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J_1–J_2–J_3 MODEL WITH LONG-RANGE LIEB–MATTIS INTERACTION

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Stimulated by the two-dimensional frustrated Heisenberg antiferromagnet with first-, second-, and third-neighbor couplings (J_1–J_2–J_3 model) we consider a corresponding three-parameter model with a long-range antiferromagnetic Lieb–Mattis interaction. This model can be solved exactly and leads to a better understanding of the role of frustration in the J_1–J_2–J_3 model. We calculate the correlations in the groundstate and consider their finite size behavior. Furthermore we present the full thermodynamic phase diagram. We find the possibility of a disordered phase at $T = 0$.

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1. Introduction

The discovery of high-temperature superconductivity renewed an interest in the study of quantum fluctuations in two-dimensional quantum antiferromagnets. How the antiferromagnetic order of high-T_c compounds is destabilized by doping is an important problem in the theoretical understanding of high-T_c superconductivity. One simple approach [1] simulating the effects of holes in lightly doped CuO_2 planes can be done by an effective two-dimensional spin-1/2 Heisenberg antiferromagnet on a square lattice with frustrating interactions, eg. the J_1–J_2–J_3 model [2–4]

$$\widehat{H}_{J_1-J_2-J_3} = J_1 \sum_{i,\delta_1} s_i s_{i+\delta_1} + J_2 \sum_{i,\delta_2} s_i s_{i+\delta_2} + J_3 \sum_{i,\delta_3} s_i s_{i+\delta_3}, \; J_1, J_2, J_3 > 0. \qquad (1)$$

Here J_1 is the interaction between nearest neighbors and J_2 and J_3 measure the frustration strength between a given spin and its second and third neighbors, respectively. Additionally, this model (1) is interesting per se as a model of a helimagnet, where the frustration [5] can produce a spiral phase in some region of parameter space.

2. Model

The J_1–J_2–J_3 model (1) can only be dealt with approximate methods, therefore we introduce a corresponding three-parameter model with the long-range Lieb–Mattis interaction [6], which is exactly solvable. To do this we separate the whole lattice in two sublattices A and B, which both are split in two further subsystems A_γ and B_γ ($\gamma = 1, 2$), respectively. As a simplification of (1) we set the interaction between every spin from A and every spin from B equal to J_1, between every spin from $A(B)_1$ and $A(B)_2$ equal to J_2 and between every spin within the four subsystems $A(B)_\gamma$ equal to J_3. We get corresponding to (1) a Lieb–Mattis model

$$\widehat{H} = \frac{8J_1}{N}\boldsymbol{S}_A\boldsymbol{S}_B + \frac{16J_2}{N}\left[\boldsymbol{S}_{A_1}\boldsymbol{S}_{A_2} + \boldsymbol{S}_{B_1}\boldsymbol{S}_{B_2}\right]$$

$$+\frac{8J_3}{N}\left[\sum_{\substack{i,j\in A_1\\ i\neq j}} \boldsymbol{s}_i\boldsymbol{s}_j + \sum_{\substack{i,j\in A_2\\ i\neq j}} \boldsymbol{s}_i\boldsymbol{s}_j + \sum_{\substack{i,j\in B_1\\ i\neq j}} \boldsymbol{s}_i\boldsymbol{s}_j + \sum_{\substack{i,j\in B_2\\ i\neq j}} \boldsymbol{s}_i\boldsymbol{s}_j\right]. \qquad (2)$$

The scaling factors cause the total strength of the J_i interaction in (2) to be the same as in the J_1–J_2–J_3 model. We use

$$\boldsymbol{S}_{A(B)_\gamma} = \sum_{i\in A(B)_\gamma} \boldsymbol{s}_i, \quad \boldsymbol{S}_{A(B)} = \sum_{i\in A(B)} \boldsymbol{s}_i = \boldsymbol{S}_{A(B)_1} + \boldsymbol{S}_{A(B)_2}, \qquad (3)$$

being the total-spin operator of the subsystems $A(B)_\gamma$ and the subsystem A, B, respectively, and N — the total number of spins ($s = 1/2$) of the system. This model can be solved exactly including the full thermodynamics. The operators $\boldsymbol{S}^2 = (\boldsymbol{S}_A + \boldsymbol{S}_B)^2$, $\boldsymbol{S}_A^2$, $\boldsymbol{S}_B^2$, $\boldsymbol{S}_{A_\gamma}^2$, $\boldsymbol{S}_{B_\gamma}^2$ and $\widehat{H}$ all commute with each other. The eigenvalues of (2) are

$$E = \frac{4}{N}\Big\{-2(J_2 - J_3)[S_{A_1}(S_{A_1}+1) + S_{A_2}(S_{A_2}+1) + S_{B_1}(S_{B_1}+1)$$

$$+S_{B_2}(S_{B_2}+1)] - (J_1 - 2J_2)[S_A(S_A+1) + S_B(S_B+1)] + J_1 S(S+1)\Big\} - 6J_3, \qquad (4)$$

where S, $S_{A(B)}$ and $S_{A(B)_\gamma}$ denote the quantum numbers of $\boldsymbol{S}^2$, $\boldsymbol{S}_{A(B)}^2$ and $\boldsymbol{S}_{A(B)_\gamma}^2$, respectively, with $S \in [|S_A - S_B|, S_A + S_B]$, $S_{A(B)} \in [|S_{A(B)_\gamma} - S_{A(B)_\gamma}|, S_{A(B)_\gamma} + S_{A(B)_\gamma}]$ and $S_{A(B)_\gamma} \in [0, N/8]$.

3. Ground state

A minimization of (4) with respect to the conditions for the quantum numbers allows us to determine a ground state phase diagram, which we present in Fig. 1a. We find $S = 0$ and due to the symmetry $S_A = S_B$ and $S_{A_1} = S_{A_2} = S_{B_1} = S_{B_2}$ in all phases. In order to characterize the different phases we introduce the staggered magnetization of the whole system ($\langle m_s^2\rangle$) and of the two subsets A and B ($\langle m_{s,A(B)}^2\rangle$)

$$\langle m_s^2\rangle = \frac{1}{N^2}\sum_{i,j=1}^{N}(-1)^{i+j}\langle \boldsymbol{s}_i\boldsymbol{s}_j\rangle, \quad \langle m_{s,A(B)}^2\rangle = \frac{4}{N^2}\sum_{i,j\in A(B)}(-1)^{i+j}\langle \boldsymbol{s}_i\boldsymbol{s}_j\rangle. \quad (5)$$

We have then $\langle m_s^2 \rangle > (=)0$ and $\langle m_{s,A(B)}^2 \rangle = (>)0$ in the Néel (collinear) phase. In the so-called paramagnetic phase both staggered magnetizations are zero. In addition we introduce correlation functions $\langle s_i s_j \rangle_{A,B}$ and $\langle s_i s_j \rangle_{A_1,A_2}$, which describe the correlation between spins from A and B and from A_1 and A_2, respectively. These definitions correspond to the correlations between nearest and second neighbors in the J_1–J_2–J_3 model. $\langle s_i s_j \rangle_{A_1}$ describes the correlation between spins within A_1 (corresponds to the third neighbor correlation). In Table we give the correlations and magnetizations at $T = 0$ and their finite size behavior. Notice that along the phase transition of the first order (i.e. at $J_2 = J_1/2$) $\langle s_i s_j \rangle_{A,B}$ and $\langle s_i s_j \rangle_{A_1,A_2}$ are equal, which indicates a canted phase.

TABLE

Zero temperature correlations and staggered magnetizations of (2) for arbitrary N for different phases and along the phase transition of the first order (at $J_2 = \frac{1}{2}J_1$) between the Néel and the collinear phase and at the tricritical point.

Phase	$\langle s_i s_j \rangle_{A,B}$	$\langle s_i s_j \rangle_{A_1,A_2}$	$\langle s_i s_j \rangle_{A_1}$	$\langle m_s^2 \rangle$	$\langle m_{s,A}^2 \rangle$
Néel	$-\left(\frac{1}{N}+\frac{1}{4}\right)$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}+\frac{1}{N}$	$\frac{1}{N}$
collinear	0	$-\left(\frac{2}{N}+\frac{1}{4}\right)$	$\frac{1}{4}$	0	$\frac{1}{4}+\frac{2}{N}$
paramagnet	0	0	$-\frac{3}{N-4}$	0	0
at $J_2 = \frac{1}{2}J_1$					
and $J_3 < J_2$	$-\left(\frac{1}{12}+\frac{2}{3N}\right)$	$-\left(\frac{1}{12}+\frac{2}{3N}\right)$	$\frac{1}{4}$	$\frac{1}{12}+\frac{2}{3N}$	$\frac{1}{6}+\frac{4}{3N}$
and $J_3 = J_2$	$-\frac{0.76}{N}$	$-\frac{0.76}{N}$	$-\frac{0.72}{N-4}$	$\frac{0.76}{N}$	$\frac{1.52}{N}$

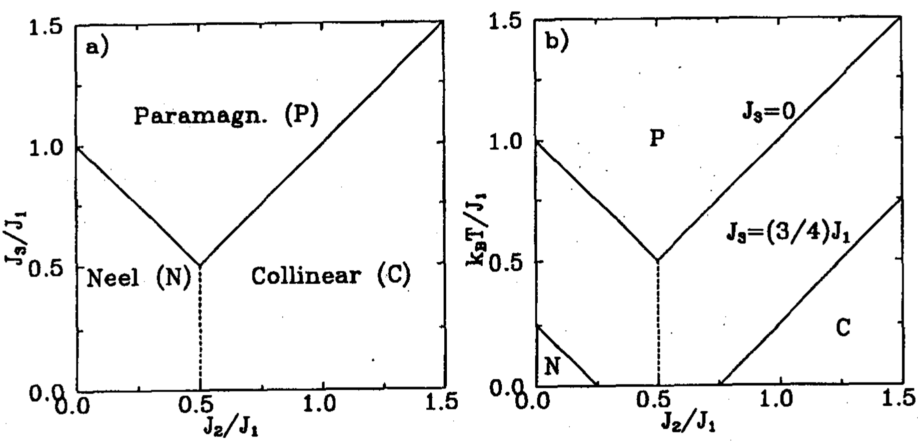

Fig. 1. Ground state (a) and full thermodynamic (b) phase diagram of (2) in the thermodynamic limit. The dashed/full lines denote phase transitions of first/second order. The phases are labelled with respect to the structure of the corresponding J_1–J_2–J_3 model.

4. Thermodynamics

For the Lieb–Mattis model the saddle-point approximation becomes exact, i.e. the partition function is given in the thermodynamic limit ($N \to \infty$) by its largest term [7]. Due to the symmetry in the thermodynamic limit we can define the normalized quantum numbers $\alpha \equiv (8/N)S_{A(B)_\gamma}$ (with $\alpha \in [0,1]$) and $\delta \equiv (4/N)S_{A(B)}$ (with $\delta \in [0, \alpha]$). We have to distinguish two cases and find

$$\delta = \begin{cases} \alpha & \text{at } J_2 < J_1/2, \text{ with } \alpha = \tanh\left[\alpha(J_1 - J_2 - J_3)/(k_\mathrm{B}T)\right] \\ 0 & \text{at } J_2 > J_1/2, \text{ with } \alpha = \tanh\left[\alpha(J_2 - J_3)/(k_\mathrm{B}T)\right] \end{cases} . \tag{6}$$

In Fig. 1b we present the thermodynamic phase diagram. Notice that J_3 has the same effect as the temperature, i.e. $k_\mathrm{B}T|_{J_3=0} = k_\mathrm{B}T + J_3$. The paramagnetic phase at $T = 0$ is characterized by the high degeneracy.

5. Summary

We have presented several exact results for a frustrated Lieb–Mattis model, which is related to the J_1–J_2–J_3 model on a square lattice (1). Varying the strength of the interactions we get a Néel, a collinear and a high degenerate paramagnetic disordered phase at $T = 0$. We found that in this model the frustration by J_3 has the same effect as thermal fluctuations.

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