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On Phase Separation in the Spherical Model of a Ferromagnet: Quasiaverage Approach

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The spherical model of a ferromagnet is investigated in the framework of the generalized quasiaverage approach where an external field positive in one half of a square lattice and negative in the other half is used. It is shown that in addition to the well-known critical point, a second one can be produced by the field. Although the main asymptotic of the free energy is analytic at this point, the next-to-leading asymptotic possesses a singularity here, as well as at the point where the free energy per site is nonanalytic. An order parameter of the model also has singularities at both critical points. The magnetization profile is studied at different scales. It is shown that (in an appropriate regime), below the new critical temperature the magnetization profile freezes, that is, becomes temperature independent.

KEY WORDS: Spherical model; magnetization profile; Gibbs states; phase transition.

1. INTRODUCTION

The spherical model of a ferromagnet introduced by Berlin and Kac[8] is definitely one of the most studied models of statistical mechanics. As soon as a question arouses interest among those who study the properties of ferromagnets, inevitably the spherical model is used to shed some light on the problem. For example, phase separation in the spherical model was studied by Abraham and Robert[2,3] following much activity on the phase separation in the Ising model (see, e.g., refs. 12, 13, 23, and 1); the spherical model in an external random field was studied by Pastur[22] after several interesting phenomena were discovered by Imry and Ma[18] for

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ferromagnets in an external random field. Effects of finite size, restricted dimensionality, and surfaces on the critical behavior of the spherical model were studied by Barber and Fisher[6] after similar analysis of the Ising model.[16] Gibbs states of the spherical model were studied by Molchanov and Sudarev[21] after an extensive study of this subject in many models of statistical mechanics by different authors (see, e.g., the book of Georgii[17] and references therein).

However, in spite of much detailed investigation of the spherical model, dark areas still exist. For instance, the influence of boundary conditions on the properties of the model has received little study. As a consequence, the structure of the set of the limit Gibbs states for the model is not completely clear, and the shape of the magnetization profile for the model with general boundary conditions is unknown (see, however, ref. 3).

The purpose of the present paper is an investigation of the distribution of the individual spin variables of the model and some macroscopic variables in the framework of the generalized quasiaverage approach.[4, 11] The quasiaverage approach can be useful, for example, for singling out different limiting Gibbs states and, as a consequence, for studying such properties as the existence of spontaneous magnetization and spontaneous symmetry breaking. In the conventional form[9] its prescription is loosely as follows: switch on an appropriate external field, calculate values of variables of interest in the thermodynamic limit, and switch off the external field. Usually the conventional quasiaverage approach is a rather rough method only allowing one to single out pure Gibbs states. The generalized quasiaverage approach[4, 14] has been proposed as a more flexible instrument allowing one to single out not only pure Gibbs states, but also their mixtures. The prescription of the generalized quasiaverage approach is as follows: switch on an appropriate external field whose magnitude $h^{(N)}$ tends to zero when the size of the system tends to infinity (e.g., $h^{(N)} = hN^{-\rho}$, $\rho > 0$) and calculate the variables of interest in the thermodynamic limit. The distinctive feature of the generalized quasiaverage approach is that switching off the external field happens not after the thermodynamic limit, but together with this limit. Although the relation between the generalized quasiaverage approach and the true instruments for singling out different Gibbs states (e.g., passing to the thermodynamic limit using different boundary conditions[20]) is not completely clear, there is a hope that the quasiaverage approach in its generalized form can model boundary conditions pretty well and hence can be quite useful, since the study of the influence of the boundary conditions may be (and usually is) very difficult.

At first sight it could seem that the presence of an external field whose magnitude depends on the size of the system makes the model very artificial and unphysical. However, many physical interpretations of such a field are possible. For instance, suppose that an experimentalist has measured the magnetization profile created by a very weak external field (so weak that the interparticle correlations are significant) in a ferromagnet sample of the "size" L. For an infinitely large sample an arbitrarily small external field reduces drastically interparticle correlations. Hence, one can expect that the profile produced by a field of the same magnitude but in a sample of "size" $2L$ will be significantly different. Thus, the following question arises: how should one change the magnitude of the field in order to obtain the same profile? The generalized quasiaverage approach produces the answer to such questions as one of its byproducts.

One might say that in part of their paper Abraham and Robert[3] made use of the (conventional) quasiaverage approach, indeed, they switched on an inhomogeneous external field positive in one half of a cubic lattice and negative in the other, calculated the shape of the magnetization profile, and then demonstrated that the width of the intermediate region between plus and minus phases tends to infinity when the external field is switched off (i.e., they found the shape of the magnetization profile in the microscopic scale, which is trivial in that case, after switching off the external field). We would like to use the generalized quasiaverage approach instead and to study the magnetization profile on a variety of scales. It turns out that some new phenomena arise for the spherical models in the framework of this approach, in particular, there appears a critical temperature below which the shape of the magnetization profile freezes, that is, no longer depends on the temperature. Moreover, order parameters of the model have a singularity at that point, although the free energy does not.

A particular form of the generalized quasiaverage approach has been used by Brankov and Danchev[10] to study the set of the limit Gibbs states (they used a homogeneous external field with the amplitude vanishing in the thermodynamic limit). They were able to single out not only pure "+" and "−" ferromagnetic limit Gibbs phases, but also their mixtures. In the present paper we will show that using an inhomogeneous external field, one can obtain distributions of the single spin variables different from those obtained in ref. 10, and hence there should exist limit Gibbs states different from those obtained in that paper.

The outline of this paper is as follows: In Section 2 the definition of the model and some preliminary results are presented. Section 3 is devoted to the study of the correction to the free energy induced by an external field. There we obtain an explicit expression for the next-to-leading asymptotic of the free energy (surface tension). The shape of the magnetization profile is studied in Section 4, where explicit expressions for the magnetization profiles are derived in different regimes. In Sections 5 and 6 the distributions of single spin variables and some thermodynamic observables are analyzed. Section 7 is devoted to a discussion of the results of the previous sections.

2. DEFINITION OF THE MODEL AND PRELIMINARY RESULTS

Consider a sequence of real-valued random variables $\{s_j\}_{j=1}^N$ (a configuration of spins) placed at the sites of a regular square lattice

$$V=\{(j_1, j_2,..., j_d)\in Z^d: j_l=1, 2,..., n_l;\ l=1, 2,..., d\}, \qquad |V|=N=n_1 n_2 \cdots n_d$$

according to the rule

$$s_j \leftrightarrow (j_1, j_2,..., j_d): \quad j=j_1+\sum_{l=2}^{d} (j_l-1) \prod_{k=1}^{l-1} n_k$$

As usual, the Hamiltonian of the spherical model is a function on the space of spin configurations R^N, and is given by the formula

$$H(s_1; s_2;...; s_N)=-2J \sum_{\langle i;j\rangle} s_i s_j - \sum_{j=1}^{N} h_j^{(N)} s_j \tag{2.1}$$

where the summation $\sum_{\langle i;j\rangle}$ runs over all pairs of nearest neighbors (on the lattice V). We impose the (Berlin–Kac) periodic boundary conditions,[8] that is, we suppose that $s_{N+k}\equiv s_k$, $k=1, 2,..., N$, and pairs of spins

$$(s_i, s_{i+1}); (s_i, s_{i+n_1}); (s_i, s_{i+n_1 n_2});...; (s_i, s_{i+n_1 n_2 \cdots n_{d-1}})$$

are pairs of nearest neighbors for any $i=1, 2,..., N$. The joint probability distribution of the random variables $\{s_j\}_{j=1}^N$ (the Gibbs distribution) is defined by the density

$$p(s_1; s_2;...; s_N)=e^{-\beta H(s_1; s_2;...; s_N)} \tag{2.2}$$

with respect to the *a priori* measure $\delta(\sum_{j=1}^N s_j^2-N)\prod_{j=1}^N ds_j$ on $(R^N; \mathscr{B}(R^N))$ [here $\prod_{j=1}^N ds_j$ is the ordinary Lebesgue measure on $(R^N; \mathscr{B}(R^N))$ and $\delta(\cdot)$ is the delta function]. The particular form of the external field $\{h_i^{(N)}=h^{(N)}\delta_i\}_{i=1}^N$ we use is

$$\delta_i=\begin{cases} +1 & \text{if } i\leftrightarrow (i_1, i_2,..., i_d) \text{ and } 0<i_1\leqslant n_1/2 \\ -1 & \text{if } i\leftrightarrow (i_1, i_2,..., i_d) \text{ and } i_1>n_1/2 \end{cases} \tag{2.3}$$

where for simplicity we suppose that n_1 is even; the opposite case can be treated with minor modifications. This form of the field is chosen because it seems to be the most probable candidate for producing Dobrushin phases[12] (although, as we shall see, it does not), i.e., phases for which the single spin distribution have positive mean in one part of the lattice [say, for all $i\leftrightarrow (i_1, i_2,..., i_d)$ with $i_1<-l$], negative in the other ($i_1>l$), with a transitional region of finite thickness in between.

The main object of our investigation will be the probability distributions of the random variables s_j, $j=1, 2,..., N$, and the macroscopic observables $N^{-\kappa} \sum_{j=1}^{N} s_j$ (normalized total spin, or magnetization) and $N^{-\nu} \sum_{j=1}^{N} \delta_j s_j$ generated by the Gibbs distribution in the thermodynamic limit ($N \to \infty$). Exact values of the parameters ν and κ will be specified later to obtain nontrivial distributions. For simplicity we consider the thermodynamic limit over the sequence of d-dimensional cubes, that is, we suppose $n_l N^{-1/d} \to 1$ as $N \to \infty$ for any $l = 1, 2,..., d$.

We will be concerned mainly with an investigation of the properties of the homogeneous spherical model (in the absence of any external field). The external field in (2.1) will serve as an auxiliary tool; its role will be similar to that of boundary conditions in the investigations of the lattice spin models. The influence of boundary conditions on the free energy per spin is usually negligible in the thermodynamic limit; to have a similar situation with an external field we will switch it off in the limit $N \to \infty$, choosing $h^{(N)} = N^{-\rho} h$, $h, \rho > 0$. It turns out, however, that there is a qualitative difference in the behavior of some other thermodynamic quantities in the thermodynamic limit, depending on the value of ρ; see below.

One can use the well-known technique after Berlin and Kac[8] to calculate the mean value of a function $f(s_1, s_2,..., s_N)$ [with respect to the Gibbs distribution (2.2)]

$$\langle f(s_1, s_2,..., s_N) \rangle_N \equiv \Theta_N^{-1} \int_R \cdots \int_R \prod_{j=1}^{N} ds_j\, \delta\left(\sum_{l=1}^{N} s_l^2 - N \right)$$

$$\times f(s_1, s_2,..., s_N) \exp\left[2\beta J \sum_{\langle i,j \rangle} s_i s_j + \beta \sum_{j=1}^{N} h_j^{(N)} s_j \right]$$

where Θ_N is the partition function,

$$\Theta_N = \int_R \cdots \int_R \prod_{j=1}^{N} ds_j\, \delta\left(\sum_{l=1}^{N} s_l^2 - N \right)$$

$$\times \exp\left[2\beta J \sum_{\langle i,j \rangle} s_i s_j + \beta \sum_{j=1}^{N} h_j^{(N)} s_j \right] \qquad (2.4)$$

That technique involves a change of the integration variables from $\{s_i\}_{i=1}^{N}$ to $\{y_i\}_{i=1}^{N}$ implemented by an orthogonal transformation which diagonalizes the quadratic form $\sum_{\langle i,j \rangle} s_i s_j$ and the introduction of an integral representation for the delta function.

As is well known,[8] the orthogonal eigenvectors $\mathbf{V}^{(k)}$, $k = 1, 2,..., N$, of the (symmetric) interaction matrix C_{ij} (defined by $2\sum_{\langle i,j\rangle} s_i s_j \equiv \sum_{i,j=1}^{N} C_{ij} s_i s_j$) are

$$\mathbf{V}^{(k)} = \left\{ V_l^{(k)} = \frac{1}{\sqrt{N}} \left(\cos\left[\frac{2\pi(k-1)(l-1)}{N}\right] + \sin\left[\frac{2\pi(k-1)(l-1)}{N}\right] \right) \right\}_{l=1}^{N} \tag{2.5}$$

with corresponding eigenvalues given by

$$\lambda_k^{(d)} = 2 \sum_{j=1}^{d} \cos\left[2\pi(k-1) \prod_{l=j}^{d} n_l^{-1} \right]$$

The interaction matrix is diagonalized by the following change of variables:

$$s_j = \sum_{l=1}^{N} V_j^{(l)} y_l; \qquad j = 1, 2,..., N \tag{2.6}$$

which yields

$$\langle f(s_1, s_2,..., s_N) \rangle_N = \Theta_N^{-1} \int_R \cdots \int_R \prod_{j=1}^{N} dy_j \, \delta\left(\sum_{l=1}^{N} y_l^2 - N \right) \tilde{f}(y_1, y_2,..., y_N)$$
$$\times \exp\left[\beta \sum_{l=1}^{N} (J\lambda_l^{(d)} y_l^2 + h^{(N)} \alpha_l y_l) \right] \tag{2.7}$$

where

$$\tilde{f}(y_1, y_2,..., y_N) = f\left(\sum_{l=1}^{N} V_1^{(l)} y_l, \sum_{l=1}^{N} V_2^{(l)} y_l,..., \sum_{l=1}^{N} V_N^{(l)} y_l \right)$$

and a similar formula for Θ_N. In the last expression we introduced coefficients α_l defined by the relation

$$\sum_{j=1}^{N} h_j^{(N)} s_j = h^{(N)} \sum_{j=1}^{N} \sum_{l=1}^{N} \delta_j V_j^{(l)} y_l \equiv h^{(N)} \sum_{l=1}^{N} \alpha_l y_l \tag{2.8}$$

Hence, using (2.3), one has the following expression for these coefficients:

$$\alpha_l = \sum_{k=1}^{n_2 n_3 \cdots n_d} \left[\sum_{j=1}^{n_1/2} V_{j+n_1(k-1)}^{(l)} - \sum_{j=n_1/2+1}^{n_1} V_{j+n_1(k-1)}^{(l)} \right]$$

The summations can be performed explicitly (see Appendix A for details), yielding

$$\alpha_l = \begin{cases} \dfrac{2\sqrt{N}}{n_1} \left[1 + \dfrac{\sin[2\pi(l-1)/N]}{1 - \cos[2\pi(l-1)/N]} \right] \\ \qquad \text{if} \quad l = 1 + (2m-1)N/n_1, \quad m = 1, 2,..., n_1/2 \\ 0 \qquad \text{otherwise} \end{cases} \tag{2.9}$$

The integral representation for the delta function used is[8]

$$\delta(x)=\frac{1}{2\pi i}\int_{-i\infty}^{i\infty} e^{\tau x}\, d\tau \tag{2.10}$$

We shall use the formulas (2.7) and (2.9) as a starting point in the next sections.

3. CORRECTION TO THE LEADING ASYMPTOTIC OF THE FREE ENERGY

After introduction of the new integration variables (2.6) in the formula (2.4) and the integral representation (2.10) for the delta function one can perform the integration over the variables y_l, $l=1, 2,..., N$, obtaining the following expression for the partition function:

$$\Theta_N=\frac{\beta J}{\pi i}\left(\frac{\pi}{2\beta J}\right)^{N/2}\int_{z_0-i\infty}^{z_0+i\infty} dz\, \exp[2N\beta J\Phi_N(z)] \tag{3.1}$$

where $z_0>d$,

$$\Phi_N(z)=z-\frac{1}{4N\beta J}\sum_{j=1}^{N}\log\left(z-\frac{1}{2}\lambda_j^{(d)}\right)+T_{n_1}(z) \tag{3.2}$$

and

$$T_{n_1}(z)\equiv\left[\frac{h^{(N)}}{2n_1 J}\right]^2\sum_{m=1}^{n_1/2}\left[1+\frac{\sin(2\pi(2m-1)/n_1)}{1-\cos(2\pi(2m-1)/n_1)}\right]^2 \times\frac{1}{1-\lambda^{(d)}_{1+(2m-1)n_2\cdots n_d}/2} \tag{3.3}$$

is the field-induced term. Summation over the variable m (see Appendix B for details) yields

$$T_{n_1}(z)=\frac{(h^{(N)})^2}{4J^2(z-d)}\left[\frac{1}{4}-\frac{1}{n_1[(z-d+1)^2-1]^{1/2}}\frac{x_2^{n_1/2}-1}{x_2^{n_1/2}+1}\right] \tag{3.4}$$

where

$$x_{1,2}=(z-d+1)\mp[(z-d+1)^2-1]^{1/2}$$

When $N\to\infty$ the field-induced term $T_{n_1}(z)$ converges uniformly to $T(z)=h_0^2/16J^2(z-d)$ (where $h_0=\lim_{N\to\infty} h^{(N)}$) for z contained in any set of the form $[a; -\infty)$, $a>d$. Evaluation of the integral in Eq. (3.1) can be performed using the saddle-point method directly if the limiting function $\Phi(z) \equiv \lim_{N\to\infty} \Phi_N(z)$ has a minimum on the real axis at a point $z^* > d$ [there exists at most one minimum on $(d; \infty)$]; otherwise this integral needs special investigation. One can formulate the result (if $z^* > d$) as follows.

For $z \in (d; \infty)$

$$\Phi(z) = z - \frac{1}{4\beta J} L(z) + \left(\frac{h_0}{4J}\right)^2 \frac{1}{z-d}$$

where

$$L(z) = \frac{1}{(2\pi)^d} \int_0^{2\pi} \cdots \int_0^{2\pi} \prod_{l=1}^{d} d\omega_l \log\left(z - \sum_{l=1}^{d} \cos\omega_l\right) \tag{3.5}$$

Let assume $\Phi(z)$ has a unique minimum at a point $z^* > d$. Then

$$\Theta_N = \left[\frac{\beta J}{N\Phi_N''(z_N^*)\pi}\right]^{1/2} \left(\frac{\pi}{2\beta J}\right)^{N/2} \exp[2N\beta J\Phi_N(z_N^*)] \left[1 + O\left(\frac{1}{N}\right)\right] \tag{3.6}$$

as $N \to \infty$, where (for each N) z_N^* is the minimum of the function $\Phi_N(z)$ on the interval $[d; \infty)$.

The condition $z^* > d$ is definitely satisfied if for $z \geqslant d$ the function

$$\phi(z) = z - \frac{L(z)}{4\beta J} \tag{3.7}$$

has a unique minimum at some $z_\phi^* > d$. According to Berlin and Kac,[8] for $d \geqslant 3$ there exists a $\beta_c < \infty$ such that $\phi(z)$ has a unique minimum z_ϕ^* for $\beta < \beta_c$, and for $\beta \geqslant \beta_c$ the function $\phi(z)$ increases for $z > d$ and has a minimum at $z = d$. The range of β, $\beta < \beta_c$, we shall call the high-temperature region. If $\beta < \beta_c$, $z > d$, and $h^{(N)} = hN^{-\rho}$, $\rho < 1/2$, one can write down [see Appendix C for an estimate of the asymptotic behavior of the sum $\sum_{j=1}^{N} \log(z - \frac{1}{2}\lambda_j^{(d)})$]

$$\Phi_N(z) = z - \frac{L(z)}{4\beta J} + N^{-2\rho} \frac{h^2}{16J^2(z-d)} + O(N^{-2\rho - 1/d})$$

as $N \to \infty$. Consequently, if $\beta < \beta_c$, one has the following asymptotic formulas for the minimum of $\Phi_N(z)$:

$$z_N^* = z_\phi^* + N^{-2\rho} \frac{\beta h^2}{4JL''(z_\phi^*)(z_\phi^* - d)^2} + o(N^{-2\rho})$$

and free energy:

$$F_N(\beta) \equiv -\frac{1}{\beta} \log \Theta_N = Nf(z_\phi^*) - N^{1-2\rho} \frac{h^2}{8J(z_\phi^* - d)} + o(N^{1-2\rho}) \quad (3.8)$$

where z_ϕ^* is the unique (for $z \geqslant d$) minimum of the function $\phi(z)$ and the value of the function

$$f(z) \equiv \frac{L(z)}{2\beta} - 2Jz - \frac{1}{2\beta} \log\left(\frac{\pi}{2\beta J}\right) \quad (3.9)$$

at the point z_ϕ^* is the free energy per site of the spherical model without an external field. When $\rho \geqslant 1/2$ the free energy has only the usual high-temperature $\log N$ correction [due to the presence of $N^{-1/2}$ in (3.6)].

The condition $z^* > d$ is also satisfied if $h^{(N)}$ tends to a nonzero limit h_0 (as $N \to \infty$). To eliminate the dependence on N produced by $h^{(N)}$ let $h^{(N)} \equiv h_0$ (the additional dependence on N produced by a nonconstant $h^{(N)}$ can be considered in the same way as for $h_0 = 0$ and $\beta < \beta_c$). Then [see Eq. (3.4) and Appendix C]

$$\Phi_N(z) = \Phi(z) - n_1^{-1} g(z) + O(\exp(-N^\delta))$$

uniformly on $\{z: a \leqslant z < \infty,\ a > d\}$ for some positive δ, where

$$g(z) = \frac{h_0^2}{4J^2(z-d)^{3/2}\,(2+z-d)^{1/2}}$$

Consequently, for $h_0 \neq 0$ the unique (for $z > d$) minimum of $\Phi_N(z)$ possesses the following asymptotic behavior:

$$z_N^* = z^* + n_1^{-1} \frac{g'(z^*)}{\Phi''(z^*)} + O(n_1^{-2})$$

Taking into account $\Phi'(z^*) = 0$, we obtain the asymptotic formula for the free energy

$$F_N(\beta) = N\left[f(z^*) - \frac{h_0^2}{8J(z^* - d)}\right] + N^{1-1/d} 2Jg(z^*) + O(N^{1-2/d}) \quad (3.10)$$

Let us notice that for $z > d$ the function $\Phi_N(z)$ coincides with the corresponding function of the spherical model in a homogeneous external field[8] up to corrections $O(n_1^{-1})$ produced by $T_{n_1}(z)$. Consequently, the following two conclusions about the situation when $h_0 \neq 0$ can be drawn.

(i) An arbitrary weak (that is, for any $h_0 > 0$) external field of the form (2.3) destroys the phase transition (that is, the free energy per spin becomes an analytic function of the temperature).

(ii) The interface between areas of different dominant spin orientation (which exists for any temperature if $h_0 \neq 0$; see next section) produces an $N^{1-1/d}$ correction to the free energy, as is widely accepted (see, e.g., ref. 5).

We now study the low-temperature region (in the case $h^{(N)} = N^{-\rho}h$, $\rho > 0$) by first investigating the behavior of the field-induced term $T_{n_1}(z)$ in the vicinity of the point $z = d$. Let us notice first of all that, being a sum of functions steadily decreasing to zero for $z \geqslant d$ [see formula (3.3)], the field-induced term has this property itself. For the same reason the first derivative of this term is steadily increasing for $z \geqslant d$, having the modulus decreasing to zero. Because $T_{n_1}(z)$ is continuous (for any $N < \infty$) at $z = d$, one can calculate $T_{n_1}(d)$ by passing to the limit $z \to d + 0$ in Eq. (3.4); this leads to

$$T_{n_1}(d) = \frac{h^2}{4J^2 N^{2\rho}} \left(\frac{N^{2/d} + 8}{96} \right)$$

Similarly, for the derivative of $T_{n_1}(z)$ at the point d one obtains

$$T'_{n_1}(d) = \frac{h^2}{4J^2 N^{2\rho}} \left(\frac{N^{4/d}}{1920} + \frac{N^{2/d}}{192} + \frac{1}{30} \right)$$

So, it is possible to anticipate that there exist three different regimes for the behavior of the model, depending on whether $T'_{n_1}(d) \to \infty$ (strong-field regime), or $T'_{n_1}(d) \to C$, $0 < C < \infty$ (moderate-field regime), or $T'_{n_1}(d) \to 0$ (weak-field regime) as $N \to \infty$.

3.1. Strong-Field Regime ($0 < \rho < 2/d$)

It is convenient to introduce a "natural" scale for the integration variable z in (3.1). In the strong-field regime this can be done by introducing a new integration variable ζ defined by $z - d = \zeta N^{-\rho}$ (in the low-temperature region), obtaining

$$\begin{aligned} \Theta_N = {} & \left(\frac{\pi}{2\beta J} \right)^{N/2} \frac{\beta J}{\pi i} N^{-\rho/2} \exp\left[2\beta J N d - \frac{1}{2} \sum_{j=2}^{N} \log\left(d - \frac{1}{2} \lambda_j^{(d)} \right) \right] \\ & \times \int_{\zeta_0 - i\infty}^{\zeta_0 + i\infty} \frac{d\zeta}{\sqrt{\zeta}} \exp\left\{ 2\beta J N^{1-\rho} \left[\zeta - \frac{N^{\rho-1}}{4\beta J} \sum_{j=2}^{N} \log\left(1 + \frac{\zeta N^{-\rho}}{d - \frac{1}{2}\lambda_j^{(d)}} \right) \right. \right. \\ & \left. \left. + \left(\frac{h}{4J} \right)^2 \frac{1}{\zeta} + O(N^{\rho/2 - 1/d}) \right] \right\} \end{aligned} \tag{3.11}$$

for the partition function. Note that in the low-temperature region the saddle-point equation determines the value of a correction to the main ($\sim N$) asymptotic of the free energy.

The integral in (3.11) is in a form convenient for an application of the saddle-point method in the sense that the saddle point does not tend to any point of nonanalyticity of the subintegral function when $N \to \infty$, in contrast to the formula (3.1) for $\beta \geqslant \beta_c$, where the saddle point tends to the branch point (this phenomenon is known as "sticking" of the saddle point).

For $d \geqslant 3$ as $N \to \infty$ the following (uniform in ζ in any bounded subset of the positive real semiaxis) asymptotic formula holds:

$$\frac{N^{\rho-1}}{4\beta J} \sum_{j=2}^{N} \log\left(1 + \frac{\zeta N^{-\rho}}{d - \frac{1}{2}\lambda_j^{(d)}}\right) = \zeta \frac{W(d)}{4\beta J} + O(N^{-\rho/2})$$

where

$$W(z) = \frac{1}{(2\pi)^d} \int_0^{2\pi} \cdots \int_0^{2\pi} \prod_{l=1}^{d} d\omega_l \frac{1}{z - \sum_{l=1}^{d} \cos \omega_l}$$

is the Watson function. Evaluating the integral in (3.11) using the saddle-point method, one obtains [for $\beta > \beta_c = W(d)/4J$]

$$F_N(\beta) = Nf(d) - N^{1-\rho} h \left(1 - \frac{\beta_c}{\beta}\right)^{1/2} + o(N^{1-\rho}) \tag{3.12}$$

where $f(d)$ is given by (3.9) and we made use of the result of Appendix C,

$$\sum_{j=2}^{N} \log(d - \tfrac{1}{2}\lambda_j^{(d)}) = NL(d) + O(\log(N))$$

Taking into account Eq. (3.8), we conclude that the $N^{1-\rho}$ correction to the leading behavior of the free energy $f_1(\beta)$ in the strong-field regime has a nonanalyticity at β_c,

$$-f_1(\beta) = \begin{cases} 0 & \text{if } \beta < \beta_c \\ h\left(1 - \dfrac{\beta_c}{\beta}\right)^{1/2} & \text{if } \beta > \beta_c \end{cases}$$

3.2. Moderate-Field Regime ($\rho = 2/d$)

As in the strong-field regime, it is convenient to introduce a new integration variable $\zeta = N^{2/d}(z - d)$ in (3.1) to perform integration on the "natural" scale. This yields a formula similar to (3.11) except that the field-induced term becomes (see Fig. 1)

$$N^{2/d}T_{n_1}(z) \to T(\zeta) = \frac{h^2}{4J^2\zeta}\left\{\frac{1}{4} - \frac{1}{(2\zeta)^{1/2}} \tanh\left[\frac{1}{2}\left(\frac{\zeta}{2}\right)^{1/2}\right]\right\}$$

Consequently one can calculate the correction to the free energy using the same procedure as in the strong-field regime, provided the corresponding sequence of saddle points does not tend to a point of nonanalyticity of the integrand, in which case one obtains, similar to (3.12),

$$F_N(\beta) = Nf(d) - N^{1-2/d}2Jq(\zeta^*) + o(N^{1-2/d}) \tag{3.13}$$

where $q(\zeta)$ is given by

$$q(\zeta) = \zeta\left(1 - \frac{\beta_c}{\beta}\right) + \left(\frac{h}{4J}\right)^2 \frac{1}{\zeta}\left\{1 - 2\left(\frac{2}{\zeta}\right)^{1/2} \tanh\left[\frac{1}{2}\left(\frac{\zeta}{2}\right)^{1/2}\right]\right\} \tag{3.14}$$

and ζ^* its unique point of minimum on the interval $(0; \infty)$. The range of temperatures where Eq. (3.13) is valid is determined by the condition $\zeta^* > 0$. Let us notice that the function

$$\xi(\zeta) = \frac{1}{\zeta}\left\{1 - 2\left(\frac{2}{\zeta}\right)^{1/2} \tanh\left[\frac{1}{2}\left(\frac{\zeta}{2}\right)^{1/2}\right]\right\} \tag{3.15}$$

is monotonically decreasing on the interval $[0; \infty)$ with an increasing negative first derivative (see Fig. 1). Hence, if the first derivative of $q(\zeta)$ is negative in the vicinity of $\zeta = 0$, then there is a unique minimum of this

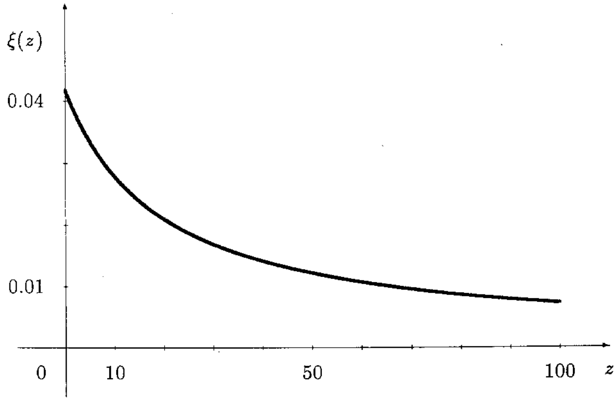

Fig. 1. Plot of the function $\xi(\zeta)$ given by Eq. (3.15), showing the perturbation of the saddle-point equation in the moderate-field regime due to the presence of an external field.

function on the interval $(0; \infty)$, otherwise $q(\zeta)$ attains its unique minimum on $[0; \infty)$ at the point $\zeta = 0$. The Taylor expansion of the function $\xi(\zeta)$ is

$$\xi(\zeta) = \frac{1}{24} - \frac{\zeta}{480} + O(\zeta^2) \tag{3.16}$$

Consequently, if

$$\frac{1}{480}\left(\frac{h}{4J}\right)^2 > 1$$

then for $\beta > \beta_c$ there always exists a unique minimum of $q(\zeta)$ for some $\zeta > 0$. If

$$\frac{1}{480}\left(\frac{h}{4J}\right)^2 \leqslant 1$$

than one gets a second "sticking" point at

$$\tilde{\beta}_c = \frac{\beta_c}{1 - (1/480)(h/4J)^2}$$

"Sticking" signals that the scale $z - d = N^{-2/d}\zeta$ is not the "natural" one for $\beta > \tilde{\beta}_c$. The "natural" scale for z in (3.1) now becomes $z - d = \zeta/N$. Hence, instead of (3.11), one obtains

$$\begin{aligned}\Theta_N = {} & \left(\frac{\pi}{2\beta J}\right)^{N/2} \frac{\beta J}{i\pi\sqrt{N}} \\ & \times \exp\left[2\beta J N d - \frac{1}{2}\sum_{j=2}^{N} \log\left(d - \frac{1}{2}\lambda_j^{(d)}\right) + N^{1-2/d}\frac{\beta J}{12}\left(\frac{h}{4J}\right)^2\right] \\ & \times \int_{\zeta_0 - i\infty}^{\zeta_0 + i\infty} \frac{d\zeta}{\sqrt{\zeta}} \exp\left\{2\beta J\left[\zeta - \frac{1}{4\beta J}\sum_{j=2}^{N}\log\left(1 + \frac{\zeta N^{-1}}{d - \frac{1}{2}\lambda_j^{(d)}}\right)\right.\right. \\ & \left.\left. - \left(\frac{h}{4J}\right)^2 \frac{\zeta}{480}\left[1 + o(1)\right]\right]\right\}\end{aligned} \tag{3.17}$$

where the integral produces only a contribution of order N^0 and does not make a contribution to the next to the leading asymptotic of the free energy. From (3.17) one obtains

$$F_N(\beta) = Nf(d) - N^{1-2/d}\frac{J}{12}\left(\frac{h}{4J}\right)^2 + o(N^{1-2/d})$$

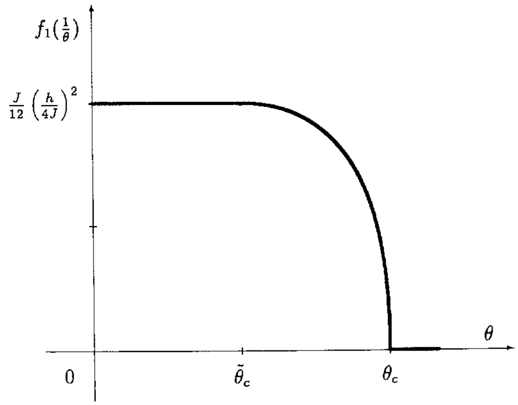

Fig. 2. The $O(N^{1+2/d})$ asymptotic of the free energy in the moderate-field regime.

Summarizing, we conclude that the correction to the leading behavior of the free energy in the moderate-field regime has two points of nonanalyticity (see Fig. 2),

$$-f_1(\beta)=\begin{cases}0 & \text{if } \beta<\beta_c\\ 2J\min\limits_{\zeta\in(0;\,\infty)} q(\zeta) & \text{if } \beta_c<\beta<\tilde{\beta}_c\\ \dfrac{J}{12}\left(\dfrac{h}{4J}\right)^2 & \text{if } \tilde{\beta}_c<\beta\end{cases}$$

3.3. Weak-Field Regime ($\rho<2/d$)

In this regime the "natural" scale for the integration variable in (3.1) is introduced by the change of variable $z-d=\zeta/N$ for all $\beta>\beta_c$, which yields for the field-induced term

$$T_{n_1}(d+N^{-1}\zeta)=N^{2/d-2\rho}\frac{h^2}{16J^2}\left[\frac{1}{24}-N^{2/d-1}\frac{\zeta}{480}+O(N^{4/d-2})\right]$$

For the partition function one obtains a formula similar to (3.17), whence one derives the correction to the free energy

$$F_N(\beta)=Nf(d)-N^{1-2\rho+2/d}f_1(\beta)+o(N^{1-2\rho+2/d})$$

where

$$f_1(\beta)=\begin{cases}0 & \text{if } \beta<\beta_c\\ \dfrac{J}{12}\left(\dfrac{h}{4J}\right)^2 & \text{if } \beta_c<\beta\end{cases}$$

and we suppose $1-2\rho+2/d>0$. Note that $f_1(\beta)$ does not depend on β for $\beta>\beta_c$ and coincides with a similar function in the moderate-field regime for $\beta>\tilde{\beta}_c$.

4. MEAN VALUES OF SINGLE SPIN VARIABLES

To calculate the average value of a single spin variable s_k one has to substitute $f(s_1, s_2,..., s_N)=s_k$ in Eq. (2.7). Then we introduce the integral representation for the delta function and integrate over $\{y_m\}_{m=1}^N$ to obtain

$$\langle s_k\rangle_N=\sum_{l=1}^N V_k^{(l)}\langle y_l\rangle_N=\frac{h^{(N)}}{4J}\sum_{l=1}^N V_k^{(l)}\left\langle\frac{\alpha_l}{z-\frac{1}{2}\lambda_l^{(d)}}\right\rangle_{z,N} \tag{4.1}$$

where we employed the notation

$$\langle f(z)\rangle_{z,N}=\Theta_N^{-1}\frac{\beta J}{\pi i}\left(\frac{\pi}{2\beta J}\right)^{N/2}\int_{z_0-i\infty}^{z_0+i\infty}dz\, f(z)\exp[2N\beta J\Phi_N(z)] \tag{4.2}$$

and $\Phi_N(z)$ is given by (3.2). One can evaluate this integral directly if the function $\Phi(z)\equiv\lim_{N\to\infty}\Phi_N(z)$ attains its unique minimum (on $[d,\infty)$) at a point $z^*>d$ which occurs in the high-temperature region if $h^{(N)}=hN^{-\rho}$ and for all temperatures if $h^{(N)}\to h_0\neq 0$ [in which cases the scale of the integration variable z in (4.1) is the "natural" one]. In the former case the magnetization profile is trivial,

$$\langle s_k\rangle\equiv\lim_{N\to\infty}\langle s_k\rangle_N=0$$

uniformly over $k\in\{1, 2,..., N\}$. In the latter case, taking into account formulas (2.5) and (2.9), one obtains the following result:

$$\begin{aligned}\langle s_k\rangle=\lim_{N\to\infty}\frac{h_0}{2Jn_1}\sum_{m=1}^{n_1/2}&\left[\cos\frac{2\pi}{n_1}(2m-1)(k-1)+\sin\frac{2\pi}{n_1}(2m-1)(k-1)\right]\\&\times\left[1+\frac{\sin(2\pi/n_1)(2m-1)}{1-\cos(2\pi/n_1)(2m-1)}\right]\\&\times\frac{1}{z_N^*-d+1-\cos(2\pi/n_1)(2m-1)}\end{aligned} \tag{4.3}$$

Note that $\langle s_k\rangle_N$ is a periodic function of k, i.e., $\langle s_k\rangle_N=\langle s_{k-n_1}\rangle_N$ for $k>n_1$ and hence it is sufficient to study just one row of the square lattice. So, all the formulas below describe a single (but arbitrary) row of the lattice. Performing the summation in (4.3) (see Appendix B), we come to

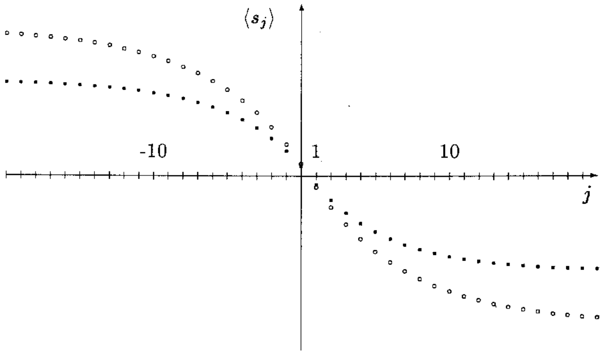

Fig. 3. The magnetization profile [see (4.4)] for $\beta = 10$, $h_0 = 0.1$, and $J = 2$ (circles) and for $\beta = 0.1$, $h_0 = 0.1$, and $J = 2$ (dots).

a result similar to that of Abraham and Robert[3] (they considered an external field a bit different from ours)

$$\langle s_k \rangle \equiv \lim_{N \to \infty} \langle s_{n_1/2+k} \rangle_N = \frac{h}{2J} \begin{cases} \dfrac{1}{z^* - d}\left(\dfrac{1}{2} - \dfrac{x_2^k}{1 + x_2}\right) & \text{if} \quad k \leqslant 0 \\ -\dfrac{1}{(z^* - d)}\left(\dfrac{1}{2} - \dfrac{x_1^k}{1 + x_1}\right) & \text{if} \quad k \geqslant 1 \end{cases} \tag{4.4}$$

(see Fig. 3 for plots of the "typical" $h \neq 0$ shapes of the magnetization profile).

When $h = 0$ one needs to change the integration variable in (4.1) in the low-temperature region (as we did in the previous section) to get into the "natural" scale.

4.1. Strong-Field Regime

Introducing the new integration variable $\zeta = N^\rho(z - d)$ and using the saddle-point method [cf. (3.11)], one obtains the following asymptotic for $\langle y_l \rangle_N$ (as $N \to \infty$):

$$\langle y_l \rangle_N = \frac{h\alpha_l}{4JN^\rho(d + N^{-\rho}\zeta^* - \frac{1}{2}\lambda_l^{(d)})} [1 + o(1)]$$

where ζ^* is the "limiting" saddle point of the integral (3.11). Let us introduce, instead of the original lattice index j, a shifted and rescaled variable γ according to $j = n_1/2 + \gamma N^{\rho/2}$. Then, using (4.1) and (B.9) from

Appendix B, one obtains the expression for the magnetization profile in the strong-field regime (in the limit $N \to \infty$)

$$\langle s_\gamma \rangle = -\operatorname{sgn}(\gamma)\left(1-\frac{\beta_c}{\beta}\right)^{1/2}\left\{1-\exp\left[-|\gamma|\left(\frac{h}{2J}\right)^{1/2}\left(\frac{\beta}{\beta-\beta_c}\right)^{1/4}\right]\right\} \tag{4.5}$$

where γ is a continuous variable, $\gamma \in (-\infty; \infty)$.

Comparison with the rescaled magnetization profile in the two-dimensional Ising model,[1] which in notations adapted to ours can be written as

$$\langle s_\gamma \rangle = m^* \operatorname{sgn}(\gamma)\, \Phi(b\,|\gamma|)$$

where $\Phi(x) = (2/\sqrt{\pi}) \int_0^x e^{-u^2}\,du$, m^* is the spontaneous magnetization, and b some constant which depends on the parameters of the model, suggests that the interface fluctuations in the spherical model have an essentially different character from those in the 2D Ising model.

4.2. Moderate-Field Regime

Due to the appearance of the second critical point at $\beta = \tilde{\beta}_c$ in the moderate-field regime the "natural" scale for the integration variable in (4.1) differs above and below $\tilde{\beta}_c$. For the integral in (4.1) one gets a formula similar to (3.17), and using the saddle-point method, we obtain the following results.

(i) For $\beta_c < \beta < \tilde{\beta}_c$

$$\langle y_s \rangle_N = \frac{h\alpha_s}{4JN^{2/d}(d + N^{-2/d}\zeta^* - \frac{1}{2}\lambda_s^{(d)})}\,[1 + o(1)] \tag{4.6}$$

as $N \to \infty$, where $\zeta^* > 0$, the point of minimum of the function (3.14). Introducing a rescaled variable $\gamma = j/n_1$, one has in the limit $N \to \infty$ from formulas (4.1) and (B.9)

$$\langle s_\gamma \rangle = \frac{h}{4J\zeta^*}\operatorname{sgn}(1-2\gamma)\left\{1 - \frac{\cosh[(|2\gamma - 1| - \frac{1}{2})(\zeta^*/2)^{1/2}]}{\cosh[\frac{1}{2}(\zeta^*/2)^{1/2}]}\right\} \tag{4.7}$$

where γ is a continuous variable satisfying $0 \leqslant \gamma \leqslant 1$. In particular, in the limit $\zeta^* \to 0$ one gets the steepest possible magnetization profile,

$$\langle s_\gamma \rangle = \frac{h}{4J}\begin{cases} \dfrac{\gamma}{2} - \gamma^2 & \text{if } \; 0 \leqslant \gamma \leqslant \dfrac{1}{2} \\[2ex] \gamma^2 - \dfrac{3\gamma}{2} + \dfrac{1}{2} & \text{if } \; \dfrac{1}{2} \leqslant \gamma \leqslant 1 \end{cases} \tag{4.8}$$

(see Fig. 4 for the plot of the magnetization profiles in this regime).

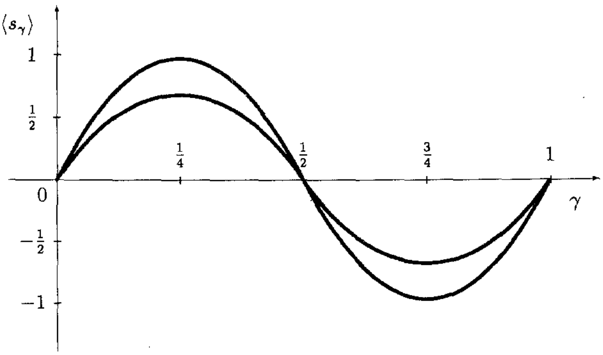

Fig. 4. The magnetization profile in the moderate-field regime [see Eqs. (4.7) and (4.8)]. The curve with the higher amplitude corresponds to the steepest possible magnetization profile and is given by Eq. (4.8).

(ii) For $\beta > \tilde{\beta}_c$ instead of (4.6) one gets

$$\langle y_s \rangle_N = \frac{h\alpha_s}{4JN^{2/d}} \left[\int_{\zeta_0 - i\infty}^{\zeta_0 + i\infty} d\zeta\, \zeta^{-1/2} \exp\left\{ 2J\beta\zeta \left[1 - \frac{\beta_c}{\beta} - \frac{1}{480}\left(\frac{h}{4J}\right)^2 \right] \right\} \right]^{-1}$$
$$\times \int_{\zeta_0 - i\infty}^{\zeta_0 + i\infty} d\zeta \frac{\exp\{2J\beta\zeta[1 - \beta_c/\beta - (1/480)(h/4J)^2]\}}{\sqrt{\zeta}\,(d + N^{-1}\zeta - \frac{1}{2}\lambda_s^{(d)})} [1 + o(1)] \tag{4.9}$$

because of the different "natural" scale. From (B.9) we see that for this temperature range the magnetization profile "freezes," that is, becomes independent of the value of β and is given by (4.8).

4.3. Weak-Field Regime

In the weak-field regime for $\beta > \beta_c$ the "natural" scale for the variable z is introduced by the change of variable $z - d = \zeta/N$ (as in the moderate-field regime for $\beta > \tilde{\beta}_c$). So, for the magnetization profile one gets a formula similar to that for $\beta > \tilde{\beta}_c$ in the moderate-field regime, but the magnitude of the external field now scales as $hN^{-\rho}$, $\rho > 2/d$ [cf. (4.9)]. Hence, the average value of a spin variable tends to zero and the following estimate for the rate of convergence is valid:

$$\max_{j=1,2,\ldots,N} \langle s_j \rangle = O(N^{2/d-\rho}) \qquad \text{as} \quad N \to \infty$$

5. DISTRIBUTIONS OF THE SINGLE SPIN VARIABLES

To find the limiting distribution of the random variable s_j it is sufficient to calculate its characteristic function $\langle e^{its_j}\rangle \equiv \lim_{N\to\infty}\langle e^{its_j}\rangle_N$. After standard transformations one obtains [using the notation (4.2)] from (2.7)

$$\langle e^{its_j}\rangle_N = \langle \phi_j(z, t)\rangle_{z,N} \tag{5.1}$$

where

$$\phi_j(z, t) = \exp\left[-\frac{t^2}{8\beta J}\sum_{m=1}^{N}\frac{(V_m^{(j)})^2}{z-\frac{1}{2}\lambda_m^{(d)}} + it\frac{h^{(N)}}{4J}\sum_{m=1}^{N}\frac{\alpha_m V_m^{(j)}}{z-\frac{1}{2}\lambda_m^{(d)}}\right]$$

One can simplify the expression for $\phi_j(z, t)$ if one takes into account the identity

$$\sum_{m=1}^{N}\frac{\sin[2\pi(m-1)(k-1)/N]\cos[2\pi(m-1)(k-1)/N]}{z-\frac{1}{2}\lambda_m^{(d)}} = 0 \tag{5.2}$$

which can be proven exactly as the formula for Σ_2 in Appendix B. The identity (5.2) yields [using the notation of (B.8)]

$$\phi_j(z, t) = \exp\left[\frac{-t^2}{8\beta JN}\sum_{m=1}^{N}\frac{1}{z-\frac{1}{2}\lambda_m^{(d)}} + it\frac{h^{(N)}}{2J}\langle s_j\rangle_{n_1}(z)\right]$$

and hence the characteristic functions (5.1) have the same periodicity property as $\langle s_j\rangle_{n_1}(z)$, namely,

$$\langle e^{its_j}\rangle_{n_1} = \langle e^{its_{j+n_1}}\rangle_{n_1}$$

So, again, it is sufficient to consider only one row (say $1 \leqslant j \leqslant n_1$) of the original square lattice. As in the previous section it is convenient to introduce rescaled coordinates

$$\gamma = \frac{j-\frac{1}{2}n_1}{N^\sigma}, \qquad j = 1, 2,..., n_1, \qquad \sigma \in \left[0, \frac{1}{d}\right]$$

where σ determines the scale; $\sigma = 0$ corresponds to the microscopic scale (i.e., its unit length is of the order of an elementary cell of the lattice), $\sigma = d^{-1}$ corresponds to the macroscopic scale (i.e., the size of the system is several unit lengths).

In the high-temperature phase the influence of the field-induced term is negligible (when $h^{(N)} = N^{-\rho}h$, $\rho > 0$) on all scales and we obtain formulas for the characteristic function (5.1) and the corresponding distribution density (with respect to Lebesgue measure on R^1) which coincide with that of the spherical model without any external field (and $\beta < \beta_c$) (see, e.g., ref. 24)

$$\langle e^{its_k} \rangle = e^{-t^2/2}, \qquad \text{which implies} \quad p(s) = (2\pi)^{-1/2}\, e^{-s^2/2}$$

We next examine the characteristic function in the low-temperature regime.

5.1. Strong-Field Regime

In this regime, after again performing the change of the scale $z - d = N^{-\rho}\zeta$, we evaluated the integral in (5.1) using the saddle-point method. Taking into account the definition of β_c, one obtains in the different scales (we let j be N dependent according to $j = N^{\sigma}\gamma + \frac{1}{2}n_1$)

$$\langle \exp(its_\gamma) \rangle \equiv \lim_{N\to\infty} \langle \exp(its_{N^\sigma\gamma + n_1/2}) \rangle_N$$

$$= \begin{cases} \exp\left(-\dfrac{\beta_c}{2\beta}t^2\right) & \text{if} \quad 0 \leqslant \sigma < \dfrac{\rho}{2} \\[2ex] \exp\left(-\dfrac{\beta_c}{2\beta}t^2 + it\langle s_\gamma \rangle\right) & \text{if} \quad \sigma = \dfrac{\rho}{2} \\[2ex] \exp\left[-\dfrac{\beta_c}{2\beta}t^2 - it\,\mathrm{sgn}(\gamma)\left(1 - \dfrac{\beta_c}{\beta}\right)^{1/2}\right] & \text{if} \quad \dfrac{\rho}{2} < \sigma \leqslant \dfrac{1}{d} \end{cases} \tag{5.3}$$

where $\langle s_\gamma \rangle$ is given by the formula (4.5). The corresponding distribution density is again Gaussian

$$p_\gamma(s) = \left(\frac{\beta_c}{2\pi\beta}\right)^{1/2} \begin{cases} \exp\left(-\dfrac{\beta_c s^2}{2\beta}\right) & \text{if} \quad 0 \leqslant \sigma < \dfrac{\rho}{2} \\[2ex] \exp\left[-\dfrac{\beta_c(s - \langle s_\gamma \rangle)^2}{2\beta}\right] & \text{if} \quad \sigma = \dfrac{\rho}{2} \\[2ex] \exp\left\{-\dfrac{\beta_c[s - \mathrm{sgn}(\gamma)(1 - \beta_c/\beta)^{1/2}]^2}{2\beta}\right\} & \text{if} \quad \dfrac{\rho}{2} < \sigma \leqslant \dfrac{1}{d} \end{cases} \tag{5.4}$$

The following conclusion can be drawn from (5.4): there is no interface in the scales with $0 \leqslant \sigma < \rho/2$; there is a smooth interface between areas of different dominant spin orientation in the scale $\sigma = \rho/2$; there is a sharp interface (similar to the Heaviside θ function) in the scales $\rho < \sigma \leqslant d^{-1}$.

Let us notice that in the thermodynamic limit the second moment of the random variables s_k equals β_c/β (when k is nonrescaled and finite), which indicates that the model is not a very good approximation for realistic ferromagnets in the low-temperature region. Note, in contrast, that the generalized spherical model, which is the infinite-component limit of the n-vector model, has the local condition $\langle s_k^2 \rangle = 1$. Only in the scales $\sigma > \rho/2$, $\gamma = j/N^\sigma$, does one get the right value of the second moment $\langle s_\gamma^2 \rangle = 1$.

5.2. Moderate-Field Regime

In the range of temperature $\tilde{T}_c < T < T_c$ one obtains essentially the same results as in the strong-field regime, because the integral in (5.1), after the change of scale $z - d = N^{-2/d}\zeta$, can be evaluated using the saddle-point method. For the distribution function of a spin variable one obtains

$$p_\gamma(s) = \left(\frac{\beta_c}{2\pi\beta}\right)^{1/2} \begin{cases} \exp\left(-\dfrac{\beta_c s^2}{2\beta}\right) & \text{if } 0 \leqslant \sigma < \dfrac{1}{d} \\ \exp\left[-\dfrac{\beta_c(s - \langle s_\gamma \rangle)^2}{2\beta}\right] & \text{if } \sigma = \dfrac{1}{d} \end{cases}$$

where $\langle s_\gamma \rangle$ for $\sigma = d^{-1}$ is given by Eq. (4.7). For $T < \tilde{T}_c$ we cannot evaluate the integral in (5.1) using the saddle-point method. However, after the change of integration variable in (5.1) according to $z - d = \zeta/N$ one obtains [cf. (3.17)]

$$\langle \exp(its_\gamma) \rangle = \exp\left[-\frac{\beta_c t^2}{2\beta} + it\langle s_\gamma \rangle\right] \left[\int_{c-i\infty}^{c+i\infty} \frac{d\zeta}{\sqrt{\zeta}} \exp(\zeta)\right]^{-1} \times \int_{c-i\infty}^{c+i\infty} \frac{d\zeta}{\sqrt{\zeta}} \exp\left(\zeta - \frac{t^2 m^*}{4\zeta}\right) \tag{5.5}$$

where $c > 0$ and m^* is given by

$$m^* = 1 - \frac{\beta_c}{\beta} - \frac{1}{480}\left(\frac{h}{4J}\right)^2 \tag{5.6}$$

This yields the following formula for the characteristic function[24]:

$$\langle \exp(its_\gamma) \rangle = \exp\left(-\frac{t^2}{2}\frac{\beta_c}{\beta}\right) \begin{cases} \cos(t\sqrt{m^*}) & \text{if } 0 \leqslant \sigma < 1/d \\ \cos(t\sqrt{m^*}) \exp(it\langle s_\gamma \rangle) & \text{if } \sigma = 1/d \end{cases} \tag{5.7}$$

where $\langle s_\gamma \rangle$ is now given by the formula (4.8). The corresponding distribution functions are given by

$$p_\gamma(s) = \frac{1}{2}\left(\frac{\beta_c}{2\pi\beta}\right)^{1/2} \times \begin{cases} \exp\left[-\frac{\beta_c(s-m^*)^2}{2\beta}\right] + \exp\left[-\frac{\beta_c(s+m^*)^2}{2\beta}\right] \\ \quad \text{if} \quad 0 \leqslant \sigma < \frac{1}{d} \\ \exp\left[-\frac{\beta_c(s-\langle s_\gamma\rangle - m^*)^2}{2\beta}\right] + \exp\left[-\frac{\beta_c(s-\langle s_\gamma\rangle + m^*)^2}{2\beta}\right] \\ \quad \text{if} \quad \sigma = \frac{1}{d} \end{cases} \tag{5.8}$$

Note that a smooth interface in the moderate-field regime appears only in the macroscopic scale and it is never sharp (i.e., θ function).

5.3. Weak-Field Regime

In this regime the influence of the external field is negligible and one obtains the same formula for the distribution of the single spin variables as in the spherical model without external field (see, e.g., ref. 24). One can obtain it formally from (5.8) by putting $h = 0$.

6. DISTRIBUTION OF SOME MACROSCOPIC VARIABLES

The distribution of the properly normalized magnetization $N^{-\nu}\sum_{j=1}^N s_j$ and of $\Pi_\nu \equiv N^{-\nu}\sum_{j=1}^N \delta_j s_j$ [see (2.3)] (which we will see plays the role of an order parameter) are of the most interest. To find both of them we shall calculate their characteristic functions. By the standard procedure one obtains for the magnetization

$$\chi_{N,\nu}^{(m)}(t) \equiv \left\langle \exp\left[itN^{-\nu}\sum_{j=1}^N s_j\right]\right\rangle_N = \left\langle \exp\left[-\frac{t^2 N^{-2\nu+1}}{8\beta J(z-d)}\right]\right\rangle_{z,N} \tag{6.1}$$

and

$$\begin{aligned}\chi_{N,\nu}^{(\Pi)}(t) &\equiv \left\langle \exp\left[itN^{-\nu}\sum_{j=1}^N \delta_j s_j\right]\right\rangle_N \\ &= \left\langle \exp\left[-\frac{t^2 N^{-2\nu}}{8\beta J}\sum_{m=1}^N \frac{\alpha_m^2}{z-\frac{1}{2}\lambda_m^{(d)}} + i\frac{tN^{-\nu-\rho}h}{4J}\sum_{m=1}^N \frac{\alpha_m^2}{z-\frac{1}{2}\lambda_m^{(d)}}\right]\right\rangle_{z,N}\end{aligned} \tag{6.2}$$

for the order parameter, where we substituted $h^{(N)} = hN^{-\rho}$. In the high-temperature region ($T > T_c$) the integrals in (6.1) and (6.2) are evaluated by the direct use of the saddle-point method. To get a nontrivial distribution of the magnetization one has to choose $\nu = 1/2$. In the high-temperature region (because the influence of the field is negligible when $\rho > 0$) we arrive at the well-known (for the spherical model without an external field) result[21]

$$\lim_{N \to \infty} \chi^{(m)}_{N;\,1/2}(t) = \exp\left[\frac{-t^2}{8\beta J(z^*_\phi - d)}\right] \tag{6.3}$$

where z^*_ϕ is the unique (on $[d; \infty)$) point of minimum of the function (3.7). That tells us that in the high-temperature region the random variable $(1/\sqrt{N}) \sum_{j=1}^N s_j$ in the thermodynamic limit has a Gaussian distribution with zero mean and variance $[4\beta J(z^*_\phi - d)]^{-1/2}$. We now turn to the variable Π_ν in the high-temperature region. Making use of (B.1) to evaluate the sum over m in (6.2), one obtains for $\chi^{(\Pi)}_\nu(t) \equiv \lim_{N \to \infty} \chi^{(\Pi)}_{N,\nu}(t)$

$$\chi^{(\Pi)}_{1-\rho}(t) = \exp\left[it\frac{h}{4J(z^*_\phi - d)}\right] \qquad \text{if} \quad 0 < \rho < \frac{1}{2}$$

$$\chi^{(\Pi)}_{1/2}(t) = \exp\left[-\frac{t^2}{8\beta J(z^*_\phi - d)} + it\frac{h}{4J(z^*_\phi - d)}\right] \qquad \text{if} \quad \rho = \frac{1}{2}$$

$$\chi^{(\Pi)}_{1/2}(t) = \exp\left[-\frac{t^2}{8\beta J(z^*_\phi - d)}\right] \qquad \text{if} \quad \frac{1}{2} < \rho$$

Hence, the distribution of $(1/N^{1-\rho}) \sum_{j=1}^N \delta_j s_j$ in the thermodynamic limit becomes degenerate and concentrated at the point $h/4J(z^*_\phi - d)$ when $0 < \rho < 1/2$. If $\rho = 1/2$, the random variable $N^{-1/2} \sum_{j=1}^N \delta_j s_j$ has a Gaussian distribution with the mean $h/4J(z^*_\phi - d)$ and variance $[4J\beta(z^*_\phi - d)]^{-1/2}$. If $\rho > 1/2$, this random variable has zero mean and the same variance as for $\rho = 1/2$.

We next study the low-temperature region, where one should rescale the integration variables in (6.1) and (6.2) prior to the application of the saddle-point method.

6.1. Strong-Field Regime

In this regime after rescaling in the integral in Eq. (6.1) according to $z - d = N^{-\rho}\zeta$, it becomes apparent that one should choose $\delta = (1 + \rho)/2$ to get a nontrivial distribution for the normalized total spin, in which case

$$\lim_{N \to \infty} \chi^{(m)}_{N;\,(1+\rho)/2}(t) = \exp\left[-\left(1 - \frac{\beta_c}{\beta}\right)^{1/2} \frac{t^2}{2\beta h}\right] \tag{6.5}$$

Equation (6.5) is essentially the same as (6.3), i.e., the distribution function of the properly normalized magnetization is Gaussian (in the thermodynamic limit) with zero mean and variance $\sigma^2 = (1/\beta h)(1-\beta_c/\beta)^{1/2}$. However, there are abnormally large fluctuations, since we have used an unusual normalization factor $N^{-(1+\rho)/2}$, where $(1+\rho)/2 > 1/2$.

For the characteristic function of $(1/N)\sum_{j=1}^{N} \delta_j s_j$, after rescaling the integration variable in (6.2), one obtains

$$\lim_{N\to\infty} \chi_{N,1}^{(\Pi)}(t) = \exp\left[it\left(1-\frac{\beta_c}{\beta}\right)^{1/2}\right] \tag{6.6}$$

Hence, the random variable $(1/N)\sum_{j=1}^{N} \delta_j s_j$ in the thermodynamic limit converges (in distribution) to a "nonrandom" limit $(1-\beta_c/\beta)^{1/2}$.

6.2. Moderate-Field Regime

As in the previous section, in the moderate-field regime there is a range of temperatures $\tilde{T}_c < T < T_c$ where the behaviors of the characteristic functions (6.1) and (6.2) are similar to those in the strong-field regime. Namely, the distribution density of the properly normalized magnetization $N^{-1/2-1/d}\sum_{j=1}^{N} s_j$ is

$$p^{(m)}(s) = \frac{1}{(2\pi)^{1/2}\sigma}\exp\left(-\frac{s^2}{2\sigma^2}\right)^{1/2}, \qquad \sigma^2 = \frac{1}{\beta h}\left(1-\frac{T}{T_c}\right)^{1/2}$$

For the random variable $(1/N)\sum_{j=1}^{N} \delta_j s_j$ one obtains

$$\lim_{N\to\infty} \chi_{N;1}^{(\Pi)}(t) = \exp\left[it\frac{h}{4J}\xi(\zeta^*)\right]$$

where the function $\xi(\zeta)$ was defined in (3.15) and $\zeta^* > 0$ is the positive minimum of the function (3.14).

For temperatures $T < \tilde{T}_c$ one need to again perform rescaling of the integration variables in (6.1) and (6.2) according to $z - d = \zeta/N$ and as a consequence one obtains significantly different results than in the strong-field regime. The characteristic function for the magnetization takes the following form:

$$\chi_1^{(m)}(t) = \cos(\sqrt{m^*}\, t)$$

where m^* is defined by formula (5.6). This tells us that the magnetization in the thermodynamic limit converges (in distribution) to a dichotomic random variable which obtains values $\pm\sqrt{m^*}$ with equal probabilities.

For the characteristic function of $(1/N)\sum_{j=1}^{N}\delta_j s_j$, using the expansion (3.16), one gets the following expression:

$$\chi_1^{(\Pi)}(t)=\exp\left(it\frac{h}{96J}\right)$$

Consequently, the random variable Π_1 converges (in distribution) to the "nonrandom" limit as $N\to\infty$,

$$\lim_{N\to\infty}\frac{1}{N}\sum_{j=1}^{N}\delta_j s_j \stackrel{\mathrm{d}}{=} \frac{h}{96J} \tag{6.7}$$

Note that the limiting value of Π_1 does not depend on temperature (for $T<\tilde{T}_c$), that is, not only is the magnetization profile frozen for $T<\tilde{T}_c$ in the moderate-field regime, but Π_1 is as well.

From (6.4), (6.6), and (6.7) we see that $\Pi_1=(1/N)\sum_{j=1}^{N}\delta_j s_j$ plays the role of an order parameter of the model, i.e., it equals zero in the high-temperature region (in a disordered phase) and is greater than zero in the low-temperature region (in an ordered phase).

7. DISCUSSION AND CONCLUDING REMARKS

Although the external field (2.3) used as an infinitesimal perturbation fails to produce translational variant Gibbs states (as was first noticed by Abraham and Robert[3]) and as a consequence the magnetization profile in the microscopic length scale, when the unit of length is the lattice spacing, is trivial (i.e., $\langle s_k\rangle=0$ in the thermodynamic limit), several important physical conclusions can be drawn. First of all, quite often experimentalists are not interested in the properties of ferromagnets on the microscopic scale, but on some rougher scale or even only on the macroscopic scale (that is, when the unit length is of the order of the size of the system). So, the absence of phase separation on the microscopic scale, that is, the infinite width of the intermediate region measured in units of the lattice spacing, does not mean that the phase separation cannot be experimentally observed. In this respect formulas (4.5) and (5.4) tell us that a "very" weak external field can produce phase separation on some appropriate scale and show how rough this scale might be for phase separation to be still observable.

The richest behavior is possessed by the model in the moderate-field regime (even a second phase transition appears). The phase diagram of the model in this regime is plotted in Fig. 5. Phase I ($\theta>\theta_c$) is the ordinary paramagnetic phase common for ferromagnets when the temperature is high enough. Phase II [$\theta<\theta_c$, $(h/4J)^2>480$] is a phase where the external

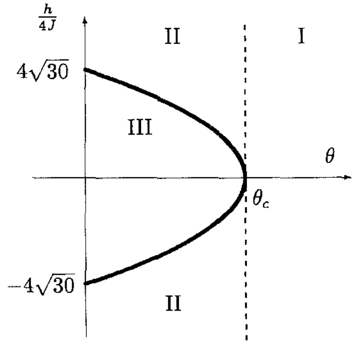

Fig. 5. The phase diagram for the model in the moderate-field regime. Phase I is the ordinary paramagnetic phase, phase II is a phase where the external field dominates over ferromagnetic interaction and temperature fluctuations, and phase III is a mixture of phase II and the ordinary ferromagnetic phase.

field (2.3) dominates over the ferromagnetic interaction (and temperature fluctuations) producing a magnetization profile (though only on the macroscopic scale). Phase III $[\theta < \theta_c, (h/4J)^2 < 480]$ is a hybrid of Phase II and an ordinary ferromagnetic phase (except for the case $h = 0$, where one has a purely ferromagnetic phase).

Brankov and Danchev[10] singled out a set of the Gibbs states for the spherical model with single spin distributions of the form

$$p_\alpha(s) = \alpha p^{(+)}(s) + (1-\alpha)\, p^{(-)}(s), \qquad 0 \leqslant \alpha \leqslant 1 \tag{7.1}$$

(in a notation adapted to ours), where

$$p^{(\pm)}(s) = \left(\frac{\beta}{2\pi\beta_c}\right)^{1/2} \exp\left\{-\frac{\beta_c}{2\beta}\left[s \mp \left(1-\frac{\beta_c}{\beta}\right)^{1/2}\right]^2\right\}$$

It becomes apparent from Section 5 that the set (7.1) is just a subset of a family of limit Gibbs states with single spin distribution of the form

$$\begin{aligned} &q_{\alpha;\mu}(s) = \alpha q_\mu^{(+)}(s) + (1-\alpha)\, q_\mu^{(-)}(s); \qquad 0 \leqslant \alpha \leqslant 1 \\ &\mu \in M_\beta \equiv \left[-\frac{h}{64J}; \frac{h}{64J}\right] \end{aligned} \tag{7.2}$$

where

$$q_\mu^{(\pm)}(s) = \left(\frac{\beta}{2\pi\beta_c}\right)^{1/2} \exp\left[-\frac{\beta_c}{2\beta}(s-\mu \mp m^*)^2\right]$$

$(1/480)(h/4J)^2 \leqslant 1$ and m^* is given by (5.6).

Pure Gibbs states with single spin distributions $q_\mu^{(\pm)}(s)$, $\mu \in M_\beta$, as well as their linear combinations can be singled out using [in addition to (2.3)] a homogeneous external field of the type used in ref. 10 (decreasing to zero sufficiently fast as $N \to \infty$). Equation (5.8) derived in Section 5 corresponds to $\alpha = 1/2$ in (7.2).

A close connection between the spherical model and the free boson gas was noticed for the first time by Gunton and Buckingham.[15] In particular they showed that critical indices for these models are identical. The most prominent phenomenon in the ideal Bose gas is Bose–Einstein condensation. It was shown in ref. 7 that, in general, noninteracting systems of bosons display two types of condensation: condensation in the ground state and condensation in several (possibly infinite) low-lying energy levels (generalized condensation). Some of these models have two critical temperatures: T_c and $\tilde{T}_c$ ($< T_c$). Above T_c there is no condensation. Generalized condensation takes place in the temperature interval $[\tilde{T}_c; T_c]$. Below $\tilde{T}_c$ both types of condensation are present.

As confirmation of the above-mentioned connection between the spherical model and the free boson gas, similar condensation phenomena have been shown to exist in the spherical model. In a recent paper[14] both types of condensation were observed. Using the "condensation" terminology from ref. 14, one can interpret the critical temperatures T_c and $\tilde{T}_c$ found in the present paper as indicating an onset of generalized condensation and condensation in the "ground state," respectively.

Several natural questions arise in connection with the results obtained in this paper. Does the presence of appropriate boundary conditions also produce the second phase transition, i.e., the freezing of the order parameter and magnetization profile? Does the same phase transition exist in more realistic models, for instance, in the generalized spherical model[19]?

APPENDIX A. FORMULA FOR THE COEFFICIENTS α_l

The following formula for the coefficients α_l defined by (2.8) holds true

$$\alpha_l = \begin{cases} \dfrac{2\sqrt{N}}{n_1}\left[1 + \dfrac{\sin[2\pi(l-1)/N]}{1-\cos[2\pi(l-1)/N]}\right] \\ \qquad \text{if} \quad l = 1 + (2m-1)N/n_1, \quad m = 1, 2,..., n_1/2 \\ 0 \qquad \text{otherwise} \end{cases} \tag{A.1}$$

We start from the expression

$$\alpha_l = \sum_{k=1}^{n_2 n_3 \cdots n_d} \left[\sum_{j=1}^{n_1/2} V^{(l)}_{j+n_1(k-1)} - \sum_{j=n_1/2+1}^{n_1} V^{(l)}_{j+n_1(k-1)}\right]$$

which is a direct consequence of the definition of the coefficients α_s and the specific form of the external field $\mathbf{h} = \{h_j\}_{j=1}^N$. Using the explicit form of the eigenvectors $\mathbf{V}^{(l)} \equiv \{V_n^{(l)}\}_{n=1}^N$ of the interaction matrix C_{ij} given in (2.5), we have

$$V^{(l)}_{j+n_1(k-1)} = \frac{1}{\sqrt{N}}\left(\cos\left\{\frac{2\pi}{N}[j-1+(k-1)n_1](l-1)\right\} + \sin\left\{\frac{2\pi}{N}[j-1+(k-1)n_1](l-1)\right\}\right)$$

As a direct consequence of the formula for the sum of a geometrical progression, one obtains

$$E_l \equiv \sum_{k=1}^{n_2 n_3 \cdots n_d}\left\{\sum_{j=1}^{n_1/2} - \sum_{j=n_1/2+1}^{n_1}\right\}\exp\left\{i\frac{2\pi}{N}[j-1+(k-1)n_1](l-1)\right\}$$
$$= \begin{cases} \dfrac{N}{n_1}\dfrac{4}{1-\exp[i2\pi(l-1)/4]} & \text{if } l = 1+(2m-1)N/n_1, \quad m = 1, 2,..., n_1/2 \\ 0 & \text{otherwise} \end{cases}$$

Because of $\alpha_l = (1/\sqrt{N})[\mathrm{Re}(E_l) + \mathrm{Im}(E_l)]$ we arrive at the following expression for the coefficients α_l:

$$\alpha_l = \frac{2\sqrt{N}}{n_1}\left[1 + \frac{\sin[2\pi(l-1)/N]}{1-\cos[2\pi(l-1)/N]}\right]$$

if $l = 1+(2m-1)N/n_1$ for some $m = 1, 2,..., n_1/2$ and zero otherwise, which coincides with (A.1).

APPENDIX B. SOME USEFUL SUMS

In this appendix we derive expressions for two sums which were used for the derivation of Eqs. (3.4), (4.4), (4.5), and (4.7).

The formula (3.4) for the field-induced term follows immediately if we can prove that

$$\Sigma \equiv \frac{1}{n^2}\sum_{m=1}^{n/2}\left[1 + \frac{\sin(2\pi/n)(2m-1)}{1-\cos(2\pi/n)(2m-1)}\right]^2 \frac{1}{z-d+1-\cos(2\pi/n)(2m-1)}$$
$$= \frac{1}{z-d}\left[\frac{1}{4} - \frac{1}{n[(z-d+1)^2-1]^{1/2}}\frac{x_2^{n/2}-1}{x_2^{n/2}+1}\right] \qquad \text{(B.1)}$$

where $x_2 = z-d+1+[(z-d+1)^2-1]^{1/2}$ and we suppose that n is even.

We start from the identity

$$\frac{1}{z-d+1-\cos[2\pi(2m-1)/n]} = \frac{2}{x_2-x_1}\left\{\frac{x_2}{x_2-\exp[2\pi i(2m-1)/n]}+\frac{x_1}{\exp[2\pi i(2m-1)/n]-x_1}\right\} \tag{B.2}$$

where $x_{1,2}=z-d+1\mp[(z-d+1)^2-1]^{1/2}$.

The following formula will also prove useful:

$$S\equiv\sum_{m=1}^{n/2}\frac{1}{x-\exp[2\pi i(2m-1)/n]}=\frac{n}{2}\frac{x^{n/2-1}}{1+x^{n/2}} \tag{B.3}$$

To obtain it, let us notice that the expressions on the left- and right-hand sides of this formula are analytic functions of x (on the whole complex plane of the variable x except for $n/2$ poles on the unit circle), so it is sufficient to prove it, say, for all real x satisfying $|x|>1$ and the rest follows by analytic continuation. Suppose that $|x|>1$; then, using the formula for the sum of a geometrical series, one can rewrite S as

$$S=\frac{1}{x}\sum_{m=1}^{n/2}\sum_{k\geqslant 0}^{\infty}x^{-k}\exp\left[\frac{2\pi i(2m-1)k}{n}\right]$$

Performing the summation over index m first, one gets

$$\sum_{m=1}^{n/2}\exp\left[\frac{2\pi i(2m-1)k}{n}\right]=\begin{cases}(-1)^r\,n/2 & \text{if}\quad k=rn/2,\quad r=0,1,2,...\\ 0 & \text{otherwise}\end{cases}$$

which yields

$$S=\frac{n}{2x}\sum_{r=0}^{\infty}(-1)^r\,x^{-nr/2}=\frac{n}{2}\frac{x^{n/2-1}}{1+x^{n/2}}$$

and (B.3) is proven. Introducing the variable $y=x^{-1}$, one can rewrite (B.3) as

$$\sum_{m=1}^{n/2}\frac{1}{1-y\exp[2\pi i(2m-1)/n]}=\frac{n}{2}\frac{1}{1+y^{n/2}} \tag{B.4}$$

Differentiating (B.4) over y and passing to the limit $y\to 1$, one obtains

$$\sum_{m=1}^{n/2}\frac{\exp[i2\pi(2m-1)/n]}{\{\exp[i2\pi(2m-1)/n]-1\}^2}=-\frac{n^2}{16} \tag{B.5}$$

Expanding the square in the lhs of (B.1), one can split the sum Σ into three parts Σ_1, Σ_2, and Σ_3.

1. $$\Sigma_1 \equiv \sum_{m=1}^{n/2} \frac{1}{z-d+1-\cos(2\pi/n)(2m-1)}$$

To calculate this sum, one needs to make use of formula (B.2) and then of (B.3). One obtains

$$\Sigma_1 = \frac{2}{x_2-x_1} \sum_{m=1}^{n/2} \left\{ \frac{x_2}{x_2-\exp[2\pi i(2m-1)/n]} + \frac{x_1}{\exp[2\pi i(2m-1)/n]-x_1} \right\}$$
$$= \frac{n}{x_2-x_1} \left(\frac{x_2^{n/2}}{1+x_2^{n/2}} - \frac{x_1^{n/2}}{1+x_1^{n/2}} \right)$$

2. $$\Sigma_2 \equiv \sum_{m=1}^{n/2} \frac{\sin(2\pi/n)(2m-1)}{1-\cos(2\pi/n)(2m-1)} \frac{1}{z-d+1-\cos(2\pi/n)(2m-1)}$$

This sum is identically zero. To prove it, let us notice first of all that

$$\Sigma_2 = \operatorname{Im} \left[\sum_{m=1}^{n/2} \frac{\exp[(2\pi i/n)(2m-1)]}{1-\cos(2\pi/n)(2m-1)} \frac{1}{z-d+1-\cos(2\pi/n)(2m-1)} \right] \tag{B.6}$$

but the sum on the right-hand side of (B.6) is a real-valued function (for any real $z \geqslant d$) because it can be reexpressed as

$$-\frac{\delta}{2(z-d+2)} + 2 \sum_{1 \leqslant m < n/4} \frac{\cos[(2\pi/n)(2m-1)]}{1-\cos(2\pi/n)(2m-1)} \times \frac{1}{z-d+1-\cos(2\pi/n)(2m-1)}$$

where $\delta = 1$ if $n/2$ is odd and $\delta = 0$ if $n/2$ is even.

3. $$\Sigma_3 \equiv \sum_{m=1}^{n/2} \left[\frac{\sin(2\pi/n)(2m-1)}{1-\cos(2\pi/n)(2m-1)} \right]^2 \frac{1}{z-d+1-\cos(2\pi/n)(2m-1)}$$

To calculate this sum, one can use formula (B.2) together with some elementary identities. One obtains

$$\Sigma_3 = \frac{2}{x_2-x_1} \sum_{m=1}^{n/2} \left[\frac{\exp[i2\pi(2m-1)/n]+1}{\exp[i2\pi(2m-1)/n]-1} \right]^2 \times \left[\frac{x_2}{x_2-\exp[i2\pi(2m-1)/n]} + \frac{x_1}{x_1-\exp[i2\pi(2m-1)/n]} \right\} \tag{B.7}$$

Now one can use the identity

$$\frac{(a+1)^2}{(a-1)^2}\frac{}{(x-a)}=\frac{4x}{(x-1)^2}\frac{a}{(a-1)^2}-\frac{4}{(x-1)^2}\frac{1}{(a-1)^2}+\frac{(x+1)^2}{(x-1)^2}\frac{1}{(x-a)}$$

to represent formula (B.7) as a sum of simple fractions, and after some algebra one obtains

$$\begin{aligned}\Sigma_3 = {} & 8\left[\frac{x_1}{(x_2-1)(x_1-1)^2}+\frac{x_2}{(x_1-1)(x_2-1)^2}\right] \\ & \times \sum_{m=1}^{n/2}\frac{\exp[i2\pi(2m-1)/n]}{\{\exp[i2\pi(2m-1)/n]-1\}^2} \\ & +\frac{2}{x_2-x_1}\left[\frac{(x_1+1)^2}{(x_1-1)^2}\sum_{m=1}^{n/2}\frac{x_1}{x_1-\exp[i2\pi(2m-1)/n]}\right. \\ & \left.-\frac{(x_2+1)^2}{(x_2-1)^2}\sum_{m=1}^{n/2}\frac{x_2}{x_2-\exp[i2\pi(2m-1)/n]}\right]\end{aligned}$$

Using (B.3) and (B.5), one arrives at the following expression for Σ_3:

$$\begin{aligned}\Sigma_3 = {} & -\frac{n^2}{2(x_2-1)(x_1-1)}\left[\frac{x_1}{x_1-1}+\frac{x_2}{x_2-1}\right] \\ & +\frac{n}{x_2-x_1}\left[\frac{(x_1+1)^2}{(x_1-1)^2}\frac{x_1^{n/2}}{1+x_1^{n/2}}-\frac{(x_2+1)^2}{(x_2-1)^2}\frac{x_2^{n/2}}{1+x_2^{n/2}}\right]\end{aligned}$$

Consequently, taking into account definition of $x_{1,2}$, one obtains

$$\Sigma_1+\Sigma_3=\frac{n^2}{4(z-d)}-\frac{4n}{x_2-x_1}\left[\frac{x_2}{(x_2-1)^2}\frac{x_2^{n/2}}{1+x_2^{n/2}}-\frac{x_1}{(x_1-1)^2}\frac{x_1^{n/2}}{1+x_1^{n/2}}\right]$$

from which the formula (B.1) follows.

Using the same technique, the following summation can be performed:

$$\begin{aligned}\langle s_j\rangle_n(z) \equiv {} & \frac{1}{n}\sum_{m=1}^{n/2}\left[\cos\frac{2\pi}{n}(2m-1)(j-1)+\sin\frac{2\pi}{n}(2m-1)(j-1)\right] \\ & \times\left[1+\frac{\sin(2\pi/n)(2m-1)}{1-\cos(2\pi/n)(2m-1)}\right]\frac{1}{z-d+1-\cos(2\pi/n)(2m-1)}\end{aligned} \tag{B.8}$$

Obviously, $\langle s_{j+n}\rangle_n(z)=\langle s_j\rangle_n(z)$, so it is sufficient to present the result just for one row of the lattice, say, for $1\leqslant j\leqslant n$,

$$\langle s_j\rangle_n(z)=\begin{cases}\dfrac{1}{z^*-d}\left(\dfrac{1}{2}-\dfrac{1}{1+x_2}\dfrac{x_2^j}{1+x_2^{n/2}}-\dfrac{1}{1+x_1}\dfrac{x_1^j}{1+x_1^{n/2}}\right) \\ \quad \text{if} \quad 1\leqslant j\leqslant\dfrac{n}{2} \\ -\dfrac{1}{z^*-d}\left(\dfrac{1}{2}-\dfrac{1}{1+x_2}\dfrac{x_2^{j-n/2}}{1+x_2^{n/2}}-\dfrac{1}{1+x_1}\dfrac{x_1^{j-n/2}}{1+x_1^{n/2}}\right) \\ \quad \text{if} \quad \dfrac{n}{2}+1\leqslant j\leqslant n\end{cases} \tag{B.9}$$

APPENDIX C. THE CONVERGENCE RATE OF SOME SUMS

In this appendix the rate of convergence of the sums

$$\begin{aligned} L_N^{(d)}(z)&=\frac{1}{N}\sum_{j=1}^{N}\log\left(z-\frac{1}{2}\lambda_j^{(d)}\right) \qquad \text{for} \quad z>d \\ \tilde{L}_N^{(d)}&\equiv\frac{1}{N}\sum_{j=2}^{N}\log\left(d-\frac{1}{2}\lambda_j^{(d)}\right)\end{aligned} \tag{C.1}$$

toward their limiting values (when $N\to\infty$) will be estimated.

One can easily calculate these sums exactly for $d=1$ using the technique of Appendix B. In this case $\lambda_j^{(1)}=2\cos(2\pi/N)(j-1)$ and one can rewrite the argument of the logarithm in (C.1) as

$$\begin{aligned} z-\cos\frac{2\pi}{N}(j-1)=\frac{z_2}{2}&\left\{1-z_1\exp\left[-i\frac{2\pi}{N}(j-1)\right]\right\} \\ &\times\left\{1-z_1\exp\left[i\frac{2\pi}{N}(j-1)\right]\right\}\end{aligned}$$

where $z_{1,2}=z\mp(z^2-1)^{1/2}$. Hence,

$$\begin{aligned} L_N^{(d)}(z)=\log\frac{z_2}{2}&+\frac{1}{N}\sum_{j=1}^{N}\log\left\{1-z_1\exp\left[-i\frac{2\pi}{N}(j-1)\right]\right\} \\ &+\frac{1}{N}\sum_{j=1}^{N}\log\left\{1-z_1\exp\left[i\frac{2\pi}{N}(j-1)\right]\right\}\end{aligned}$$

For $z_1 < 1$ (i.e., $z > 1$) one can use the Taylor expansion of $\log(1+x)$ at the point $x = 0$, which yields

$$\begin{aligned}\tilde{\sigma} &\equiv \sum_{j=1}^{N} \log\left\{1 - z_1 \exp\left[-i\frac{2\pi}{N}(j-1)\right]\right\} \\ &= -\sum_{r=1}^{\infty} \frac{z_1^r}{r} \sum_{j=1}^{N} \exp\left[-i\frac{2\pi}{N}(j-1)r\right]\end{aligned}$$

Using the formula

$$\sum_{j=1}^{N} \exp\left[-i\frac{2\pi}{N}(j-1)r\right] = \begin{cases} N & \text{if } \; r = fN \text{ for some integer } f \\ 0 & \text{otherwise}\end{cases}$$

one obtains

$$\tilde{\sigma} = -N \sum_{f \geqslant 1}^{N} \frac{(z_1^N)^f}{Nf} = \log(1 - z_1^N)$$

Consequently,

$$\begin{aligned}&\sum_{j=1}^{N} \log\left[z - \cos\frac{2\pi}{N}(j-1)\right] \\ &\quad = N \log\frac{z + (z^2-1)^{1/2}}{2} + 2\log\{1 - [z - (z^2-1)^{1/2}]^N\} \qquad \text{(C.2)}\end{aligned}$$

that is, the sum $L_N^{(1)}(z)$ converges toward its limit exponentially fast for any $z > 1$.

An exact formula for $\tilde{L}_N^{(1)}$ can be derived from (C.2),

$$\begin{aligned}N\tilde{L}_N^{(1)} &= \sum_{m=2}^{N} \log\left\{1 - \cos\left[\frac{2\pi}{N}(m-1)\right]\right\} \\ &= \lim_{z \downarrow 1}\left(\sum_{m=1}^{N} \log\left\{1 - \cos\left[\frac{2\pi}{N}(m-1)\right]\right\} - \log(z-1)\right) \\ &= (1-N)\log 2 + 2\log N\end{aligned}$$

Thus, when $N \to \infty$ the convergence rate of the sum $\tilde{L}_N^{(1)}$ toward its limiting value is $O(N^{-1}\log N)$.

Now we shall apply the $d = 1$ results to obtain estimates for the convergence rates of the sums (C.1) for $d \geqslant 2$. The results are the same as for $d = 1$, i.e., for any $z > d$ the sum $L_N^{(d)}(z)$ converges toward its limit exponentially fast, and the convergence rate for the sum $\tilde{L}_N^{(d)}$ is $O(N^{-1}\log N)$. For the sake of notational simplicity we shall present a derivation only for the case $d=3$. Generalization to other dimensions is straightforward.

For $d=3$ one has

$$NL_N^{(d)}(z)=\sum_{j=1}^{N}\log\left(z-\frac{1}{2}\lambda_j^{(d)}\right)$$
$$=\sum_{l=1}^{n_2}\sum_{m=1}^{n_3}\sum_{k=1}^{n_1}\log\left\{z_{m,l}-\cos\frac{2\pi}{N}\right.$$
$$\left.\times[m-1+(l-1)n_3+(k-1)n_2n_3]\right\}$$

where

$$z_{m,l}=z-\cos\frac{2\pi n_1}{N}[m-1+(l-1)n_3]-\cos\frac{2\pi n_1 n_2}{N}(m-1)$$

does not depend on k. One can perform summation over k repeating (and slightly modifying) our calculations for the case $d=1$, which yields [cf. (C.2)]

$$NL_N^{(d)}(z)=\sum_{l,m}n_1\log[\tfrac{1}{2}z_{m,l}^{(+)}]+\Delta_1$$

where

$$\Delta_1=\sum_{l,m}\log\left\{1-2[z_{m,l}^{(-)}]^{n_1}\cos\frac{2\pi n_1}{N}[m-1+n_3(l-1)]+[z_{m,l}^{(-)}]^{2n_1}\right\}\tag{C.3}$$

and $z_{m,l}^{(\pm)}=z_{m,l}\pm(z_{m,l}^2-1)^{1/2}$. Note now the identity

$$\frac{1}{2\pi}\int_0^{2\pi}d\omega_1\log(z-\cos\omega_1)=\log\frac{1}{2}[z+(z^2-1)^{1/2}]$$

which can be obtained, for instance, from formula (C.2) by passing to the limit $N\to\infty$. Hence

$$NL_N^{(d)}(z)=\frac{n_1}{2\pi}\sum_{m,l}\int_0^{2\pi}d\omega_1\log\left[z-\cos\frac{2\pi n_1 n_2(m-1)}{N}\right.$$
$$\left.-\cos\frac{2\pi n_1[m-1+(l-1)n_3]}{N}-\cos\omega_1\right]+\Delta_1$$

One can consecutively perform the summations over l and m under the integral exactly as has been done over k. One obtains

$$L_N^{(d)}(z) = \iiint_0^{2\pi} \frac{d\omega_1\, d\omega_2\, d\omega_3}{(2\pi)^3} \log(z - \cos\omega_1 - \cos\omega_2 - \cos\omega_3) + \frac{\Delta_1 + \Delta_2 + \Delta_3}{N}$$

where

$$\Delta_2 = \frac{1}{2\pi} \sum_{m=1}^{n_3} \int_0^{2\pi} d\omega_1 \log\left\{1 + 2[z_m^{(-)}(\omega_1)]^{n_2} \times \cos\left[\frac{2\pi n_1 n_2 (m-1)}{N}\right] + [z_m^{(-)}(\omega_1)]^{2n_2}\right\}$$

$$z_m^{(-)}(\omega) = z_m(\omega) - [z_m^2(\omega) - 1]^{1/2}$$

$$z_m(\omega) = z - \cos\frac{2\pi n_1 n_2 (m-1)}{N} - \cos\omega$$

$$\Delta_3 = \frac{1}{2\pi^2} \iint_0^{2\pi} d\omega_1\, d\omega_2 \log\{1 + [z^{(-)}(\omega_1;\omega_2)]^{n_3}\}$$

$$z^{(-)}(\omega_1;\omega_2) = z(\omega_1;\omega_2) - [z^2(\omega_1;\omega_2) - 1]^{1/2}$$

$$z(\omega_1;\omega_2) = z - \cos\omega_1 - \cos\omega_2$$

If $z > 3$, then $z_{m,l}^{(-)} < z - 2 - [(z-2)^2 - 1]^{1/2} < 1$ and hence

$$|\Delta_1| \leqslant 2n_2 n_3 \{z - 2 - [(z-2)^2 - 1]^{1/2}\}^{n_1} + n_2 n_3 \{z - 2 - [(z-2)^2 - 1]^{1/2}\}^{2n_1}$$

This means that when $N \to \infty$ the term Δ_1 tends to zero as $o(\exp(-N^{1/3}\gamma))$ for some $\gamma > 0$. One can estimate Δ_2 and Δ_3 in a similar way and obtain finally

$$L_N^{(d)}(z) = \frac{N}{(2\pi)^3} \iiint_0^{2\pi} d\omega_1\, d\omega_2\, d\omega_3 \times \log(z - \cos\omega_1 - \cos\omega_2 - \cos\omega_3) + o(\exp(-N^{1/3}\gamma))$$

for some $\gamma = \gamma(z) > 0$ when $z > 3$.

Let now $z = 3$. As in the case $d = 1$, one can use the identity

$$\tilde{L}_N^{(3)} = \lim_{z \downarrow 3} \left[L_N^{(3)}(z) - \frac{\log(z-3)}{N}\right]$$

It is clear that, say, for $\frac{1}{6}N^{1/3} \leqslant l, m \leqslant \frac{5}{6}N^{1/3}$ the corresponding terms in the sum (C.3) are exponentially small and one can forget about them, as we are looking for an $O(N^{-1}\log(N))$ estimate. One can use the inequality $\cos(2\pi x) \leqslant 1 - 18x^2$ if $0 \leqslant x \leqslant \frac{1}{6}$ to estimate $z_{m,l}^{(-)}$ when $m, l < \frac{1}{6}N^{1/3}$ and a similar inequality for $m, l > \frac{5}{6}N^{1/3}$. This yields

$$\lim_{N \to \infty} (z_{m,l}^{(-)})^{N^{1/3}} \leqslant \exp\{-6[(l-1)^2 + (m-1)^2]^{1/2}\} \tag{C.4}$$

for any finite l (>1) and m (>1). It is clear now that one can find a constant C_1 such that for $l, m \in [C_1 \log N; N^{1/3} - C_1 \log N]$ one has

$$\max_{C_1 \log N \leqslant l,\, m \leqslant N^{1/3} - C_1 \log N} [z_{m,l}^{(-)}]^{N^{1/3}} = o\left(\frac{1}{N}\right)$$

Using (C.4), one concludes that all terms in the sum (C.3) remain uniformly bounded over $m, l > 0$ as $N \to \infty$. Hence the sum (C.3) is bounded above by $C(\log N)^2$ as $N \to \infty$ (which is already sufficient for the validity of all the results of this paper) and more careful estimates show that $\Delta_1 = O(\log N)$. Similar arguments can be applied for the estimation of Δ_2 and Δ_3 and we obtain finally $\Delta_1 + \Delta_2 + \Delta_3 = O(\log N)$ as $N \to \infty$.

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