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The Spherical Limit for n-Vector Correlations

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We investigate the $n \to \infty$ limit of the n-vector model single-spin and pair-spin correlation functions. In this limit we show that the correlation functions become those of the corresponding spherical model.

KEY WORDS: Spin correlations; n-vector model; spherical model; $n \to \infty$ limit.

1. INTRODUCTION

The "identification"[1] of the spherical model[2] as the infinite-spin-dimensionality limit of the n-vector model has added greatly to the significance of this unique statistical mechanical model. However, the "identification" is far from complete, since only the equivalence of the free energies in zero field has been established rigorously.[3] Even so, it is widely believed that in this limit other thermodynamic functions should correspond. Stanley[1] gives evidence to show that the susceptibilities should agree and many other authors simply assume that the correlation functions actually coincide. It is principally to this latter problem of correlations that we address ourselves in this paper.

Our approach to this problem originates from a recent paper by Gates and Thompson[4] in which correlation functions are investigated in the infinite-*spatial*-dimensionality limit. In essence the strategy is to introduce a nonuniform field and then to calculate the correlations from the field derivatives of the free energy. In accord with this program, we generalize the theorem of Ref. 3 to include a nonuniform field in the following section. In Section 3 the correlations are obtained by differentiation and the justification of the necessary interchanges of limits and differentiations is outlined.

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2. SPHERICAL LIMIT FOR A NONUNIFORM FIELD

Consider an n-vector model with a nonuniform field, that is, a lattice system of N, n-dimensional classical spins, $\mathbf{S}_i = (S_{i1}, S_{i2},..., S_{in})$, $i = 1, 2,..., N$, with length

$$\|\mathbf{S}_i\| = \left[\sum_{\alpha=1}^{n} S_{i\alpha}^2\right]^{1/2} = n^{1/2} \tag{1}$$

and described by the Hamiltonian

$$\mathscr{H} = -\tfrac{1}{2} \sum_{i,j=1}^{N} \rho_{ij}\mathbf{S}_i\cdot\mathbf{S}_j - \sum_{i=1}^{N} \mathbf{H}_i\cdot\mathbf{S}_i \tag{2}$$

We include the self-interacting terms in the Hamiltonian for convenience and set $\rho_{ii} = \rho_0$ large enough to ensure that the matrix ρ is positive definite. Furthermore, we choose the field $\mathbf{H}_i$ at each site i such that

$$H_{i\alpha} = n^{1/2}h_{i\alpha}, \qquad i = 1, 2,..., N \tag{3}$$

in order to guarantee a field contribution to the limiting free energy. The limiting free energy is given by

$$F\{\beta; \mathbf{H}_i\} = \lim_{N,n\to\infty} (Nn)^{-1} \log Z_N{}^n\{\beta; \mathbf{H}_i\} \tag{4}$$

where the n-vector partition function is

$$Z_N{}^n\{\beta; \mathbf{H}_i\} = \int\cdots\int_{\|\mathbf{S}_i\|=n^{1/2}} \prod_{i=1}^{N} d\mathbf{S}_i \exp\left(\tfrac{1}{2}\beta \sum_{i,j=1}^{N} \rho_{ij}\mathbf{S}_i\cdot\mathbf{S}_j + \beta\sum_{i=1}^{N} \mathbf{H}_i\cdot\mathbf{S}_i\right) \tag{5}$$

The most important feature of the nonuniform field case is that the Hamiltonian (2) is no longer translationally invariant, even for translationally invariant couplings

$$\rho_{ij} = \rho(\mathbf{r}_i - \mathbf{r}_j) \tag{6}$$

This translational invariance of the Hamiltonian is indispensable in the proof[3] that the n-vector free energy approaches the spherical free energy in the infinite-spin-dimensionality limit. We cannot therefore expect the limiting model in our nontranslationally invariant case to be the usual spherical model.

Taking the lead from Knops,[5] we consider the generalized spherical model defined by the partition function

$$Q_N\{\beta; z_i, H_i\} = \exp\left(\sum_{i=1}^{N} z_i\right) \int_{-\infty}^{\infty}\cdots\int \prod_{i=1}^{N} dx_i$$

$$\times \exp\left[\sum_{i,j=1}^{N} (\tfrac{1}{2}\beta\rho_{ij} - \delta_{ij}z_i)x_ix_j + \beta\sum_{i=1}^{N} H_ix_i\right] \tag{7}$$

within a region $\mathscr{D}$ where the "spherical fields" z_i are large enough to ensure that the quadratic form in the exponent is negative definite. The spherical fields are to be determined by the individual spherical constraints

$$\frac{\partial}{\partial z_i} \log Q_N\{\beta; z_i, H_i\} = 0, \qquad i = 1, 2,..., N \tag{8}$$

Following Knops, the generalized spherical free energy is

$$f\{\beta; H_i\} = \lim_{N\to\infty} N^{-1} \min_{z_i \in \mathscr{D}} \log Q_N\{\beta; z_i, H_i\} \tag{9}$$

where $Q_N\{\beta; z_i, H_i\}$ given by (7) factors explicitly as [see (19)]

$$Q_N\{\beta; z_i, H_i\} = Q_N\{\beta; z_i, 0\} \exp\left[\tfrac{1}{4}\beta^2 \sum_{i,j=1}^{N} (Z - \tfrac{1}{2}\beta\rho)_{ij}^{-1} H_i H_j\right] \tag{10}$$

$$= \pi^{N/2} \exp\left(\sum_{i=1}^{N} z_i\right)[\det(Z - \tfrac{1}{2}\beta\rho)]^{-1/2}$$

$$\times \exp\left[\tfrac{1}{4}\beta^2 \sum_{i,j=1}^{N} (Z - \tfrac{1}{2}\beta\rho)_{ij}^{-1} H_i H_j\right] \tag{11}$$

with the matrix Z given by

$$Z_{ij} = z_i\, \delta_{ij}; \qquad i, j = 1, 2,..., N \tag{12}$$

The theorem we want to prove can now be formulated.

Theorem. Under the condition (3) the limiting *n*-vector free energy (4) is given in terms of the spherical partition function (7) by

$$F\{\beta; \mathbf{H}_i\} = \lim_{N,n\to\infty} \min_{z_i \in \mathscr{D}} (Nn)^{-1} \log \prod_{\alpha=1}^{n} Q_N\{\beta; z_i, H_{i\alpha}\} \tag{13}$$

To prove the theorem we will obtain upper and lower bounds that coalesce in the stated limit.

Lower Bound. The derivation of the lower bound shadows that of Knops.[5] Define

$$Z_N^n\{\beta; \lambda_i, \mathbf{H}_i\} = \int_{\|\mathbf{S}_i\| = n^{1/2}\lambda_i} \cdots \int \prod_{i=1}^{N} d\mathbf{S}_i \exp\left(\tfrac{1}{2}\beta \sum_{i,j=1}^{N} \rho_{ij} \mathbf{S}_i \cdot \mathbf{S}_j + \beta \sum_{i=1}^{N} \mathbf{H}_i \cdot \mathbf{S}_i\right) \tag{14}$$

so that by direct calculation

$$\int_{-\infty}^{\infty}\cdots\int \prod_{i=1}^{N} d\lambda_i\, Z_N{}^n\{\beta;\lambda_i,H_i\}\exp\left(-\sum_{i=1}^{N} nz_i\lambda_i{}^2\right)$$
$$= n^{-N/2}\exp\left(-n\sum_{i=1}^{N} z_i\right) Q_N\{\beta; z_i, 0\}^n$$
$$\times \exp\left[\tfrac{1}{4}\beta^2 \sum_{i,j=1}^{N} (Z-\tfrac{1}{2}\beta\rho)_{ij}^{-1}\mathbf{H}_i\cdot\mathbf{H}_j\right] \quad (15)$$

Increasing the integrand in (15) to

$$\exp\left(-\frac{\pi}{2}\sum_{i=1}^{N}\lambda_i{}^2\right)\max_{0\le\lambda_i<\infty}\left[Z_N{}^n\{\beta;\lambda_i,\mathbf{H}_i\}\exp\left(-n\sum_{i=1}^{N} z_i'\lambda_i{}^2\right)\right] \quad (16)$$

with $z_i' = z_i - \pi/2n$, we obtain

$$\max_{0\le\lambda_i<\infty}\left[Z_N{}^n\{\beta;\lambda_i,\mathbf{H}_i\}\exp\left(n\sum_{i=1}^{N}(z_i - z_i'\lambda_i{}^2)\right)\right]$$
$$\geqslant n^{-N/2}Q_N\{\beta; z_i, 0\}^n \exp\left[\tfrac{1}{4}\beta^2\sum_{i,j=1}^{N}(Z-\tfrac{1}{2}\beta\rho)_{ij}^{-1}\mathbf{H}_i\cdot\mathbf{H}_j\right] \quad (17)$$

Now, by adjusting the z's in $\mathscr{D}$ so that the maximum occurs at $\lambda_1 = \lambda_2 = \cdots = \lambda_N = 1$, then replacing the right-hand side by its minimal value in $\mathscr{D}$, and finally taking the limits $N, n \to \infty$, we obtain straightforwardly

$$\lim_{N,n\to\infty}(Nn)^{-1}\log Z_N{}^n\{\beta;\mathbf{H}_i\}$$
$$\geqslant \lim_{N,n\to\infty}\max_{z_i\in\mathscr{D}}\left[\frac{1}{N}\log Q_N\{\beta; z_i, 0\} + \frac{\beta^2}{4Nn}\sum_{i,j=1}^{N}(Z-\tfrac{1}{2}\beta\rho)_{ij}^{-1}\mathbf{H}_i\cdot\mathbf{H}_j\right] \quad (18)$$

Upper Bound. The derivation of the upper bound is based on the well-known identity

$$\exp\left(\tfrac{1}{2}\beta\sum_{i,j=1}^{N}\rho_{ij}\mathbf{S}_i\cdot\mathbf{S}_j\right)$$
$$= (2\pi)^{-Nn/2}(\det\rho)^{-n/2}\int_{-\infty}^{\infty}\cdots\int\prod_{i=1}^{N} d\mathbf{x}_i$$
$$\times\exp\left(-\tfrac{1}{2}\sum_{i,j=1}^{N}\rho_{ij}^{-1}\mathbf{x}_i\cdot\mathbf{x}_j + \beta^{1/2}\sum_{i=1}^{N}\mathbf{x}_i\cdot\mathbf{S}_i\right) \quad (19)$$

which is valid for any positive-definite matrix ρ and n-dimensional vectors

$\mathbf{S}_i$. Using this identity, we have from (5), after an interchange in orders of integration,

$$Z_N^n\{\beta;\mathbf{H}_i\} = (2\pi)^{-Nn/2}(\det\rho)^{-n/2}\int_{-\infty}^{\infty}\cdots\int\prod_{i=1}^{N}d\mathbf{x}_i\exp\left(-\tfrac{1}{2}\sum_{i,j=1}^{N}\rho_{ij}^{-1}\mathbf{x}_i\cdot\mathbf{x}_j\right)$$
$$\times\int_{\|\mathbf{S}_i\|=n^{1/2}}\cdots\int\prod_{i=1}^{N}d\mathbf{S}_i\exp\left[\beta^{1/2}\sum_{i=1}^{N}(\mathbf{x}_i+\beta^{1/2}\mathbf{H}_i)\cdot\mathbf{S}_i\right] \tag{20}$$

Translation of the "local fields" leads to our final representation

$$Z_N^n\{\beta;\mathbf{H}_i\} = (2\pi)^{-Nn/2}(\det\rho)^{-n/2}\int_{-\infty}^{\infty}\cdots\int\prod_{i=1}^{N}d\mathbf{x}_i$$
$$\times\exp\left\{-\tfrac{1}{2}\sum_{i,j=1}^{N}\left[\rho_{ij}^{-1}(\mathbf{x}_i-\beta^{1/2}\mathbf{H}_i)\cdot(\mathbf{x}_j-\beta^{1/2}\mathbf{H}_j)\right.\right.$$
$$\left.\left.-\frac{\beta}{2z_i}\delta_{ij}\mathbf{x}_i\cdot\mathbf{x}_j\right]\right\}\cdot\prod_{i=1}^{N}\Phi_i(\beta^{1/2}\mathbf{x}_i) \tag{21}$$

where

$$\Phi_i(\mathbf{y}) = [\exp(-\|\mathbf{y}\|^2/4z_i)]\int_{\|\mathbf{S}\|=n^{1/2}}\cdots\int\exp(\mathbf{y}\cdot\mathbf{S})\,d\mathbf{S} \tag{22}$$

Now, to obtain an upper bound, we replace each Φ_i in (21) by the majorization [Knops, Eq. (2.25)]

$$\Phi_i \leqslant A_n\exp[(n/2)(2z_i-1-\log 2z_i+\epsilon_i)] \tag{23}$$

where

$$A_n = 2\pi^{n/2}n^{(n-1)/2}/\Gamma(n/2) \tag{24}$$

and

$$\epsilon_i = n^{-1}(2+2\log 2z_i) \tag{25}$$

The remaining integral in (21) can be recast into the form

$$(2\pi)^{-Nn/2}(\det\rho)^{-n/2}\left(\exp\left(-\tfrac{1}{2}\beta\sum_{i,j=1}^{N}\rho_{ij}^{-1}\mathbf{H}_i\cdot\mathbf{H}_j\right)\right)$$
$$\times\int_{-\infty}^{\infty}\cdots\int d^N\mathbf{x}\exp\left[-\tfrac{1}{2}\sum_{i,j=1}^{N}\left(\rho_{ij}^{-1}-\frac{\beta}{2z_i}\delta_{ij}\right)\mathbf{x}_i\cdot\mathbf{x}_j+\beta^{1/2}\sum_{i,j=1}^{N}\rho_{ij}^{-1}\mathbf{x}_i\cdot\mathbf{H}_j\right] \tag{26}$$
$$= [\det(I-\tfrac{1}{2}\beta\rho Z^{-1})]^{-n/2}\exp\left[-\tfrac{1}{2}\beta\sum_{i,j=1}^{N}\rho_{ij}^{-1}\mathbf{H}_i\cdot\mathbf{H}_j\right.$$
$$\left.+\tfrac{1}{2}\beta\sum_{i,j=1}^{N}(\rho^{-1}-\tfrac{1}{2}\beta Z^{-1})_{ij}^{-1}\sum_{k=1}^{N}\rho_{ik}^{-1}\mathbf{H}_k\cdot\sum_{l=1}^{N}\rho_{jl}^{-1}\mathbf{H}_l\right] \tag{27}$$

The Gaussian integrals have been evaluated using (19), with the z_i chosen such that the matrix $I - \frac{1}{2}\beta\rho Z^{-1}$ is positive definite, that is, $z_i \in \mathscr{D}$.

The matrix of the quadratic form in the exponent of (27) can now be written

$$A \equiv -\rho^{-1} + \rho^{-1}(\rho^{-1} + \tfrac{1}{2}\beta\rho Z^{-1})\rho^{-1} = \tfrac{1}{2}\beta(Z - \tfrac{1}{2}\beta\rho)^{-1} \tag{28}$$

This identity is easily proved by expanding the matrix expression $A(Z - \frac{1}{2}\beta\rho)$.

Combining (22)–(28), we have

$$Z_N{}^n\{\beta; \mathbf{H}_i\} \leqslant [\det(I - \tfrac{1}{2}\beta\rho Z^{-1}]^{-n/2} \exp\left[\tfrac{1}{4}\beta^2 \sum_{i,j=1}^{N} (Z - \tfrac{1}{2}\beta\rho)_{ij}^{-1}\mathbf{H}_i\cdot\mathbf{H}_j\right]$$

$$\times (A_n)^N \exp\left[\tfrac{1}{2}n \sum_{i=1}^{N} (2z_i - 1 - \log 2z_i + \epsilon_i)\right] \tag{29}$$

Finally, minimizing the right-hand side with respect to the z's and applying Stirling's formula to A_n we obtain

$$\lim_{N,n\to\infty} (Nn)^{-1} \log Z_N{}^n\{\beta; \mathbf{H}_i\}$$

$$\leqslant \lim_{N,n\to\infty} \min_{z_i\in\mathscr{D}}\left[-\frac{1}{2} N^{-1} \log\det\left(Z - \frac{1}{2}\beta\rho\right)\right.$$

$$\left. + \frac{\beta^2}{4Nn} \sum_{i,j=1}^{N} \left(Z - \frac{1}{2}\beta\rho\right)_{ij}^{-1} \mathbf{H}_i\cdot\mathbf{H}_j + \frac{1}{2}\log\pi + N^{-1}\sum_{i=1}^{N} z_i\right] \tag{30}$$

As argued by Knops,[5] the error term $\frac{1}{2}N^{-1} \sum_i z_i$ vanishes in the limit.

In view of (10) and (11) and the lower bound (18), the theorem is established.

3. THE CORRELATION FUNCTIONS

First let us rewrite the theorem (13) in the form

$$F\{\beta; \mathbf{H}_i\} = \lim_{N,n\to\infty} F_N{}^n\{\beta; \mathbf{h}_i\} \tag{31}$$

where

$$F_N{}^n\{\beta; \mathbf{h}_i\} = \frac{1}{2}\log\pi + \frac{1}{N}\sum_{i=1}^{N} z_i^* - \frac{1}{2N}\log\det\left(Z^* - \frac{1}{2}\beta\rho\right)$$

$$+ \frac{\beta^2}{4N}\sum_{i,j=1}^{N}\left(Z^* - \frac{1}{2}\beta\rho\right)_{ij}^{-1} \mathbf{h}_i\cdot\mathbf{h}_j \tag{32}$$

We have assumed that the minimum in (13) is attained for

$$z_i = z_i^*\{\mathbf{h}_i\} \tag{33}$$

in terms of the scaled field (3).

Consider now the limit of the n-vector single-spin correlation function

$$\lim_{n\to\infty} n^{1/2}\langle S_{i\alpha}\rangle_n = \lim_{N,n\to\infty} \frac{\partial}{\partial(\beta h_{i\alpha})} (Nn)^{-1} \log Z_N{}^n\{\beta; \mathbf{h}_i\} \tag{34}$$

Since $\log Z_N{}^n\{\beta; \mathbf{h}_i\}$ is a convex function of $h_{i\alpha}$, the right-hand side of (34) is equal to

$$\frac{\partial}{\partial(\beta h_{i\alpha})} \lim_{N,n\to\infty} (Nn)^{-1} \log Z_N{}^n\{\beta; \mathbf{h}_i\} \tag{35}$$

wherever (35) defines a continuous function of $h_{i\alpha}$. This theorem on the interchange of limits and differentiation is due to Griffiths.[6] Note also that, because the limiting n-vector free energy $F\{\beta; \mathbf{h}_i\}$ is a convex function of $h_{i\alpha}$, the derivative (35) is a monotonic increasing function and thus is continuous everywhere except, possibly, at a countable number of jump discontinuities. Now, by our theorem (31), we can write (35) as

$$\frac{\partial}{\partial(\beta h_{i\alpha})} \lim_{N,n\to\infty} F_N{}^n\{\beta; \mathbf{h}_i\} \tag{36}$$

$$= \lim_{N,n\to\infty} \frac{\partial}{\partial(\beta h_{i\alpha})} F_N{}^n\{\beta; \mathbf{h}_i\} \tag{37}$$

if we again invoke Griffiths' theorem.[6] The limit (37) can now be readily calculated using the facts that

$$\frac{\partial}{\partial h_{i\alpha}} G\{z_k{}^*(h_{i\alpha}), h_{i\alpha}\} = \sum_{k=1}^{N} \frac{\partial G}{\partial z_k{}^*} \frac{\partial z_k{}^*}{\partial h_{i\alpha}} + \left.\frac{\partial G}{\partial h_{i\alpha}}\right|_{z_k^* \text{ const}} \tag{38}$$

and

$$\frac{\partial F_N{}^n}{\partial z_k{}^*} = 0, \qquad k = 1, 2,..., N \tag{39}$$

We thus obtain

$$\lim_{N,n\to\infty} \frac{\partial}{\partial(\beta h_{i\alpha})} F_N{}^n\{\beta; \mathbf{h}_i\} = \lim_{N\to\infty} \frac{\beta}{2N} \sum_{j=1}^{N} \left(Z^* - \frac{1}{2}\beta\rho\right)_{ij}^{-1} h_{j\alpha} \tag{40}$$

If we now let each $h_{i\alpha} \to h$, it is easily seen that the right-hand side of (40) is precisely the generalized spherical single-spin correlation in a uniform field $H_i = h$,[7] which we denote by $\langle S_i\rangle$. Moreover, in this $h_{i\alpha} \to h$ limit, by invariance under rotation about a uniform field, the n-vector spin component correlations and, in particular, $\langle S_{i\alpha}\rangle_n$ are independent of the value of α. Hence we conclude that for a uniform field ($H_{i\alpha} = n^{1/2}h$)

$$\lim_{n\to\infty} \|\langle S_i\rangle_n\| = \lim_{n\to\infty} \left(\sum_{\alpha=1}^{n} \langle S_{i\alpha}\rangle_n{}^2\right)^{1/2} = \lim_{n\to\infty} n^{1/2}\langle S_{i\alpha}\rangle_n = \langle S_i\rangle \tag{41}$$

We can now obtain the limit of the n-vector pair correlations by considering

$$\lim_{n\to\infty} n(\langle S_{i\alpha}S_{j\alpha}\rangle_n - \langle S_{i\alpha}\rangle_n\langle S_{j\alpha}\rangle_n)$$
$$= \lim_{N,n\to\infty} \beta^{-2} \frac{\partial^2}{\partial h_{i\alpha}\partial h_{j\alpha}} (Nn)^{-1} \log Z_N{}^n\{\beta; \mathbf{h}_i\} \tag{42}$$

The previous arguments lead to the conclusion that for a uniform field

$$\lim_{n\to\infty} (\langle \mathbf{S}_i\cdot\mathbf{S}_j\rangle_n - \langle S_i\rangle_n\langle S_j\rangle_n) = \langle S_iS_j\rangle - \langle S_i\rangle\langle S_j\rangle \tag{43}$$

Unfortunately, we have been unable to find a generalization of Griffiths' Theorem[6] to obtain this result with absolute rigor. However, given that the necessary interchanges of limits and differentiations are valid, we can conclude that

$$\lim_{n\to\infty} \langle \mathbf{S}_i\cdot\mathbf{S}_j\rangle_n = \langle S_iS_j\rangle \tag{44}$$

by using (41) and the fact that each $\langle \mathbf{S}_i\rangle_n$ is parallel to the uniform field.

Finally, we observe that in a uniform field and for periodic, translationally invariant interactions the generalized spherical model reduces to the mean spherical model. Moreover, if the field is nonzero, the mean spherical correlations agree with the usual spherical model correlations.[8]

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