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Néel Order in the Ground State of Spin-1/2 Heisenberg Antiferromagnetic Multilayer Systems

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We show existence of Néel order for the ground state of a system with M two-dimensional layers with spin 1/2 and Heisenberg antiferromagnetic coupling, provided $M \geqslant 8$. The method uses the infrared bounds for the ground state combined with ideas introduced by Kennedy, Lieb, and Shastry.

KEY WORDS: Heisenberg antiferromagnet; multilayer systems; Néel order; ground state; infrared bounds; dimensional interpolation.

1. INTRODUCTION

The existence of Néel order in the ground state of two-dimensional spin-1/2 Heisenberg antiferromagnets remains an open problem.[1] For spin $S \geqslant 1$, Jordão Neves and Perez[2] adapted the techniques of Dyson *et al.*[4] to show long range order (LRO) in the ground state (actually, due to a numerical oversight corrected in ref. 3, the result was claimed to be valid only for $S \geqslant 3/2$). Nevertheless, the method is not sharp enough to obtain order for the $S = 1/2$ case even for the ground state of the three-dimensional model.[5] Later, Kennedy *et al.*[1] improved these techniques to show Néel order for $S > 1/2$ and $d \geqslant 3$.

In this note we consider the ground state of a system composed of an even number M of two-dimensional layers with $S \geqslant 1/2$. Each layer is an infinite two-dimensional square lattice, so that the finite-volume Hamiltonian is given by

$$\mathscr{H}_{M,N} = \sum_{x \in \Lambda} \sum_{i=1}^{3} \mathbf{S}_x \cdot \mathbf{S}_{x+1_i}$$

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where $\Lambda = \{1,..., N\}^2 \times \{1,..., M\}$, N is even, and $\mathbf{1}_i$ is the unit vector in the i direction. We are interested in the thermodynamic limit $N \to \infty$ with fixed M. For $M = 1$ we would have the two-dimensional model and in the limit $M \to \infty$ we obtain the $d = 3$ system, so that our Hamiltonian interpolates between two and three dimensions.

We shall take periodic boundary conditions in all directions. The model with open boundary conditions in the third direction, the relevant one when dealing with real systems of layers, cannot be controlled with our methods, since the use of periodic boundary conditions is essential to the derivation of the crucial infrared bound. On intuitive grounds one would expect to need a greater number of layers for Néel order to appear.

We show the existence of Néel order provided $M \geqslant 8$ for $S = 1/2$.

It should be stressed that the Mermin–Wagner argument applies to the system under consideration, so that Néel order is absent for any positive temperature. This is in contrast to the three-dimensional model proposed and discussed in ref. 1, where the coupling constant in the third dimension was affected by a factor r, with $0 \leqslant r \leqslant 1$, thus simulating an interpolation between the two- and three-dimensional models ($r = 0, 1$, corresponding respectively, to two and three dimensions). For the latter model Néel order was shown to hold both for the ground state and sufficiently low temperatures, if $r \geqslant 0.16$.

2. THE TECHNIQUE

Our proof is carried out along the same lines as in Ref. 1. After defining

$$S_q = \frac{1}{|\Lambda|^{1/2}} \sum_{x \in \Lambda} S_x^3 \exp\{-iqx\}$$

and $g_q = \langle S_{-q} S_q \rangle$, where by $\langle \cdot \rangle$ we mean the expectation value in the ground state, we have the sum rule

$$I \equiv \frac{1}{M} \sum_{q_3 \in B_M} \frac{1}{(2\pi)^2} \int g_q \, d^2 q = \frac{S(S+1)}{3} \tag{2.1}$$

Here the summation on q_3 is taken over $B_M = \{(2\pi/M)\, k, k = 1, 2,..., M\}$. We also have the infrared bound[2]

$$0 \leqslant g_q \leqslant f_q = \left(\frac{\langle [[S_q, \mathscr{H}_M], S_{-q}] \rangle}{4E_{q-Q}} \right)^{1/2} \tag{2.2}$$

where

$$E_q = \sum_{i=1}^{3} (1 - \cos q_i) \tag{2.3}$$

and Q is the point (π, π, π).

Under the assumption of absence of LRO we have the following formula:

$$\frac{1}{M} \sum_{q_3 \in B_M} \frac{1}{(2\pi)^2} \int g_q(\cos q_1 + \cos q_2 + \cos q_3)\, d^2q = -\frac{e_0}{3} \tag{2.4}$$

where $-e_0$ is the ground-state energy per site of the system.

We then maximize the integral I over all functions g_q satisfying both the infrared bound (2.2) and the constraint (2.4). If $I_{\max}$, the maximum value so obtained, is less than $S(S+1)/3$, we have a contradiction, implying the existence of LRO.

3. THE RESULTS

The expectation value of the double commutator in (2.2) can be calculated explicitly and equals

$$\tfrac{2}{3}[(2 - \cos q_1 - \cos q_2)\,\rho_1 + (1 - \cos q_3)\,\rho_3]$$

where

$$\rho_1 = -\langle \mathbf{S}_x \cdot \mathbf{S}_{x+l_1} \rangle \qquad \text{and} \qquad \rho_3 = -\langle \mathbf{S}_x \cdot \mathbf{S}_{x+l_3} \rangle$$

It should first be remarked that ρ_1 and ρ_3 are nonnegative. This result is a Griffith inequality of the first type for the system. Its proof can be reduced to the proof given by Ginibre[6] of a class of such inequalities for quantum ferromagnetic spin systems. This is achieved by performing a rotation on the system by an angle π around the third spin direction, on the even sublattice. This transforms the Hamiltonian of the system into

$$\mathscr{H}'_{M,N} = \sum_{x \in A} \sum_{i=1}^{3} (-S_x^1 \cdot S_{x+l_i}^1 - S_x^2 \cdot S_{x+l_i}^2 + S_x^3 \cdot S_{x+l_i}^3)$$

The method used in the proof of the Corollary of Theorem 5, p. 110, of ref. 6 applies to the expectation values in the ground state of the modified system (as the sign of the coupling in the third direction is irrelevant), so that for any pair of sites x and y

$$\langle S_x^1 S_y^1 + S_x^2 S_y^2 \rangle' \geq 0$$

Remark. Actually Ginibre's proof is given for a positive-temperature state, but the inequality clearly survives the limit $\beta \to \infty$.

Undoing the transformation, we obtain for the original system and for any pair of nearest neighbor sites x and y

$$\langle S_x^1 S_y^1 + S_x^2 S_y^2 \rangle \leq 0$$

Using the isotropy in the spin variable, we finally get, for any pair of nearest neighbor sites x and y

$$\langle \mathbf{S}_x \cdot \mathbf{S}_y \rangle = \langle S_x^1 S_y^1 + S_x^2 S_y^2 + S_x^3 S_y^3 \rangle \leq 0$$

At this point our method departs from the one used in ref. 1, as we have not been able to estimate ρ_1 and ρ_3 in terms of the ground state energy density e_0. So we consider separately two situations: (1) $\rho_1 \leq e_0/4, \rho_3 \leq e_0$; and (2) $\rho_1 \leq e_0/2, \rho_3 \leq e_0/2$. One of these two cases always holds, since $e_0 = 2\rho_1 + \rho_3$, $\rho_1 \geq 0$, and $\rho_3 \geq 0$. We shall compute I_{max} for each case. The conclusion follows if we get $I_{max} < S(S+1)/3$ in both cases.

As in ref. 1, the maximum of I for all g_q subject to (2.2) is attained by

$$g_q = f_q \chi(\cos q_1 + \cos q_2 + \cos q_3 < \alpha)$$

where α is a positive constant and $\chi(\cdot) = 1$ when condition $(\cdot)$ is true and zero otherwise. We perform a numerical calculation in order to determine the value of α so that the constraint (2.4) is satisfied. A lower bound for e_0 can be obtained by using the Néel state as a variational trial ground state. For our system it is given by $e_0 \geq e_0^{(N)} = 0.75$. Replacing e_0 by $e_0^{(N)}$, we compute the value of $\alpha^{(N)}$ for $M = 8$:

Case 1. $\alpha_1^{(N)} = 0.71160$.

Case 2. $\alpha_1^{(N)} = 0.72056$.

For both of these values the integral I_{max} is calculated and shown to be less than $S(S+1)/3$:

Case 1. $\alpha_{max,1}^{(N)} = 0.24388$.

Case 2. $\alpha_{max,2}^{(N)} = 0.24650$.

By monotonicity we have that $I_{\max,1} \leqslant I^{(N)}_{\max,1}$ and $I_{\max,2} \leqslant I^{(N)}_{\max,2}$, implying $I_{\max} < S(S+1)/3$, which concludes the proof.

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