and in the vicinity of a first-order phase transition.[13-17] Its relation to other current problems in the theory of phase transitions and criticality is outlined in ref. 18.

In this paper we consider the ferromagnetic mean spherical model[4] with periodic boundary conditions in fully finite geometry. The model

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Hamiltonian is defined on a d-dimensional torus $\mathbb{T}_N = \{1,..., N_0\}^d$ of $N = N_0^d$ sites and has the form

$$\mathscr{H}_N = -\frac{1}{2}\sum_{\mathbf{r},\mathbf{r}'} J(|\mathbf{r}-\mathbf{r}'|)\,\sigma_{\mathbf{r}}\sigma_{\mathbf{r}'} - H\sum_{\mathbf{r}} \sigma_{\mathbf{r}} \tag{1.1}$$

where $\mathbf{r} \in \mathbb{T}_N$, $\sigma_{\mathbf{r}} \in \mathbb{R}^1$ is the spin variable at site $\mathbf{r}$, $J(|\boldsymbol{l}|)$ is the pair interaction potential, and $H \in \mathbb{R}^1$ is an external magnetic field. The exact partition function of the finite mean spherical model depends on the interaction only through its Fourier transform

$$\hat{J}(\mathbf{q}) = \sum_{\boldsymbol{l} \in \mathbb{S}_N} J(|\boldsymbol{l}|)\exp(-i\boldsymbol{l}\cdot\mathbf{q}), \qquad \mathbf{q} = 2\pi\mathbf{p}/N_0, \quad p_\alpha = 1,..., N_0 \tag{1.2}$$

where

$$\mathbb{S}_N = \left\{-\frac{N_0-1}{2},..., 0,..., \frac{N_0-1}{2}\right\}^d$$

and is given by the expression

$$Z_N(s\,|\,\beta, H) = \pi^{N/2}\exp\left\{\frac{\beta^2H^2N}{4(s-\frac{1}{2}\beta\hat{J}(0))}\right\}\prod_{\mathbf{p}\in\mathbb{T}_N}\left[s-\frac{1}{2}\beta\hat{J}\left(\frac{2\pi\mathbf{p}}{N_0}\right)\right]^{-1/2} \tag{1.3}$$

Here $\beta > 0$ is the inverse temperature and the Lagrange multiplier $s = s_N(\beta, H)$ obeys the mean spherical constraint

$$-\frac{\partial}{\partial s}\log Z_N(s\,|\,\beta,\ H) = N \tag{1.4}$$

If we set

$$s = \tfrac{1}{2}\beta\hat{J}(0)(\phi+1)$$

then the equation for the spherical field (1.4) takes the form

$$W_d^{(N)}(\phi) = \beta\hat{J}(0)\{1-[H/\hat{J}(0)\phi]^2\} \tag{1.5}$$

where

$$W_d^{(N)}(\phi) = N_0^{-d}\sum_{\mathbf{p}\in\mathbb{T}_N}[\phi+\lambda(2\pi\mathbf{p}/N_0)]^{-1} \tag{1.6}$$

$$\lambda(\mathbf{q}) = 1-\hat{J}(\mathbf{q})/\hat{J}(0) \tag{1.7}$$

The study of the difference between the d-fold sum (1.5) at large N_0 and small ϕ and its limiting d-dimensional integral

$$W_d(\phi) = (2\pi)^{-d} \int_{-\pi}^{\pi} \cdots \int d^d\theta \, [\phi + \lambda(\boldsymbol{\theta})]^{-1} \tag{1.8}$$

is the cornerstone in the derivation of finite-size effects in the mean spherical model. There exist several approaches to the solution of this problem: direct evaluation of the closeness of the sum to the limiting integral,[17] methods based on the Poisson summation formula,[8,10,11] and the Ewald summation technique.[12]

The use of the Poisson summation formula makes possible the explicit separation of finite-size effects from the bulk contribution.[8,10,11] This approach is readily applicable to systems with short-range interactions, when the Fourier transform (1.2) has a quadratic long-wavelength asymptotic form.[3] Then one has to calculate the d-dimensional Fourier transform of $(\tilde{\phi} + q^2)^{-1}$, $\tilde{\phi} = 2d\phi$, which can be easily performed by using the elementary identity

$$(\tilde{\phi} + q^2)^{-1} = \int_0^{\infty} dt \exp(-\tilde{\phi}t) \prod_{\alpha=1}^{d} \exp(-q_\alpha^2 t) \tag{1.9}$$

This trick reduces the problem to the calculation of one-dimensional Gaussian integrals over $-\pi < q_\alpha \leqslant \pi$, $\alpha = 1,..., d$.

On the other hand, an arbitrary long-range interaction, decaying at large distances as $1/r^{d+\sigma}$ with $\sigma > 0$, has a Fourier transform with the long-wavelength asymptotics[5,19,20]

$$\hat{J}(\mathbf{q}) = \hat{J}(0)[1 - \rho_\sigma |\mathbf{q}|^\sigma + O(|\mathbf{q}|^{\sigma+\delta})], \qquad 0 < \sigma < 2, \quad \delta > 0 \tag{1.10}$$

The finite-size effects in this case have been studied only by the direct evaluation method and near the first-order phase boundary.[17]

One of the motivations of the present work was the wish to study finite-size effects in the spherical model with long-range ferromagnetic interaction of the type (1.10) in the critical region as well. The main idea of our approach becomes transparent when one considers the identity (1.9) as a Laplace transformation of the function $\exp(-\tilde{\phi}t)$. Then, for interactions (1.10) with arbitrary $\sigma \in (0, 2)$, instead of (1.9) we write

$$[\tilde{\phi} + (q^2)^{\sigma/2}]^{-1} = \int_0^{\infty} dt \, F_{\sigma/2}(\tilde{\phi}, t) \prod_{\alpha=1}^{d} \exp(-q_\alpha^2 t) \tag{1.11}$$

[3] By comparing the results of refs 8 and 10 with those of ref. 11, one concludes that the finite-size scaling is determined by the leading asymptotic form of the function $\hat{J}(\mathbf{q})$ and does not depend on its detailed behavior.

which also reduces the problem to the calculation of one-dimensional Gaussian integrals and the evaluation of their asymptotic behavior. The most surprising fact is that the explicit form of the function $F_{\sigma/2}(\tilde{\phi}, t)$, the Laplace transform of which is $(\tilde{\phi}+q^{\sigma})^{-1}$, is even of no importance. This makes it possible to study in a very simple and uniform way both cases of short-range ($\sigma=2$) and long-range ($0<\sigma<2$) interactions. We expect that the application of the present approach is not restricted to the spherical model only.

The paper is organized as follows. In Section 2 we explicitly show that the finite-size effects in the critical scaling regime do not depend on the details of the interaction (which for simplicity we assume isotropic), but only on the exponent σ of the Fourier transform $\hat{J}(\mathbf{q})$. This enables us to replace $\hat{J}(\mathbf{q})$ by its leading asymptotic form all over the Brillouin zone. In Section 3 we evaluate the d-dimensional Fourier transform of $(\tilde{\phi}+q^{\sigma})^{-1}$, which appears in the finite-size term derived by the application of the Poisson summation formula. The leading scaling behavior of the bulk and finite-size terms is derived in Section 4. There we obtain the main result of this paper: a new representation of the equation for the spherical field, valid for any $\sigma>0$ and $\sigma<d<2\sigma$. A straightforward, although not rigorous, derivation of our representation is given in Section 5 together with a brief discussion. Comments on some mathematical problems arising in our approach are given in the Appendix.

2. THE LONG-WAVELENGTH ASYMPTOTICS AND FINITE-SIZE EFFECTS

The derivation of the finite-size scaling equation is considerably facilitated by the consideration, instead of the original interaction $J(|\mathbf{l}|)$, of a model asymptotic one, $J^{as}(|\mathbf{l}|)$, the Fourier transform of which is exactly

$$\hat{J}^{as}(\mathbf{q}) = \hat{J}(0)[1-\rho_0 |q|^{\sigma}] \tag{2.1}$$

all over the Brillouin zone $-\pi<q_{\alpha}\leqslant\pi$, $\alpha=1,\ldots,d$. That is why we first prove that the error produced by such a replacement does not affect the leading finite-size terms, which are of the order[17] $O(N_0^{-d+\sigma})$ for $\sigma<d\leqslant 2\sigma$. It is assumed that the original interaction is isotropic (for simplicity of notation) and ferromagnetic, i.e., that $\hat{J}(\mathbf{q})$ reaches its unique maximum at $\mathbf{q}=0$.

By following the usual procedure based on the Poisson sum formula, one may cast the d-fold sum in Eq. (1.6) into the form[8,10,11]

$$W_d^{(N)}(\phi) = W_d(\phi) + \sum_{\mathbf{k}\in\mathbb{Z}^d}' \hat{g}(\phi; N_0\mathbf{k}) \tag{2.2}$$

where the prime in the sum over $\mathbf{k} \in \mathbb{Z}^d$ denotes the omission of the $\mathbf{k}=0$ term. In the right-hand side of Eq. (2.2) $W_d(\phi) = \hat{g}(0;0)$ is the bulk term (1.8), and $\hat{g}(\phi;\mathbf{k})$ is the Fourier transform of the summand in (1.6):

$$\hat{g}(\phi;\mathbf{k}) = N_0^{-d} \int_0^{N_0} \cdots \int_0^{N_0} d^d p \, [\phi + \lambda(2\pi \mathbf{p}/N_0)]^{-1} \exp(-2\pi i \mathbf{k}\cdot\mathbf{p}/N_0)$$
$$= (2\pi)^{-d} \int_{-\pi}^{\pi} \cdots \int_{-\pi}^{\pi} d^d\theta \, [\phi + \lambda(\boldsymbol{\theta})]^{-1} \exp(-i\mathbf{k}\cdot\boldsymbol{\theta}) \tag{2.3}$$

Now, along with $\hat{g}(\phi;\mathbf{k})$, we define

$$\hat{g}^{\mathrm{as}}(\phi;\mathbf{k}) = (2\pi)^{-d} \int_{-\pi}^{\pi} \cdots \int_{-\pi}^{\pi} d^d\theta \, (\phi + \rho_\sigma |\boldsymbol{\theta}|^\sigma)^{-1} \exp(-i\mathbf{k}\cdot\boldsymbol{\theta}) \tag{2.4}$$

Considering first the approximation error in the bulk term when $\phi = 0$, we use the identity

$$\hat{g}^{\mathrm{as}}(\phi;0) - \hat{g}(\phi;0)$$
$$= (2\pi)^{-d} \int_{-\pi}^{\pi} \cdots \int_{-\pi}^{\pi} d^d\theta \, f_\sigma(\boldsymbol{\theta}) - \phi(2\pi)^{-d} \int_{-\pi}^{\pi} \cdots \int_{-\pi}^{\pi} d^d\theta \, f_\sigma(\boldsymbol{\theta}) \, h_\sigma(\theta;\phi) \tag{2.5}$$

where

$$f_\sigma(\boldsymbol{\theta}) = \frac{\lambda(\boldsymbol{\theta}) - \rho_\sigma |\boldsymbol{\theta}|^\sigma}{\rho_\sigma |\theta|^\sigma \lambda(\boldsymbol{\theta})} = O(|\boldsymbol{\theta}|^{\delta-\sigma}) \tag{2.6}$$

$$h_\sigma(\boldsymbol{\theta};\phi) = \frac{\phi + \rho_\sigma |\boldsymbol{\theta}|^\sigma + \lambda(\boldsymbol{\theta})}{[\phi + \rho_\sigma |\boldsymbol{\theta}|^\sigma][\phi + \lambda(\boldsymbol{\theta})]} \tag{2.7}$$

The first integral on the right-hand side of Eq. (2.5) converges at $\boldsymbol{\theta} = 0$ for all $d > \sigma - \delta$ and we set

$$A_{d,\sigma} = (2\pi)^{-d} \int_{-\pi}^{\pi} \cdots \int_{-\pi}^{\pi} d^d\theta \, f_\sigma(\boldsymbol{\theta}), \qquad d > \sigma - \delta \tag{2.8}$$

Next, since $h_\sigma(\boldsymbol{\theta};0) = O(|\boldsymbol{\theta}|^{-\sigma})$, the second integral in Eq. (2.5) converges at $\phi \to 0$ for all $d > 2\sigma - \delta$ to the constant

$$B_{d,\sigma} = (2\pi)^{-d} \int_{-\pi}^{\pi} \cdots \int_{-\pi}^{\pi} d^d\theta \, f_\sigma(\boldsymbol{\theta}) \, h_\sigma(\boldsymbol{\theta};0), \qquad d > 2\sigma - \delta \tag{2.9}$$

Now let $\sigma - \delta < d < 2\sigma - \delta$. By writing

$$B_{d,\sigma}(\phi) \equiv (2\pi)^{-d} \int_{-\pi}^{\pi} \cdots \int_{-\pi}^{\pi} d^d\theta \, f_\sigma(\boldsymbol{\theta}) \, h_\sigma(\boldsymbol{\theta}; \phi)$$

$$= (2\pi)^{-d} \int_{-\pi}^{\pi} \cdots \int_{-\pi}^{\pi} d^d\theta \, f_\sigma(\boldsymbol{\theta}) \, h_\sigma(\boldsymbol{\theta}; \phi) + (2\pi)^{-d} \int_{-\pi}^{\pi} \cdots \int_{-\pi}^{\pi} d^d\theta \, f_\sigma(\boldsymbol{\theta}) \, h_\sigma(\boldsymbol{\theta}; \phi) \tag{2.10}$$

and using the asymptotic form (1.10) of $\hat{J}(\boldsymbol{\theta})$ for $|\boldsymbol{\theta}| \leqslant \varepsilon$, where ε is sufficiently small, together with the property of $\lambda(\boldsymbol{\theta})$ to have a unique maximum at $\boldsymbol{\theta} = 0$, we obtain the following estimates:

(a) $\sigma - \delta < d < 2\sigma - \delta$,

$$B_{d,\sigma}(\phi) = O(\phi^{-1} \varepsilon^{d+\delta-\sigma}) + O(\varepsilon^{d+\delta-2\sigma}) \tag{2.11}$$

The choice of $\varepsilon > 0$ on the right-hand side of (2.11) can be optimized by setting $\varepsilon = O(\phi^{1/\sigma})$, which results in the estimate

$$B_{d,\sigma}(\phi) = O(\phi^{(d+\delta-2\sigma)/\sigma}) \tag{2.12}$$

(b) $d = 2\sigma - \delta$,

$$B_{d,\sigma}(\phi) = O(\phi^{-1} \varepsilon^{\sigma}) - O(\log \varepsilon) \tag{2.13}$$

The optimal choice is again $\varepsilon = O(\phi^{1/\sigma})$, which leads to

$$B_{d,\sigma}(\phi) = -O(\log \phi) \tag{2.14}$$

Combining Eqs. (2.5) and (2.8) with the corresponding estimate (2.9), (2.12), or (2.14), we obtain

$$\hat{g}^{\mathrm{as}}(\phi; 0) - \hat{g}(\phi; 0) - A_{d,\sigma} = \begin{cases} O(\phi^{(d-\sigma+\delta)/\sigma}), & \sigma - \delta < d < 2\sigma - \delta \\ O(\phi \log \phi), & d = 2\sigma - \delta \\ O(\phi), & d > 2\sigma - \delta \end{cases} \tag{2.15}$$

It is well known (see, e.g., refs. 17 and 20) that the Watson-type integral (1.8) has the following asymptotic form when $\phi \to 0$:

$$W_d(\phi) = \begin{cases} W_d(0) - Q_{d,\sigma} \phi^{(d-\sigma)/\sigma}, & \sigma < d < 2\sigma \\ W_d(0) + Q_{d,2d} \phi \log \phi, & d = 2\sigma \\ W_d(0) - Q_{d,\sigma} \phi, & d > 2\sigma \end{cases} \tag{2.16}$$

By comparing (2.15) and (2.16), we conclude that for all d such that $\sigma < d \leqslant 2\sigma$, the deviation of the actual Fourier transform $\hat{J}(\mathbf{q})$ from its leading asymptotic form (2.1) is irrelevant to the bulk critical properties (i.e., whenever $\phi \to 0$); it may affect just the value of the critical temperature.

Next we consider the finite-size term in Eq. (2.2). Due to the presence of the rapidly oscillating factor $\exp(-iN_0\mathbf{k}\cdot\boldsymbol{\theta})$ in the integrand, one has

$$\begin{aligned}
&\hat{g}^{\mathrm{as}}(\phi, N_0\mathbf{k}) - \hat{g}(\phi, N_0\mathbf{k}) \\
&\quad = (2\pi)^{-d}\int_{-\pi}^{\pi}\cdots\int_{-\pi}^{\pi} d^d\theta \exp(-iN_0\mathbf{k}\cdot\boldsymbol{\theta}) \frac{\lambda(\boldsymbol{\theta}) - \rho_\sigma|\boldsymbol{\theta}|^\sigma}{[\phi + \rho_\sigma|\boldsymbol{\theta}|^\sigma][\phi + \lambda(\boldsymbol{\theta})]} \\
&\quad \simeq \phi^{(d+\delta-\sigma)/\sigma} b(N_0\phi^{1/\sigma}\mathbf{k}; \phi)
\end{aligned} \tag{2.17}$$

where, at $\phi \to 0$ and finite $N_0\phi^{1/\sigma}$,

$$\begin{aligned}
&b(N_0\phi^{1/\sigma}\mathbf{k}; \phi) \\
&\quad \simeq b(N_0\phi^{1/\sigma}\mathbf{k}; 0) \\
&\quad = (2\pi)^{-d}\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty} d^dx\, [\exp(-iN_0\phi^{1/\sigma}\mathbf{k}\cdot\mathbf{x})]\, O(|\mathbf{x}|^{\delta+\sigma})[1 + \rho_\sigma|\mathbf{x}|^\sigma]^{-2}
\end{aligned} \tag{2.18}$$

Since the scaled spherical field[17] ϕN_0^σ is finite in the critical region [see Eq. (4.20) below], the $|\mathbf{k}| \to \infty$ asymptotics of (2.18)

$$b(N_0\phi^{1/\sigma}\mathbf{k}; 0) = O(|\mathbf{k}|^{-d-\sigma-\delta}) \tag{2.19}$$

ensures the absolute convergences of the d-fold series

$$\sum_{\mathbf{k}\in\mathbb{Z}^d}{}' b(N_0\phi^{1/\sigma}\mathbf{k}; 0) = b(N_0\phi^{1/\sigma}) \tag{2.20}$$

Therefore,

$$\sum_{\mathbf{k}}{}' \hat{g}(\phi; N_0\mathbf{k}) = \sum_{\mathbf{k}}{}' \hat{g}^{\mathrm{as}}(\phi; N_0\mathbf{k}) - O(N_0^{-d+\sigma-\delta})(\phi^{1/\sigma}N_0)^{d-\sigma+\delta} b(\phi^{1/\sigma}N_0) \tag{2.21}$$

which implies that the leading $O(N_0^{-d+\sigma})$ finite-size terms are determined solely by the $|\mathbf{q}|^\sigma$ asymptotics of $\hat{J}(\mathbf{q})$. This fact has been used in ref. 17.

Summarizing, without loss of generality, we may confine ourselves to the study of the simplest representative of each universality class, namely the one with $\hat{J}(\mathbf{q})$ of the form (2.1) for all $\mathbf{q}$, $-\pi < q_\alpha \leqslant \pi$, $\alpha = 1,\ldots, d$.

3. EVALUATION OF THE d-DIMENSIONAL FOURIER TRANSFORM

Here we present our method of evaluation of the leading asymptotic form of the Fourier transform $\hat{g}^{\text{as}}(\phi; N_0\mathbf{k})$. For simplicity of notation, in the remainder we set $\tilde{\phi} = \phi/\rho_\sigma$.

Suppose that the function $F_\mu(t)$ is defined by its Laplace transform

$$(1 + s^\mu)^{-1} = \int_0^\infty F_\mu(t)\, e^{-st}\, dt \tag{3.1}$$

for $s, \mu > 0$. Then

$$\begin{aligned}
&\rho_\sigma \hat{g}^{\text{as}}(\phi; N_0\mathbf{k}) \\
&= (2\pi)^{-d} \int_{-\pi}^{\pi} \cdots \int_{-\pi}^{\pi} d^d\theta\, (\tilde{\phi} - |\boldsymbol{\theta}|^\sigma)^{-1} \exp(-iN_0\mathbf{k}\cdot\boldsymbol{\theta}) \\
&= \tilde{\phi}^{2/\sigma - 1} \int_0^\infty dx\, F_{\sigma/2}(\tilde{\phi}^{2/\sigma}x) \prod_{\alpha=1}^{d} \left\{ \frac{1}{2\pi} \int_{-\pi}^{\pi} d\theta_\alpha \exp(-iN_0 k_\alpha \cdot \theta_\alpha - x\theta_\alpha^2) \right\} \\
&= \frac{\tilde{\phi}^{2/\sigma - 1}}{2^d \pi^{d/2}} \int_0^\infty dx\, F_{\sigma/2}(\tilde{\phi}^{2/\sigma}x)\, x^{-d/2} \left(\exp \frac{-N_0^2 k^2}{4x} \right) \prod_{\alpha=1}^{d} \operatorname{Re}\{\Phi(z_\alpha)\}
\end{aligned} \tag{3.2}$$

Here $\Phi(z_\alpha)$ is the error function of a complex variable z_α,

$$z_\alpha = \pi x^{1/2} + \tfrac{1}{2} i N_0 k_\alpha x^{-1/2}$$

and $\operatorname{Re}\{\Phi(z_\alpha)\}$ denotes its real part.

Since for $k_\alpha \neq 0$

$$|z_\alpha|^2 \geqslant \pi N_0 |k_\alpha| \to \infty, \qquad N_0 \to \infty \tag{3.3}$$

uniformly in $x \geqslant 0$, one may use the known large-$|z|$ asymptotic expansion

$$\pi^{1/2} z e^{z^2} [1 - \Phi(z)] = 1 + O(z^{-2}) \tag{3.4}$$

and prove that the leading asymptotic form of the right-hand side of Eq. (3.2) results by setting $\Phi(z_\alpha) = 1$, $\alpha = 1, \ldots, d$, i.e.,

$$\begin{aligned}
&\rho_\sigma \hat{g}^{\text{as}}(\phi; N_0\mathbf{k}) \\
&\simeq \frac{\tilde{\phi}^{2/\sigma - 1}}{2^d \pi^{d/2}} \int_0^\infty dx\, F_{\sigma/2}(\tilde{\phi}^{2/\sigma}x)\, x^{-d/2} \exp \frac{-N_0^2 k^2}{4x} \\
&= \frac{\tilde{\phi}^{2/\sigma - 1}}{2^d \pi^{d/2}} \left(\frac{2\pi}{N_0} \right)^{d-2} \int_0^\infty dt\, F_{\sigma/2}(y^2 t)\, t^{-d/2} \exp \frac{-\pi^2 k^2}{t}
\end{aligned} \tag{3.5}$$

where

$$y = \tilde{\phi}^{1/\sigma} N_0 / 2\pi \tag{3.6}$$

4. EQUATION FOR THE SPHERICAL FIELD

Here we obtain the leading scaling behavior of the bulk and finite-size terms in (2.2) and derive the corresponding asymptotic form of the equation for the spherical field (1.5).

By substituting (3.5) into the sum on the right-hand side of Eq. (2.21) and exchanging the order of summation and integration, one obtains

$$\sum_{\mathbf{k}\in\mathbb{Z}^d}' \hat{g}(\phi; N_0\mathbf{k}) \simeq \frac{\bar{\phi}^{2/\sigma-1}}{\rho_\sigma 2^d \pi^{d/2}} \left(\frac{2\pi}{N_0}\right)^{d-2} \int_0^\infty dt\, F_{\sigma/2}(y^2 t) t^{-d/2} \sum_{\mathbf{k}\in\mathbb{Z}^d}' e^{-\pi^2 k^2/t} \tag{4.1}$$

Next, following refs. 8 and 11, we use Jacobi's identity

$$\sum_{\mathbf{k}}' e^{-\pi^2 k^2/t} = \left(\frac{t}{\pi}\right)^{d/2} \left(\sum_{\mathbf{k}}' e^{-k^2 t} + 1\right) - 1 \tag{4.2}$$

to transform expression (4.1) into

$$\sum_{\mathbf{k}}' \hat{g}(\phi; N_0\mathbf{k}) = \rho_\sigma^{-1} (2\pi y)^{-\sigma} N_0^{\sigma-d} [1 + y^2 I(y^2)] \tag{4.3}$$

where

$$I(y^2) = \int_0^\infty dt\, F_{\sigma/2}(y^2 t) \left[\sum_{\mathbf{k}}' e^{-k^2 t} - \left(\frac{\pi}{t}\right)^{d/2}\right] \tag{4.4}$$

We notice that the two terms in the square brackets in Eq. (4.4) cannot be integrated separately, since the d-fold sum

$$\sum_{\mathbf{k}\in\mathbb{Z}^d}' \int_0^\infty dt\, F_{\sigma/2}(y^2 t) e^{-k^2 t} = y^{-2} \sum_{\mathbf{k}}' [1 + (k/y)^\sigma]^{-1} \tag{4.5}$$

diverges ar $d \geqslant \sigma$ and so does the integral

$$\pi^{d/2} \int_0^\infty dt\, F_{\sigma/2}(y^2 t) t^{-d/2} \tag{4.6}$$

Nevertheless, we can transform further Eq. (4.4) by using the small-argument asymptotics of $F_{\sigma/2}(t)$, which follows from the definition (3.1):

$$F_{\sigma/2}(t) = t^{\sigma/2-1}/\Gamma(\sigma/2) - t^{\sigma-1}/\Gamma(\sigma) + O(t^{3\sigma/2-1}) \tag{4.7}$$

For $\sigma < d < 2\sigma$ we write (4.4) identically in the form

$$I(y^2) = I_1(y^2) + I_2(y^2) \tag{4.8}$$

where

$$I_1(y^2) = \int_0^\infty dt\,[F_{\sigma/2}(y^2t) - (y^2t)^{\sigma/2-1}/\Gamma(\sigma/2)]\left[\sum_{\mathbf{k}}{}' e^{-k^2t} - (\pi/t)^{d/2}\right]$$

$$= \sum_{\mathbf{k}}{}' \left\{\int_0^\infty dt\, F_{\sigma/2}(y^2t))e^{-k^2t} - \int_0^\infty dt\,[(y^2t)^{\sigma/2-1}/\Gamma(\sigma/2)]e^{-k^2t}\right\}$$

$$- \int_0^\infty dt\, F_{\sigma/2}(y^2t) - (y^2t)^{\sigma/2-1}/\Gamma(\sigma/2)](\pi/t)^{d/2}$$

$$= -y^2 \sum_{\mathbf{k}}{}' (k/y)^{-\sigma}[(k/y)^\sigma + 1]^{-1} + (2\pi)^d y^{d-2} D_{d,\sigma} \tag{4.9}$$

and

$$I_2(y^2) = \int_0^\infty dt\,[(y^2t)^{\sigma/2-1}/\Gamma(\sigma/2)]\left[\sum_{\mathbf{k}}{}' e^{-k^2t} - (\pi/t)^{d/2}\right]$$

$$= \lim_{\delta\to 0} \int_\delta^\infty dt\,[(y^2t)^{\sigma/2-1}/\Gamma(\sigma/2)]\left[\sum_{\mathbf{k}}{}' e^{-k^2t} - (\pi/t)^{d/2}\right]$$

$$= [y^{\sigma-2}/\Gamma(\sigma/2)] \lim_{\delta\to 0}\left\{\sum_{\mathbf{k}}{}' \int_\delta^\infty dt\, t^{\sigma/2-1}e^{-k^2t} - \pi^{d/2}\int_\delta^\infty dt\, t^{(\sigma-d)/2-1}\right\}$$

$$= y^{\sigma-2} C_{d,\sigma}/\Gamma(\sigma/2) \tag{4.10}$$

In (4.9) we have introduced the notation $D_{d,\sigma}$ for the integral

$$D_{d,\sigma} = -2^{-d}\pi^{-d/2}\int_0^\infty dx\, x^{-d/2}[F_{\sigma/2}(x) - x^{\sigma/2-1}/\Gamma(\sigma/2)] \tag{4.11}$$

and in (4.10) $C_{d,\sigma}$ denotes the Madelung-type constant (see, e.g., ref. 21)

$$C_{d,\sigma} = \lim_{\delta\to 0}\left\{\sum_{\mathbf{k}\in\mathbb{Z}^d}{}' \Gamma(\sigma/2, \delta k^2)k^{-\sigma} - \int_{-\infty}^\infty \cdots \int_{-\infty}^\infty d^dk\, \Gamma(\sigma/2, \delta k^2)k^{-\sigma}\right\} \tag{4.12}$$

Here $\Gamma(\alpha, x)$ is the incomplete gamma function.

Finally, from (4.3), (4.9), and (4.10) we obtain

$$\sum_{\mathbf{k}\in\mathbb{Z}^d}{}' \hat{g}(\phi; N_0\mathbf{k})$$

$$\simeq \rho_\sigma^{-1} N_0^{-d+\sigma}\left\{1/\bar{\phi}N_0^\sigma + C_{d,\sigma}/(2\pi)^\sigma\Gamma(\sigma/2)\right.$$

$$\left. + D_{d,\sigma}(\bar{\phi}N_0^\sigma)^{d/\sigma-1} - \bar{\phi}N_0^\sigma \sum_{\mathbf{k}\in\mathbb{Z}^d}{}' (2\pi k)^{-\sigma}[(2\pi k)^\sigma + \bar{\phi}N_0^\sigma]^{-1}\right\} \tag{4.13}$$

The leading asymptotic form of the bulk term can be obtained by setting $k_\alpha = 0$, $\alpha = 1, \ldots, d$, in Eq. (3.2) and then separating the small-argument asymptotics of $F_{\sigma/2}(t)$:

$$\begin{aligned}
\rho_\sigma \hat{g}^{\rm as}(\phi; 0) &= \frac{\tilde{\phi}^{2/\sigma - 1}}{2^d \pi^{d/2}} \int_0^\infty dx\ x^{-d/2} F_{\sigma/2}(\tilde{\phi}^{2/\sigma} x) [\Phi(\pi x^{1/2})]^d \\
&= \frac{\tilde{\phi}^{d/\sigma - 1}}{2^d \pi^{d/2}} \left\{ \int_0^\infty dt\, t^{-d/2} \left[F_{\sigma/2}(t) - \frac{t^{\sigma/2 - 1}}{\Gamma(\sigma/2)} \right] [\Phi(\pi t^{1/2} \tilde{\phi}^{-1/\sigma})]^d \right. \\
&\quad \left. + \frac{1}{\Gamma(\sigma/2)} \int_0^\infty dt\, t^{(\sigma - d - 2)/2} [\Phi(\pi t^{1/2} \tilde{\phi}^{-1/\sigma})]^d \right\} \\
&\simeq \rho_\sigma \hat{g}^{\rm as}(0; 0) - D_{d,\sigma} \tilde{\phi}^{d/\sigma - 1}
\end{aligned} \tag{4.14}$$

Here

$$\rho_\sigma \hat{g}^{\rm as}(0; 0) = [2^d \pi^{d/2} \Gamma(\sigma/2)]^{-1} \int_0^\infty dx\, x^{(\sigma - d - 2)/2} [\Phi(\pi x^{1/2})]^d \tag{4.15}$$

and $D_{d,\sigma}$ is the constant defined by Eq. (4.11).

Now we are ready to write down the equation for the spherical field $\tilde{\phi} = \phi/\rho_\sigma$ in the critical region. Taking into account the definition of the bulk critical temperature

$$\beta_c \hat{J}(0) = W_d(0) \tag{4.16}$$

and collecting the results (1.5), (2.2), (4.13), and (4.14), we obtain

$$\begin{aligned}
1/\tilde{\phi} N_0^\sigma + C_{d,\sigma}/(2\pi)^\sigma\, \Gamma(\sigma/2) - \tilde{\phi} N_0^\sigma \sum_{\mathbf{k}}{}' (2\pi k)^{-\sigma} [(2\pi k)^\sigma + \tilde{\phi} N_0^\sigma]^{-1} \\
= [(\beta - \beta_c) \rho_\sigma \hat{J}(0) - \beta H^2/\rho_\sigma \hat{J}(0) \tilde{\phi}^2] N_0^{d - \sigma}
\end{aligned} \tag{4.17}$$

By introducing the appropriate scaled variables

$$\begin{aligned}
x_1 &= \beta_c \rho_\sigma \hat{J}(0)(1 - \beta/\beta_c - \varepsilon_N) N_0^{d - \sigma} \\
x_2 &= [\beta/\rho_0 \hat{J}(0)]^{1/2}\, H N_0^{(d + \sigma)/2}
\end{aligned} \tag{4.18}$$

where ε_N is the finite-size temperature shift

$$\varepsilon_N = -C_{d,\sigma} [\beta_c \rho_\sigma \hat{J}(0) (2\pi)^\sigma\, \Gamma(\sigma/2) N_0^{d - \sigma}]^{-1} \tag{4.19}$$

we can write Eq. (4.17) in the universal form

$$\frac{1}{\tilde{\phi} N_0^\sigma} - \tilde{\phi} N_0^\sigma \sum_{\mathbf{k} \in \mathbb{Z}^d}{}' (2\pi k)^{-\sigma} [(2\pi k)^\sigma + \tilde{\phi} N_0^\sigma]^{-1} = -x_1 - \left(\frac{x_2}{\tilde{\phi} N_0^\sigma} \right)^2 \tag{4.20}$$

5. DISCUSSION

There is a very straightforward, although not exact and rigorous, derivation of Eq. (4.20). It starts with Eqs. (1.5) and (1.6) and the identity

$$N_0^{-d} \sum_{\mathbf{p} \in \mathbb{T}_N} \left[\phi + \lambda\left(\frac{2x\mathbf{p}}{N_0}\right)\right]^{-1}$$
$$= N_0^{-d} \sum_{\mathbf{p} \in \mathbb{T}_N}' \left[\lambda\left(\frac{2\pi\mathbf{p}}{N_0}\right)\right]^{-1}$$
$$+ N_0^{\sigma-d}\left\{\frac{1}{\phi N_0^{\sigma}} - \phi N_0^{-\sigma} \sum_{\mathbf{p} \in \mathbb{T}_N}' \left[\lambda\left(\frac{2\pi\mathbf{p}}{N_0}\right)\right]^{-1}\left[\phi + \lambda\left(\frac{2\pi\mathbf{p}}{N_0}\right)\right]^{-1}\right\} \quad (5.1)$$

The first term on the right-hand side of Eq. (5.1) is of order unity for $d > \sigma$ and we may set

$$N_0^{-d} \sum_{\mathbf{p} \in \mathbb{T}_N}' \left[\lambda\left(\frac{2\pi\mathbf{p}}{N_0}\right)\right]^{-1} = \beta_c \hat{J}(0)(1 - \varepsilon_N) \quad (5.2)$$

where $\varepsilon_N \to 0$ as $N_0 \to \infty$. The large-N_0 and small-ϕ asymptotic form of the last term on the right-hand side of Eq. (5.1) for $\sigma < d < 2\sigma$ is determined by the small-argument behavior of $\lambda(\mathbf{q})$; thus, we have the approximation

$$\phi N_0^{-\sigma} \sum_{\mathbf{p} \in \mathbb{T}_N}' \left[\lambda\left(\frac{2\pi\mathbf{p}}{N_0}\right)\right]^{-1}\left[\phi + \lambda\left(\frac{2\pi\mathbf{p}}{N_0}\right)\right]^{-1}$$
$$\simeq \phi\rho_\sigma^{-1} N_0^{\sigma} \sum_{\mathbf{p} \in \mathbb{T}_N}' (2\pi p)^{-\sigma}[\phi N_0^{\sigma} + \rho_\sigma(2\pi p)^{\sigma}]^{-1}$$
$$\simeq \rho_\sigma^{-1}\tilde{\phi} N_0^{\sigma} \sum_{\mathbf{p} \in \mathbb{Z}^d}' (2\pi p)^{-\sigma}\,[(2\pi p)^{\sigma} + \tilde{\phi} N_0^{\sigma}]^{-1} \quad (5.3)$$

Combining the above results with Eq. (1.5), we recover exactly Eq. (4.17), provided the values of ε_N is specified according to Eq. (4.19).

Thus, one of the main contributions of our work consists in suggesting a method of justification of the approximations involved in Eq. (5.3). Some mathematical problems arising in our approach are discussed in the Appendix.

Next, we have given an analytic definition of the temperature shift ε_N that makes connection to the Madelung-type lattice constants.[24] The result of Shapiro and Rudnick[12] is based on numerical approximations. Expression (62) of ref. 12 for the temperature shift in our notations takes the form

$$\varepsilon_N^{\mathrm{SR}} = \frac{d}{4\pi(d-2)}(\beta_c J N_0^{d-2})^{-1} \quad (5.4)$$

On the other hand, in the case of a simple cubic lattice with nearest neighbor interactions of strength J, one has $\sigma = 2$ and $\rho_2 \hat{J}(0) = J$, which simplifies expression (4.19) to

$$\varepsilon_N = -\frac{C_{d,2}}{4\pi^2} (\beta_c J N_0^{d-2})^{-1} \tag{5.5}$$

The numerical value of $C_{3,2}$ found by Harris and Monkhorst[24] (see also ref. 21) is $C_{3,2} = -8.913\,633$. This gives for the numerical prefactor in Eq. (5.8) the value of 0.225 785, which is to be compared to the corresponding value of 0.238 732 in the approximation (5.4).

We believe that Eq. (4.20) provides a very natural basis for deriving useful asymptotic expressions for the spherical field. We mention here two limiting cases.

When $\tilde{\phi} N_0^\sigma \gg 1$, for $\sigma < d < 2\sigma$ we may approximate the sum in Eq. (4.20) by an integral[17]:

$$\begin{aligned}
&\tilde{\phi} N_0^\sigma \sum_{\mathbf{k} \in \mathbb{Z}^d}{}' (2\pi k)^{-\sigma} [(2\pi k)^\sigma + \tilde{\phi} N_0^\sigma]^{-1} \\
&\quad = (2\pi y)^{-\sigma} \sum_{\mathbf{k} \in \mathbb{Z}^d}{}' (k/y)^{-\sigma} [(k/y)^\sigma + 1]^{-1} \\
&\quad \simeq \frac{2\pi^{d/2} y^{d-\sigma}}{\Gamma(d/2)(2\pi)^\sigma} \int_0^\infty \frac{r^{d-\sigma-1}\, dr}{1 + r^\sigma} \\
&\quad = G_{d,\sigma} (\tilde{\phi} N_0^\sigma)^{(d-\sigma)/\sigma}
\end{aligned} \tag{5.6}$$

where [cf. Eq. (3.22) in ref. 17]

$$G_{d,\sigma} = \frac{2\pi}{\sigma (4\pi)^{d/2} \Gamma(d/2) \,|\sin(\pi d/\sigma)|}$$

The above asymptotic form has been derived by Fisher and Privman[17]; at $\sigma = 2$ it agrees with the corresponding expression derived by Hall.[25] With the use of (5.6) one finds the asymptotic solution of Eq. (4.20), which to the leading order in $x_1 \gg 1$ is (for x_2 finite)

$$\tilde{\phi} \cong [\beta_c \rho \sigma \hat{J}(0)/G_{d,\sigma}]^{\sigma/(d-\sigma)} (1 - \beta/\beta_c)^{\sigma/(d-\sigma)} \tag{5.7}$$

i.e., it recovers the familiar bulk high-temperature, zero-field result.[5]

Whenever Eq. (4.20) has a solution $\tilde{\phi} N_0^\sigma \ll 1$, use can be made of the asymptotic expansion[26]

$$\sum_{\mathbf{k} \in \mathbb{Z}^d}{}' (2\pi k)^{-\sigma} [(2\pi k)^\sigma + \tilde{\phi} N_0^\sigma]^{-1} = (2\pi)^{-2\sigma} \sum_{\mathbf{k} \in \mathbb{Z}^d}{}' k^{-2\sigma} + O(\tilde{\phi} N_0^\sigma) \tag{5.8}$$

The constant

$$b_{d,\sigma} = \sum_{\mathbf{k} \in \mathbb{Z}^d}' k^{-2\sigma} \tag{5.9}$$

has been calculated for $d=3$ and $\sigma=2$ by Zasada and Pathria[26]: $b_{3,2}=16.53232$.

Taking into account Eq. (5.8), in the limit $x_1 \ll -1$ one finds

$$\tilde{\phi} N_0^{\sigma} \cong [(1+4\,|x_1|\,x_2^2)^{1/2}+1]/2\,|x_1| \tag{5.10}$$

This result can be put into the familiar first-order finite-size scaling form[15,17]

$$m_N(T, H) = m_0(T)\, Y_0(y_N) \tag{5.11}$$

where $m_N(T, H)$ is the average magnetization per spin,

$$m_N(T, H) = H/\rho_\sigma \hat{J}(0)\tilde{\phi}$$

$m_0(T)=(1-\beta_c/\beta)^{1/2}$ is the spontaneous magnetization, $y_N = m_0(T)\,\beta H N_0^d$ is the dimensionless scaling variable, and $Y_0(y)$ is the scaling function.

Finally, we note that the approximations to Eq. (4.20) that follow from Eqs. (5.6) and (5.8) can be used to derive corrections to the known low- and high-temperature asymptotic behavior of the spherical field.

APPENDIX: SOME MATHEMATICAL PROBLEMS

The formal derivation of Eq. (4.20), carried out for any $\sigma > 0$, $\sigma < d < 2\sigma$, raises some mathematical problems, the solution of which is a premise for developing a rigorous theory. Such problems are:

1. Existence and properties of the original $F_\mu(t)$ of the Laplace transformation (3.1).
2. Are the conditions of an appropriate Tauberian theorem sufficient for the derivation of the asymptotic expansion (4.7) satisfied?
3. Justification of the exchangeability of the order of summation over $\mathbf{k} \in \mathbb{Z}^d$ and integration over $t \in [0, \infty)$, tacitly assumed in the derivation of Eq. (4.13).
4. Is it possible to define a Madelung-type constant [see Eq. (4.12)] for noninteger dimensionality d?

Without attempting at completeness, we give here some comments on these questions.

As already mentioned, one of the major advantages of the suggested approch is its universality with respect to the value of σ, $0<\sigma<2$, and the apparent redundance of the explicit form of $F_{\sigma/2}(t)$. However, some properties of $F_\mu(t)$ are necessary, e.g., for solving problem 2. Needless to say, we could not find in standard tables of Laplace transforms[22] any explicit expression for $F_\mu(t)$ except for the special cases $\mu=1$ and $\mu=1/2$.

As usual, the domain of definition of Eq. (3.1) can be extended to the complex s-plane by setting

$$s^\mu = \exp(\mu \operatorname{Log} s) \tag{A.1}$$

where $\operatorname{Log} s$ is defined as an analytic function in the complex plane with a cut along the negative real axis:

$$\operatorname{Log} s = \log|s| + i \arg s, \qquad |s| \neq 0, \quad -\pi < \arg s \leqslant \pi \tag{A.2}$$

Thus we consider Eq. (3.1) as defining a Laplace transformation in the half-plane $\operatorname{Re} s>0$, where (a) $f_\mu(s)$ is analytical, (b) $|f_\mu(s)|<|s|^{-\mu}$, and, moreover, (c) for any $x>0$, the integral

$$\frac{1}{2\pi i}\, \mathrm{P} \int_{x-i\infty}^{x+i\infty} e^{ts} f_\mu(s)\, ds = F_\mu(t) \tag{A.3}$$

where P means the principle value, converges uniformly with respect to t in the interval $t \geqslant t_0 > 0$, t_0 any positive number. According to a theorem,[23] the above conditions guarantee that $f_\mu(s)$ at $\operatorname{Re} s>0$ is a Laplace transform of the function $F_\mu(t)$, continuous in $t>0$, given by Eq. (A.3).

For any $t>0$ the integral in Eq. (A.3) does not depend on x for all $x>0$. In the limit $x \to 0$ one obtains

$$F_\mu(t) = \frac{1}{\pi} \int_0^\infty dy\, \frac{(1+ay^\mu)\cos(ty) + by^\mu \sin(ty)}{1+2ay^\mu + y^{2\mu}} \tag{A.4}$$

where

$$a = \cos(\mu\pi/2), \qquad b = \sin(\mu\pi/2) \tag{A.5}$$

One can check that this expression gives the particular cases

$$F_1(t) = \frac{1}{\pi} \int_0^\infty dy\, \frac{\cos(ty) + y\sin(ty)}{1+y^2} = e^{-t} \tag{A.6}$$

and

$$F_{1/2}(t) = \frac{1}{\pi}\int_0^\infty dy \frac{[1+(y/2)^{1/2}]\cos(ty) + (y/2)^{1/2}\sin(ty)}{1+(2y)^{1/2}+y}$$
$$= (\pi t)^{-1/2} - e^t[1-\Phi(t^{1/2})] \quad \text{(A.7)}$$

In the case of $0<\mu<1$ one can obtain a more convenient representation of $F_\mu(t)$ by deforming the contour of integration in (A.3) to the rims of the cut along the negative axis. Thus we find

$$F_\mu(t) = \frac{\sin(\mu\pi)}{\pi}\int_0^\infty dy \frac{y^\mu e^{-ty}}{1+2y^\mu\cos(\mu\pi)+y^{2\mu}} \quad \text{(A.8)}$$

As far as problem 3 is concerned, we note that the Jacobi identity (4.2) converts a series uniformly convergent in the interval $0 \leqslant t \leqslant T_0$, with any $T_0 \in (0, \infty)$, into a series uniformly convergent in the interval $t_0 \leqslant t < \infty$, with any $t_0 > 0$. Since the integrand contains a factor $F_{\sigma/2}(y^2 t)$, which for $\sigma < 2$ is singular at $t=0$, this may cause a problem [see Eq. (4.5)]. To avoid it, we subtract from $F_\mu(t)$ its singular asymptotics (as $t \to 0$) and study separately the convergence of the integral containing it [see Eq. (4.10)]. The latter is just the term giving rise to the Madelung-type constants. We will note pursue here any further the subtleties involved in this problem.

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