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Large-*n* Limit of the Heisenberg Model: The Decorated Lattice and the Disordered Chain

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The critical temperature of the generalized spherical model (large-component limit of the classical Heisenberg model) on a cubic lattice, whose every bond is decorated by L spins, is found. When $L \to \infty$, the asymptotics of the temperature is $T_c \sim aL^{-1}$. The reduction of the number of spherical constraints for the model is found to be fairly large. The free energy of the one-dimensional generalized spherical model with random nearest neighbor interaction is calculated.

KEY WORDS: Spherical model; decorated lattice; critical temperature; Jacobi matrix.

1. Considerable interest has recently been displayed in the behavior of quasi-one-dimensional systems (see refs. 1 and 2 and lists of references therein). Particles in such systems interact predominantly along specific directions of a d-dimensional space, so that there are two length scales. One of them determines the sizes in which the system may be regarded as one-dimensional; the other one is the sample size.

Therefore it is reasonable to consider a simple but sufficiently instructive, exactly solvable model defined on a geometry that is restricted in some way. In particular, a version of the spherical model on a d-dimensional cubic lattice with each bond decorated by L spins (Fig. 1), which below will be referred to as just as decorated, was considered in ref. 2. The authors regarded their results as modeling certain aspects of helium superfluidity in porous media.

However, interpretation of the results of ref. 2 involved a problem. As is known, in the translationally invariant case the spherical model (charac-

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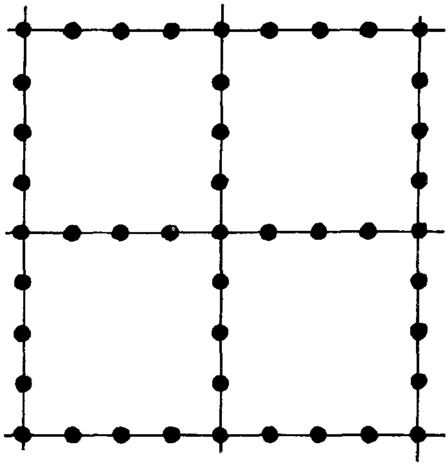

Fig. 1. Two-dimensional decorated lattice with $L = 3$.

terized by a single spherical condition) is a large-n limit of the classical (n-vector) Heisenberg model[3,4] and describes sufficiently well the behavior of the latter even for $n = 3$[5]. In the absence of the translational invariance, this is generally speaking not the case (see, e.g., ref. 6 presenting a counter-example). According to refs. 7 and 4, in the limit $n \to \infty$, we obtain a generalized spherical model (GSM), in which the number of spherical constraints depends on the degree of inhomogeneity. For example, in the disordered case there arises a macroscopic number of such constraints, while for a decorated lattice there are generally speaking $1 + (L+1)/2$ constraints. However, the version of the spherical model proposed in ref. 2, for any L, contains only two spherical conditions. Therefore, the physically very important relationship of this model to the large-n limit of the Heisenberg model is not at all clear.

Here we propose a simple method to determine the critical temperature T_c of the GSM (of the large-n limit of the Heisenberg model) on the decorated lattice, which in particular leads to the asymptotics $T_c \sim aL^{-1}$ for $L \to \infty$ [see formulas (19)–(21) below]. This asymptotics has the same form as that found in ref. 2, but with a different constant a.[2]

The present study may be of interest not only in the context of quasi-one-dimensional systems. The reason is that the spherical constraints which are a kind of self-consistency condition represent a system of transcendental equations whose solution is the basis of the study of the thermodynamics

[2] Note here that for the Ising model on the decorated lattice the analogous asymptotics is $T_c \sim (lnL)^{-1}$.[13]

of the GSM. The inhomogeneous GSM is therefore very complicated even for qualitative analysis to be made. Until now exact solutions have been known for it only in the cases where this system consists of two equations,[8-10] and qualitative analysis only covers a single example.[10] Thus, we are providing another and richer example [the number of equations being $1+(L+1)/2$], where the exact solution of the system can be found. Note also that our calculation yields not only the critical temperature, but also the fact that the GSM on the decorated lattice for any L is determined by only three spherical conditions.

The main trick enabling us to obtain the final expressions (19)–(21) is application of the Cauchy problem solutions for the second-order finite-difference equation (11) generated by the Jacobi matrix (6) for the analysis of the spherical conditions. This fact is due to the quasi-one-dimensionality of the problem and is fairly general in nature. In Section 4 we demonstrate it by similarly calculating the free energy of a one-dimensional GSM with random nearest-neighbor interaction.

2. Let us define the GSM on the decorated lattice. Any site of such a lattice may be represented as $R=r+j\,\delta_m$, where $r\in(L+1)\,\mathbb{Z}^d$, δ_m ($m=1,\dots,d$) is the orthonormal basis of $\mathbb{Z}^d$, and $j=0, 1,\dots, L$. The free energy of the model in a finite volume V, $V=\{R\in\mathbb{Z}^d,\ R=r+j\,\delta_m;\ r_m=0,\ L+1,\dots,(N-1)(L+1),\ m=1,\dots,d;\ j=0,\ 1,\dots,L\}$ is as follows[7]:

$$f_V=\max_{\{z_R\}_{R\in V}\in D} F(\{z_R\})$$

where

$$F(\{z_R\})=-\frac{1}{\beta\,|V|}\ln\int_{\mathbb{R}^{|V|}}\exp\left\{-\frac{\beta}{2}\left[-\sum_{\langle R,R'\rangle}x_R x_{R'}\right.\right.$$

$$\left.\left.+\sum_{R\in V}(z_R x_R^2-z_R)\right]\right\}\prod_{R\in V}dx_R \tag{1}$$

and the set D consists of those spherical constants $\{z_R\}_{R\in V}$ for which the quadratic form

$$(Hx,x)=-\sum_{\langle R,R'\rangle}x_R x_{R'}+\sum_{R\in V}z_R x_R^2 \tag{2}$$

is positively defined. The symbol $\sum_{\langle R,R'\rangle}$ denotes summation over the pairs of nearest neighbors from V, taking into account periodic boundary conditions. Note that the maximum in (1) is attained for those z_R for which

$$\langle x_R^2 \rangle = 1, \qquad R \in V \tag{3}$$

Let T_m, $m = 1,..., d$, be translations in $\mathbb{Z}^d$ on the vectors $(L+1)\,\delta_m$, and let Q_m be reflections in $\mathbb{Z}^d$ with respect to the planes $R_m = (L+1)/2$. The function $F(\{z_R\}_{R \in V})$ in (1) is upward convex and takes on infinitely large negative values at the boundary of the set D, and the system (3) is invariant under the actions T_m and Q_m. Therefore, the unique solution (3) of D is also invariant under T_m and Q_m. Thus, we may restrict ourselves from the very beginning to those $\{z_R\}_{R \in V}$ for which

$$\begin{aligned} &z_{r+j\delta_m} \equiv z_j, \qquad r \in (L+1)\,\mathbb{Z}^d, \qquad j = 1,..., d \\ &z_j \equiv z_{L+1-j} \end{aligned} \tag{4}$$

Let us assume that L is an odd number, i.e., $L = 2l - 1$ (the case of even L is treated similarly). In view of (4), the free energy of the GSM on the decorated lattice is as follows:

$$f = \lim_{|V| \to \infty} f_V, \qquad f_V = \max_{(z_0,..., z_l) \in D} F(z_0,..., z_l)$$

where

$$\begin{aligned} F(z_0,..., z_l) = &-\frac{1}{2\beta} \ln \frac{2\pi}{\beta} + \frac{1}{2\beta\,|V|} \ln \det H \\ &- \frac{1}{2(1+Ld)} (z_0 + 2dz_1 + \cdots + 2dz_{l-1} + dz_l) \end{aligned} \tag{5}$$

H is an operator generated by the quadratic form (2) and $D = \{(z_0,..., z_l)$: $H > 0\}$.

Let us calculate $\det H$, using the structure of H. Since it commutes with the operators T_m, its eigenvectors ψ have the Bloch form

$$\psi_R = \exp\left(i \sum_{m=1}^{d} \frac{K_m R_m}{L+1}\right) U_R$$

and therefore $\det H = \prod_{K \in V^*} \det H_K$, where $V^* = \{(K_1,..., K_d)$: $K_m = 2\pi q_m/N$, $q_m = 0, 1,..., N-1\}$, and the matrices H_K are as follows:

$$\left(\begin{array}{c|c|c|c}
Z_0 & -1\ 0\cdots 0\ -e^{iK_1} & -1\ 0\cdots 0\ -e^{iK_2} & -1\ 0\cdots 0\ -e^{iK_d} \\ \hline
\begin{matrix}-1\\ 0\\ \vdots\\ 0\\ -e^{iK_1}\end{matrix} & J & 0 & 0 \\ \hline
\begin{matrix}-1\\ 0\\ \vdots\\ 0\\ -e^{-iK_2}\end{matrix} & 0 & J & 0 \\ \hline
\begin{matrix}-1\\ 0\\ \vdots\\ 0\\ -e^{-iK_d}\end{matrix} & 0 & 0 & J
\end{array}\right)$$

where the diagonal blocks J are the Jacobi matrices

$$J=\begin{pmatrix}
z_1 & -1 & & & & & \\
-1 & z_2 & -1 & & & 0 & \\
& \ddots & & \ddots & & & \\
& & -1 & z_l & -1 & & \\
& & & \ddots & & \ddots & \\
& 0 & & & -1 & z_2 & -1 \\
& & & & & -1 & z_1
\end{pmatrix} \tag{6}$$

By expanding first det H_K by the first row and then every resulting cofactor by the first column, we obtain the following:

$$\det H_K = (\det J)^d \left[z_0 - 2d(G_{1,1} + G_{1,2l-1}) + E(K) G_{1,2l-1}\right] \tag{7}$$

where G is the matrix inverse to J and

$$E(K) = 2 \sum_{m=1}^{d} (1 - \cos K_m)$$

Substituting (7) into (5) and performing the thermodynamic limit, we find the free energy of the GSM on the decorated lattice:

$$f = \max_{(z_0,\dots,z_l)\in D} F(z_0,\dots,z_l),$$

$$\begin{aligned} F(z_0,\dots,z_l) = &-\frac{1}{2\beta}\ln\frac{2\pi}{\beta}+\frac{1}{2(1+Ld)} \\ &\times\left\{\frac{d}{\beta}\ln\det J+\frac{1}{\beta}\int_{[0,2\pi]^d}\ln\right. \\ &\times[z_0-2d(G_{1,1}+G_{1,2l-1})+E(K)G_{1,2l-1}]\frac{dK}{(2\pi)^d} \\ &\left.-(z_0+2dz_1+\cdots+2dz_{l-1}+dz_l)\right\} \end{aligned} \tag{8}$$

If there is no phase transition, the maximum in (8) is attained at the unique point $(z_0,\dots,z_l)\in D$, for which $\partial F(z_0,\dots,z_l)/\partial z_j=0$, $j=0,\dots,l$. By differentiating $F(z_0,\dots,z_l)$, we arrive at the system of equations

$$\begin{gathered} \frac{1}{\beta}\int_{[0,2\pi]^d}\frac{1}{z_0-2d(G_{1,1}+G_{1,2l-1})+E(K)G_{1,2l-1}}\frac{dK}{(2\pi)^d}=1 \\ \frac{1}{\beta}G_{j,j}+\frac{1}{\beta}\int_{[0,2\pi]^d}\frac{(G_{1,j}+G_{j,2l-1})^2-[E(K)/d]\,G_{1,j}G_{j,2l-1}}{z_0-2d(G_{1,1}+G_{1,2l-1})+E(K)G_{1,2l-1}}\frac{dK}{(2\pi)^d},\quad j=1,\dots,l, \end{gathered} \tag{9}$$

for finding the spherical constants $z_0,\dots,z_l$.

As is known, the mathematical mechanism of the phase transition in the spherical model is the sticking of the solution (7) to the boundary ∂D of the set $D^{(3)}$. The sticking means that the maximum in (8) for $\beta\geqslant\beta_c$ is attained at $(z_0,\dots,z_l)\in\partial D$ and the system (9) has no solution. For $d=1$ and $d=2$ the system (9) always has a solution in D and thus the phase transition is absent. If $d\geqslant 3$, then, because $z_0=2d(G_{1,1}+G_{1,2l-1})$ on the boundary of the set D, the critical temperature $T_c=\beta_c^{-1}$ can be found by solution of the system of equations

$$\begin{gathered} \frac{\beta_0}{\beta_c G_{1,2l-1}}=1 \\ \frac{1}{\beta_c}G_{j,j}+(G_{1,j}+G_{j,2l-1})^2-\frac{1}{d\beta_c}\frac{G_{1,j}G_{j,2l-1}}{G_{1,2l-1}}=1,\qquad j=1,\dots,l \end{gathered} \tag{10}$$

for $\beta_c, z_1,..., z_l$. The symbol β_0 denotes here the integral

$$\beta_0 = \int_{[0,2\pi]^d} \frac{1}{E(K)} \frac{dK}{(2\pi)^d}$$
$$= \int_{[0,2\pi]^d} \frac{1}{2\sum_{m=1}^d (1-\cos K_m)} \frac{dK}{(2\pi)^d}$$

Note that β_0^{-1} coincides with the critical temperature of the standard Berlin–Kac spherical model on the cubic lattice $\mathbb{Z}^d$.[3]

3. To solve the system of equations (10) let us use the representation[11]

$$G_{j,m} = \begin{cases} \dfrac{y_j w_m}{W}, & j \geqslant m \\ \dfrac{y_m w_j}{W}, & j \leqslant m \end{cases}$$

where y_j and w_j are the solutions of the Cauchy problem for the finite-difference second-order equation generated by the Jacobi matrix (6) for the case of $\lambda = 0$, namely

$$\begin{aligned} &y_1(\lambda) = 1; \qquad -y_2(\lambda) = (\lambda - z_1)\, y_1(\lambda) \\ &-y_{j+1}(\lambda) = (\lambda - z_j)\, y_j(\lambda) + y_{j-1}(\lambda), \qquad j = 1,..., l \\ &-y_{l+j+1}(\lambda) = (\lambda - z_{l-j})\, y_{l+j}(\lambda) + y_{l+j-1}(\lambda), \qquad j = 1,..., l-1 \\ &w_j(\lambda) = y_{2l-j}(\lambda), \qquad j = 1,..., 2l-1 \end{aligned} \tag{11}$$

and $W = y_{j+1} w_j - y_j w_{j+1} \equiv \text{const}$.

The system (10) then becomes as follows:

$$\begin{aligned} &\beta_0 W = \beta_c \\ &\frac{d-1}{d}\, y_j w_j + \beta_0 (y_j + w_j)^2 = \beta_c W, \qquad j = 1,..., l \end{aligned} \tag{12}$$

Having solved it, we shall find β_c and $z_1,..., z_l$ by formulas (11).

Let

$$\tau_{\pm} = \left(\frac{d-1}{d} + \beta_0\right)^{1/2} \pm \left(\frac{d-1}{d}\right)^{1/2},$$

$$\tilde{y}_j = \tau_+ y_j + \tau_- w_j, \qquad \tilde{w}_j = \tau_- y_j + \tau_+ w_j$$

Then

$$\tilde{W} = \tilde{y}_{j+1}\tilde{w}_j - \tilde{y}_j\tilde{w}_{j+1} = \alpha W$$
$$\alpha = \left[\frac{d-1}{d}\left(\frac{d-1}{d} + 4\beta_0\right)\right]^{1/2} \tag{13}$$

and the last l equations of (12) will become

$$\tilde{y}_j\tilde{w}_j = \frac{\beta_c}{\alpha}\tilde{W}, \qquad j = 1,\ldots, l \tag{14}$$

From (13) and (14) it follows that y_{j+1}/y_j satisfy the equations

$$\frac{\tilde{y}_{j+1}}{\tilde{y}_j} - \frac{\tilde{y}_j}{\tilde{y}_{j+1}} = \frac{\alpha}{\beta_c}, \qquad j = 1,\ldots, l-1 \tag{15}$$

The condition $(z_0,\ldots, z_l) \in \partial D$ under which we are to solve (10) implies the inequality $J > 0$. Since the eigenvalues of J coincide with the roots of the polynomial $y_{2l}(\lambda)$, (11), and the roots of the polynomials $y_j(\lambda)$ and $y_{j+1}(\lambda)$ are intermittent, then all $y_j = y_j(0)$ for such $z_0,\ldots, z_l$ should have the same signs. Therefore, it follows from (15) that

$$\tilde{y}_{j+1} = t\tilde{y}_j, \qquad t = \frac{\alpha + (\alpha^2 + 4\beta_c)^{1/2}}{2\beta_c}, \qquad j = 1,\ldots, l-1$$

Similarly, $\tilde{w}_{j+1} = t^{-1}\tilde{w}_j$, and thus, in view of $w_l = y_l$,

$$\tilde{w}_1 = t^{2l-2}\tilde{y}_1 = t^{L-1}\tilde{y}_1, \qquad \frac{\beta_c}{\alpha}\tilde{W} = (\tau_+ + \tau_- w_1)^2\, t^{L-1} \tag{16}$$

On the other hand,

$$\frac{\beta_c}{\alpha} W = (\tau_+ + \tau_- w_1)(\tau_- + \tau_+ w_1) \tag{17}$$

Comparison of (16) and (17) shows that

$$w_1 = \frac{\tau_- - \tau_+ t^{L-1}}{\tau_- t^{L-1} - \tau_+} \tag{18}$$

Substituting this expression into (16), we arrive at the equality

$$w\beta_c = t^{L-1}\,\frac{\alpha^2}{(\tau_- t^{L-1} - \tau_+)^2}$$

which, combined with the first equation of (12), yields the equation for β_c:

$$\beta_c = \beta_0^{1/2} t^{(L-1)/2} \alpha(|\tau_- t^{L-1} - \tau_+|)^{-1}$$

Since β_c and t are related as $\beta_c = \alpha t(t^2 - 1)^{-1}$, then

$$\beta_c = \left[\frac{d-1}{d}\left(\frac{d-1}{d} + 4\beta_0\right)\right]^{1/2} t_0 \Big/ (t_0^2 - 1) \tag{19}$$

where t_0 is the root of the equation

$$\frac{t}{t^2 - 1} = \frac{\beta_0^{1/2} t^{(L-1)/2}}{\tau_+ - \tau_- t^{(L-1)/2}} \tag{20}$$

lying in the interval $(1, (\tau_+/\tau_-)^{1/(L-1)})$. This requirement on t_0 is due to the inequality $w_1 > 0$ and the dependence of w_1 on t, (18). Note that the same expression for β_c is valid for even L.

From (19) and (20) it is easy to obtain the asymptotics of the critical temperature $T_c = \beta_c^{-1}$ for $L \to \infty$:

$$\begin{aligned} T_c &= \frac{2}{\alpha(L-1)} \ln \frac{\tau_+}{\tau_-} + O\left(\frac{1}{(L-1)^2}\right) \\ &= \frac{2}{(L-1)\{[(d-1)/d][(d-1)/d + 4\beta_0]\}^{1/2}} \\ &\quad \times \ln \frac{[(d-1)/d + 4\beta_0]^{1/2} + [(d-1)/d]^{1/2}}{[(d-1)/d + 4\beta_0]^{1/2} - [(d-1)/d]^{1/2}} + O\left(\frac{1}{(L-1)^2}\right) \end{aligned} \tag{21}$$

Besides the simple expression for the critical temperature for finite L and its asymptotics for $L \to \infty$, an important result of the above arguments is the reduction of the number of the spherical constants z_j. From the solution of (20), one can find y_j, w_j, and then z_j. According to (11), all z_j, $j = 2,..., l-1$, are equal. The same is the case for the solution of (9) with $T > T_c$. Thus, the set of the spherical constants z_R for the generalized spherical model on the decorated lattice (1), for any L, contains not more than three different elements (z_0, $z_1 = z_l$, $z_2 = z_3 = \cdots = z_{l-1}$). Note that the modified spherical model[2] contains only two spherical constants.

4. The technique used in the preceding section to solve the system (10) is due to the existence of one-dimensional structures on the decorated lattice. To show it in a clearer way, let us calculate in the same fashion the free energy of a one-dimensional generalized spherical model with random nearest neighbor interaction.

The partition function of the model is

$$Z=\int_{\mathbb{R}^{|V|}} \exp\left[\beta\left(\sum_{j=-N}^{N} J_j x_j x_{j+1}-\sum_{j=-N}^{N}\frac{z_j}{2}x_j^2\right)\right]\prod_{|j|\leqslant N} dx_j \tag{22}$$

where the quantities J_j form an ergodic sequence and the spherical constants z_j are to be found from the conditions

$$\langle x_j^2\rangle=1, \qquad |j|\leqslant N \tag{23}$$

By calculating the Gaussian integrals in (23), we arrive at the system of transcendental equations

$$\frac{1}{\beta}G_{j,j}=1, \qquad |j|\leqslant N \tag{24}$$

to determine $\{z_j\}_{|j|\leqslant N}$. The symbol G now denotes the matrix inverse to the matrix

$$\begin{pmatrix} z_{-N} & -J_{-N} & & & & 0 \\ -J_{-N} & z_{-N+1} & -J_{-N+1} & & & \\ & \ddots & \ddots & \ddots & & \\ 0 & & -J_{N-2} & z_{N-1} & -J_{N-1} \\ & & & -J_{N-1} & z_N \end{pmatrix} \tag{25}$$

Introduce as in the preceding section [see Eq. (11)] the solutions y_j and w_j of the Cauchy problem for the finite-difference equation generated by (25). Then the system (24) will transform to the following form [cf. (14)]:

$$y_j w_j=\beta W, \qquad |j|\leqslant N,$$
$$W=y_{j+1}w_j-y_j w_{j+1}$$

Repeating the arguments of the preceding section, we find that

$$z_j=\frac{(1+4\beta^2J_j^2)^{1/2}+(1+4\beta^2J_{j-1}^2)^{1/2}}{2\beta}, \qquad |j|<N$$

$$z_N=\frac{(1+4\beta^2J_{N-1}^2)^{1/2}+1}{2\beta}, \qquad z_{-N}=\frac{(1+4\beta^2J_{-N}^2)^{1/2}+1}{2\beta}$$

Note that earlier the solution of (24) was found for $V=\mathbb{Z}$ and used to calculate the internal energy of the model.[12]

In order to calculate the free energy of the model, let us integrate (22) with respect to the variable x_{-N}. The spherical constant z_{-N+1} will as a result be renormalized:

$$z_{-N+1} \to \tilde{z}_{-N+1} = z_{-N+1} - \frac{J_{-N}^2}{z_{-N}} = \frac{(1+4\beta^2 J_{-N+1}^2)^{1/2}+1}{2\beta}$$

and there will appear the multiplier $\{4\pi/[1+4\beta^2 J_{-N}^2)^{1/2}+1]\}^{1/2}$ before the integral. After having integrated successively with respect to the other variables, we have

$$Z = \prod_{|j| \leqslant N} \left[\frac{4\pi}{(1+4\beta^2 J_j^2)^{1/2}+1}\right]^{1/2}$$

Hence,

$$f = -\frac{\ln 2\pi}{\beta} + \frac{1}{2\beta}\mathbf{M}\left\{\ln \frac{1+(1+4\beta^2 J_0^2)^{1/2}}{2}\right\} - \mathbf{M}\left\{\frac{(1+4\beta^2 J_0^2)^{1/2}}{2\beta}\right\}$$

provided that

$$\mathbf{M}\{(1+4\beta^2 J_0^2)^{1/2}\} < +\infty$$

where $\mathbf{M}\{\cdot\}$ denotes the average over the realizations of J_j. This expression, as would be expected, coincides with the large-n limit of the free energy of the respective Heisenberg model which was directly calculated in Supplement IV of ref. 6.

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