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Absence of long-range order in three-dimensional spherical models

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The spherical model is a unique model for which an exact solution at finite temperature exists in three dimensions (3D). In this paper we prove that this model may show an absence of long-range order (LRO) in 3D if a suitable competition between exchange couplings is assumed. In particular we find an absence of LRO in wedge-shaped regions around the ferromagnet or antiferromagnet-helix transition line or in the vicinity of a degeneration line, where infinite non-equivalent isoenergetic helix configurations are possible. We evaluate explicitly the phase diagram of a tetragonal antiferromagnet with exchange couplings up to third neighbors but our conclusions apply as well to any Bravais lattice. We also discuss the connection of the spherical model or classical Heisenberg Hamiltonian for parameters lying on the degeneration line with more general spin Hamiltonians where the interaction may be written in terms of the adjacency matrix. This seems particularly promising for describing a perturbative approach to the Hubbard Hamiltonian, which is of particular interest in high-T_c superconductivity.

Very few statistical models exist that can be exactly solved, and even less that allow an exact solution in three dimensions (3D). One of these is the spherical model of Berlin and Kac.[1] It was born as an approximation to the Ising model, obtained by relaxing the Ising constraint $S_i=\pm 1$ and replacing it by the *spherical* constraint $\sum_{i=1}^{N} S_i^2=N$. In this way the partition function

$$Z_N(\beta)=\int_{-\infty}^{+\infty}\cdots\int_{-\infty}^{+\infty}\delta\left[N-\sum_i S_i^2\right]\exp(-\beta\mathcal{H})\prod_i dS_i\,, \tag{1}$$

where $\beta=1/k_BT$ and the Hamiltonian $\mathcal{H}$ is

$$\mathcal{H}=-\tfrac{1}{2}\sum_{ij}J_{ij}S_iS_j \tag{2}$$

may be exactly evaluated by replacing the δ function in (1) by its integral representation

$$\delta\left[N-\sum_i S_i^2\right]=\frac{1}{2\pi i}\int_{-i\infty}^{+i\infty}\exp\left[s\left[N-\sum_i S_i^2\right]\right]ds\,.$$

The Gaussian integrations over spin degrees of freedom appearing in (1) can be exactly performed provided that the complex integral over the Lagrangian multiplier s is evaluated on a judiciously chosen path. For a Bravais lattice it turns out[1,2] that the order of integration over S_i and s can be exchanged if

$$\mathcal{R}(s)>\tfrac{1}{2}\beta J_{\max}\,, \tag{3}$$

where $J_{\max}$ is the maximum value of the Fourier transform of the exchange coupling

$$J(\mathbf{k})=\sum_i J_{ij}e^{i\mathbf{k}\cdot(\mathbf{r}_j-\mathbf{r}_i)} \tag{4}$$

and the integration over s can be performed by applying the method of steepest descent. The free energy per spin of the model results in

$$F(\beta,\lambda)=-\frac{1}{\beta}\left[\lambda+\tfrac{1}{2}\ln\pi-\frac{v_c}{2(2\pi)^d}\times\int d^d\mathbf{k}\ln\left[\lambda-\frac{\beta}{2}J(\mathbf{k})\right]\right], \tag{5}$$

where the saddle-point implicit equation for the parameter λ is given by

$$1=\frac{v_c}{2(2\pi)^d}\int d^d\mathbf{k}\frac{1}{\lambda-(\beta/2)J(\mathbf{k})}\,. \tag{6}$$

In Eqs. (5) and (6) v_c is the volume of the d-dimensional lattice unit cell and integration is performed on the first Brillouin zone of the reciprocal lattice. When the saddle point coincides with the branch point of the integrals appearing in (5) and (6)

$$\lambda=\tfrac{1}{2}\beta J_{\max}\,, \tag{7}$$

a phase transition occurs at a critical temperature

$$\frac{1}{k_BT_c}=\frac{v_c}{(2\pi)^d}\int d^d\mathbf{k}\frac{1}{J_{\max}-J(\mathbf{k})}\,. \tag{8}$$

If the integral on the right-hand side of (8) is convergent, one obtains an ordered phase for $T<T_c$ where the saddle point λ in Eq. (5) *sticks* at the value given by Eq. (7). For $T>T_c$ Eq. (6) provides the value of λ to be inserted in Eq. (5) in order to obtain the free energy of the disordered phase. However, if the integral in (8) diverges T_c vanishes and no phase transition occurs.

Our interest in this model comes from a recent rigorous result[3] that establishes the absence of long-range order (LRO) in 3D Heisenberg models on surfaces of the parameter space determined by suitable competition of exchange couplings. The spherical model may be a good example of testing this rigorous result giving explicit equations for that surface which reduces to the ferromagnet-helix (F-H) boundary at vanishing temperature. It is worthwhile noticing that the ground state of the Heisenberg model in the classical limit ($S \to \infty$) is the same as that of the spherical model whose internal energy per spin at $T=0$ is given by

$$U(T=0) = -\tfrac{1}{2} J_{\max} \equiv -\tfrac{1}{2} J(\mathbf{Q}) , \tag{9}$$

where $\mathbf{Q}$ is the wave vector that maximizes $J(\mathbf{k})$. Even more interesting is the fact that in a number of Bravais lattices lines in the zero-temperature parameter space are found where an infinite degeneracy of the ground state of the Heisenberg model is present when the classical limit is taken.

These infinite degeneration lines may be originated by a suitable competition of the exchange couplings as for tetragonal or hexagonal lattices[4,5] or by a frustration related to the lattice structure itself as in a rhombohedral antiferromagnetic (RAF) model[6] where the interaction is limited to nearest neighbors (NN). Tetragonal and hexagonal lattices have been studied with exchange interactions up to third-nearest neighbors (TNN) in the basal plane and NN out of plane in order to assess the existence of long-range order (LRO). The NN in-plane exchange integral was assumed to be ferromagnetic in Ref. 4 and antiferromagnetic in Ref. 5. These models are useful to describe some helimagnets as $NiBr_2$ (Refs. 7 and 8), NiI_2, and CoI_2 (Ref. 9) when $J_1 > 0$ or $RbNiCl_3$, $CsNiCl_3$ (Ref. 10), $TbGa_2$ (Ref. 11), $LiCrS_2$ (Ref. 12), and VI_2 (Ref. 13) when $J_1 < 0$. In all these models an infinite degeneration line appears at $J_2 = 2J_3$, where J_2 and J_3 are the next-nearest neighbor (NNN) and TNN exchange integral, respectively.[14]

In Ref. 6 the frustration is entered by the lattice structure and is present for any $J_1 < 0$ and any coupling between planes $|J'| < |J_1|$. This model seems appropriate to describe the oxygen in its β phase at low temperature.[15]

Even more exciting seems to be the tetragonal lattice with $J_1 < 0$ where the infinite degeneration line seems to be explored by the high-T_c superconductor La_2CuO_4.[16] In this case the Hubbard Hamiltonian maps into a Heisenberg Hamiltonian with $J_1 < 0$ and $J_2 = 2J_3$.

The rigorous theorem proved in Ref. 3 was not able to establish that LRO is absent on surfaces that reduce to these infinite degeneration lines for vanishing temperatures even if simple spin wave theory supports this conjecture. This important question may be answered, on the contrary, evaluating exactly the critical temperature of the spherical model in the vicinity of the infinite degeneration lines. We anticipate the interesting result that wedge-shaped regions of absence of LRO appear in vicinity of these infinite degeneration lines as well as in the vicinity of the F-H or AF-H phase boundary.

As an example let us take a spherical model on a tetragonal lattice with NN $J_1 < 0$, NNN J_2, TNN J_3 in-plane, and NN J' out-of-plane exchange couplings.

The ground state of this model, which is the same as the corresponding classical Heisenberg model, is shown in Fig. 1 where AF, AF_1, H_1, and H_2 mean the usual antiferromagnet with $\mathbf{Q} = (\pi, \pi)$, a configuration where ferromagnetic lines of spins alternate antiferromagnetically characterized by $\mathbf{Q} = (\pi, 0)$, and two helix phases characterized by wave vectors $\mathbf{Q} = \{\pi, \cos^{-1}[-(1-2j_2)/4j_3]\}$

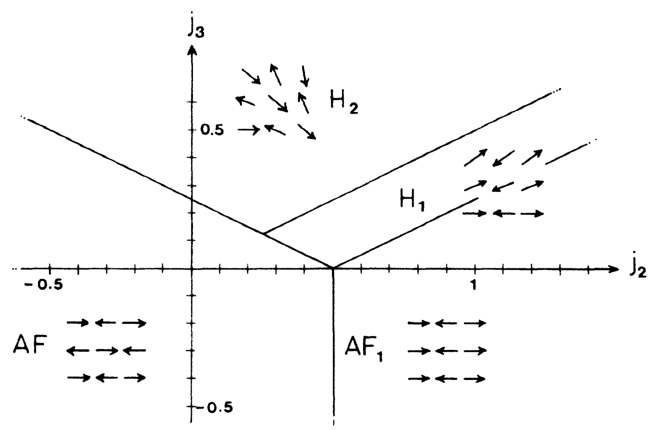

FIG. 1. Phase diagram at zero temperature of the spherical or classical Heisenberg model on a tetragonal lattice with $J_1 < 0$: AF, AF_1, H_1, H_2 mean usual antiferromagnetic phase, antiferromagnetic stacking of ferromagnetic lines, and two helical phases ($j_a \equiv J_a/J_1$).

and

$$\mathbf{Q} = \{\cos^{-1}[-1/(2j_2+4j_3)], \cos^{-1}[-1/(2j_2+4j_3)]\} ,$$

respectively. The lattice constant is assumed to be unity. The reduced exchange couplings are defined as $j_a = J_a/J_1$. The sign of J' simply determines the order along the c axis. The stacking of planes is ferromagnetic or antiferromagnetic depending on whether J' is positive or negative.

The line between the AF and H_1, H_2 phases (AF-H line) is

$$1 - 2j_2 - 4j_3 = 0, \quad j_2 < \tfrac{1}{2} . \tag{10}$$

The line between the H_1 and H_2 phases of equation

$$j_2 = 2j_3, \quad j_3 > \tfrac{1}{8} \tag{11}$$

is an infinite degeneration line where all helix wave vectors satisfying the equation

$$\cos Q_x + \cos Q_y = -\frac{1}{4j_3} \tag{12}$$

minimize the ground-state energy. The boundary line between AF_1 and H_1 phases is $1 - 2j_2 + 4j_3 = 0$, $j_2 > \frac{1}{2}$, while the one between AF and AF_1 phases is $j_2 = \frac{1}{2}$, $j_3 < 0$.

The critical temperature of the spherical model is given by Eq. (8) where the integration over k_z can be easily performed leading to the equation

$$\frac{4|J_1|}{k_B T_c} = \frac{1}{\pi^2} \int_0^{\pi} \int_0^{\pi} dk_x dk_y \frac{1}{\{a(\mathbf{k})[a(\mathbf{k}) + |j'|]\}^{1/2}} , \tag{13}$$

where

$$a(\mathbf{k}) = \gamma(\mathbf{k}) - \gamma(\mathbf{Q}), \quad j' = J'/J_1 \tag{14}$$

and

$$\gamma(\mathbf{k}) = \tfrac{1}{2}(\cos k_x + \cos k_y) + j_2 \cos k_x \cos k_y + j_3(\cos^2 k_x + \cos^2 k_y - 1) . \tag{15}$$

In Eq. (14), $\gamma(\mathbf{Q})$ is the maximum of $\gamma(\mathbf{k})$.

In order to find where the integral in (13) diverges, it is convenient to expand $a(\mathbf{k})$ around $\mathbf{k}=\mathbf{Q}$. Indeed the main (possibly divergent) contribution to the integral comes from that region. The result is

$$a(\mathbf{q})=Aq_x^2+Bq_y^2+Cq_xq_y\,, \tag{16}$$

where

$$A=-\tfrac{1}{4}\,[\cos Q_x+2j_2\cos Q_x\cos Q_y+4j_3(2\cos^2 Q_x-1)]\,,$$

$$B=-\tfrac{1}{4}\,[\cos Q_y+2j_2\cos Q_x\cos Q_y+4j_3(2\cos^2 Q_y-1)]\,,$$

$$C=j_2\sin Q_x\sin Q_y\,,$$

and $\mathbf{q}=\mathbf{k}-\mathbf{Q}$. The right-hand side of (13) diverges if $A=B=C=0$. This condition is verified on the line AF-H. Indeed in the AF phase one has

$$A=B=\tfrac{1}{4}(1-2j_2-4j_3),\quad C=0\,, \tag{17}$$

so that A and B vanish approaching the AF-H line (10) and T_c decreases logarithmically to zero as this line is approached from the AF phase. The same behavior is found approaching the AF-H line from the H_1 or H_2 phase where one has

$$A=\frac{(j_2-2j_3)(4j_3+2j_2-1)}{8j_3},\quad B=\frac{(4j_3-2j_2+1)(4j_3+2j_2-1)}{16j_3},\quad C=0 \tag{18}$$

or

$$A=B=\frac{j_3(4j_3+2j_2-1)(4j_3+2j_2+1)}{4(j_2+2j_3)^2},\quad C=\frac{j_2(4j_3+2j_2-1)(4j_3+2j_2+1)}{4(j_2+2j_3)^2}\,, \tag{19}$$

respectively. On the contrary, the critical temperature remains finite on the AF-AF_1 and AF_1-H_1 lines. On line (11) between the H_1 and H_2 phases the divergence of the integral appearing in (13) is due to the *degenerate helix* (12) which enters a *whole line* of zeros in the denominator of (13). On this line Eq. (16) becomes

$$a(\mathbf{q})=j_3(\sin Q_xq_x+\sin Q_yq_y)^2\,.$$

The divergence is easily seen replacing the integration variables q_x,q_y by the variables $q_\parallel$, $q_\perp$ defined as

$$q_\parallel=\sin Q_xq_x+\sin Q_yq_y\,,$$

$$q_\perp=-\sin Q_yq_x+\sin Q_xq_y\,,$$

which are the abscissa along the curve (12) and its perpendicular direction, respectively. With this choice the main contribution to the integral in Eq. (13) becomes

$$\frac{4|J_1|}{k_BT_c}\sim\frac{1}{(|j'|j_3)^{1/2}(\sin^2 Q_x+\sin^2 Q_y)}\times\int\int dq_\parallel dq_\perp\frac{1}{|q_\parallel|}\,, \tag{20}$$

which diverges logarithmically for $q_\parallel\to 0$ when integration over $q_\parallel$ is performed. The phase diagram at finite temperature of the spherical model is given in Fig. 2 for $|j'|=1$. As one can see a wedge-shaped region where LRO is absent in 3D onsets in the vicinity of the AF-H and H_1-H_2 lines.

The *degenerate helix* appearing on the line $J_2=2J_3$ may look like an exotic phase never to show up in any real system, since it is unstable both to the addition of some fourth-neighbor coupling[17] and with respect to quantum fluctuations.[14] However, a number of works has appeared which treated the Heisenberg-spin Hamiltonian on the square lattice with NNN and TNN just in the above proportion, as an approximation of the single-band Hubbard model with doping.[16]

In fact, the hole motion induces a superexchange coupling with spins which are NNN in the hopping sense, i.e., which are connected to the spin in the origin by a path two steps long; these are NNN and TNN in the Euclidean metric sense, and it is readily seen that the diagonal NNN are counted twice, since it is possible to reach them along two distinct paths.

Let us now make the following remark: If we assume the same interaction between spins on sites connected by the same number of steps, it is possible to write any spin-quadratic Hamiltonian in the form

$$\mathcal{H}=-\tfrac{1}{2}\sum_{ij}\mathbf{S}_i\underline{J}_{ij}\mathbf{S}_j\,, \tag{21}$$

where $\underline{J}$ is a polynomial in the adjacency matrix $\underline{A}$ of the lattice ($\underline{A}_{ij}$ is one if i and j are NN, and zero otherwise). This happens because the matrix element $(\underline{A}^n)_{ij}$ of the nth power of $\underline{A}$ is the number of n-step paths connecting i and j.[18]

This in turn implies that it is always possible to find a

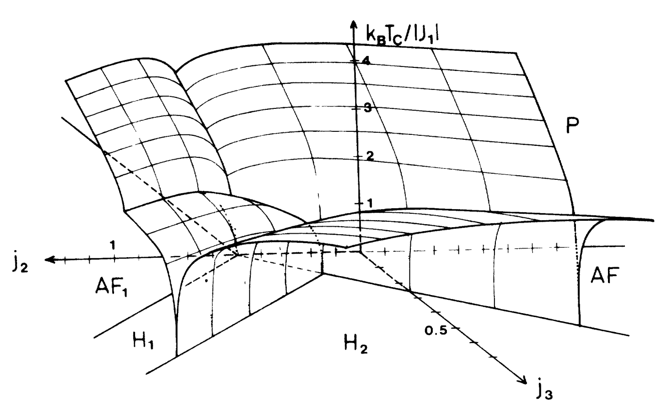

FIG. 2. Phase diagram of the spherical model at finite temperature for $j'=1$. Symbols have the same meaning as in Fig. 1. P means paramagentic phase. Notice the wedge-shaped regions of absence of LRO springing from the AF-H and H_1-H_2 phase boundaries.

combination of the coefficients in the matrix polynomial $\underline{J}$ such as to give an infinite degeneration in the classical ground state.

To show how this works, consider a classical spin model on the square lattice with NN and NNN couplings J^{I} and J^{II}, respectively; NNN are to be understood in the hopping sense. Then the Hamiltonian is

$$\mathcal{H} = -\sum_{ij} \mathbf{S}_i (J^{\mathrm{I}}\underline{A} + J^{\mathrm{II}}\underline{A}^2 - 4J^{\mathrm{II}}\underline{1})_{ij}\mathbf{S}_j \, . \tag{22}$$

Calling J_p and a_p the eigenvalues of $\underline{J} \equiv J^{\mathrm{I}}\underline{A} + J^{\mathrm{II}}\underline{A}^2 - 4J^{\mathrm{II}}\underline{1}$ and $\underline{A}$, respectively, the ground-state energy is obtained by maximizing the J_p's as functions of p. It can be readily seen[19] that the $p - J_p$ relationship is many to one when $(J^{\mathrm{II}}/J^{\mathrm{I}}) > \frac{1}{8}$, since then the maximum J_p is given by

$$J_p^{\max} = J^{\mathrm{I}} a_p^{\max} + J^{\mathrm{II}}(a_p^{\max})^2 - 4J^{\mathrm{II}} \, , \tag{23}$$

where

$$a_p^{\max} = -\frac{J^{\mathrm{I}}}{2J^{\mathrm{II}}} \, . \tag{24}$$

The last equation reads, for the square lattice $p \equiv (k_x, k_y)$,

$$\cos k_x + \cos k_y = -\frac{J^{\mathrm{I}}}{4J^{\mathrm{II}}} \, , \tag{25}$$

which has to be compared with Eq. (12), keeping in mind that J^{II} corresponds exactly to J_3. This substanciates our claim that an infinite degeneration in the ground state, of the same kind as the *degenerate helix* we have just discussed, naturally appears for the appropriate values of the exchange integrals, as soon as one considers neighborhood in terms of hopping (i.e., graph-theoretic distance) instead of Euclidean distance. This fact enables us to foresee how the infinite degeneration lines are affected by farther neighbor interactions. For instance, if one takes the three-step neighbors into account a new infinite degeneration line has to be expected for $J_2 = 2J_3$, $J_4 = 6J_6$, where J_4 and J_6 are the fourth and sixth nearest-neighbor exchange couplings, respectively.

This *persistence* of the infinite degeneration line for farther interactions could be particularly interesting in view of an application to the high-T_c superconductors. In fact, recently it has been proved[16] that the Hubbard Hamiltonian maps into a Heisenberg Hamiltonian with $J_1 < 0$ and $J_2 = 2J_3$ if the hopping is limited to second order (two steps). This map onto the infinite degeneration line could be more general since higher-order perturbation theory (more steps) should enter further neighbor interactions but always remaining on these infinite degeneration lines.

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