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Existence of Néel Order in Some Spin-1/2 Heisenberg Antiferromagnets

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The methods of Dyson, Lieb, and Simon are extended to prove the existence of Néel order in the ground state of the 3D spin-1/2 Heisenberg antiferromagnet on the cubic lattice. We also consider the spin-1/2 antiferromagnet on the cubic lattice with the coupling in one of the three lattice directions taken to be r times its value in the other two lattice directions. We prove the existence of Néel order for $0.16 \leqslant r \leqslant 1$. For the 2D spin-1/2 model we give a series of inequalities which involve the two-point function only at short distances and each of which would by itself imply Néel order.

KEY WORDS: Néel order; spin-1/2 antiferromagnets; infrared bounds; Gaussian domination.

The existence or absence of Néel order in various spin-1/2 Heisenberg antiferromagnets is still unresolved after 50 years of study. Interest in this question has been revived recently in the context of certain models proposed for high-T_c superconductors. In particular Anderson[(2)] suggested that the "resonating valence bond" (RVB) state, a state with strong antiferromagnetic correlations but without Néel order, is relevant in this context. There has been considerable subsequent debate on whether the 2D spin-1/2 Heisenberg antiferromagnet on the square lattice possesses Néel order. Recent numerical work of Liang *et al.*[(11)] shows that the energy of the RVB state is very close to the energy of Néel-like states, but other recent numerical work of Reger and Young[(13)] and Gross *et al.*[(7)] suggests the existence of Néel order. In view of the delicate nature of the question, it is important to review the rigorous results on the existence of Néel order

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for quantum antiferromagnets and to extend them to the case of spin 1/2 in two and three dimensions.

The rigorous results on the existence of Néel order in quantum Heisenberg antiferromagnets are all based on the work of Dyson *et al.*,[3] who proved that there is Néel order at low temperatures if the spin is at least 1 and if the dimension is three or more, and for spin 1/2 if the dimension is sufficiently large. This work extended the results of Fröhlich *et al.*[5] for the classical Heisenberg model. In two dimensions the Mermin–Wagner–Hohenberg theorem states that there is no Néel order at low but nonzero temperatures, but the question of whether or not there is Néel order in the ground state is nontrivial. Jordaõ-Neves and Fernando-Perez[10] observed that the methods of Dyson *et al.* can be applied to the ground state in two dimensions. These methods show that the ground state of the two-dimensional Heisenberg antiferromagnet has Néel order if the spin is at least 1. (Because of a numerical error, they asserted the result only for spin greater than 1; this numerical oversight was corrected in ref. 1.) Two of the most interesting cases from the physical point of view, spin 1/2 in two and three dimensions, have thus far eluded rigorous results.

In this paper we show that a simple extension of the above methods proves the existence of Néel order for the case of spin 1/2 in three dimensions. We also consider a spin-1/2 model which interpolates between two and three dimensions. This model is the three-dimensional cubic lattice with the coupling constant in two of the three lattice directions taken to be 1, but in the third lattice direction it is taken to be r. When $r=0$ we recover the case of two dimensions, while $r=1$ yields three dimensions. For this model we prove that there is Néel order if $1 \geqslant r \geqslant 0.16$. (Although we only consider the ground states of these models, the techniques we use may be combined with the techniques of Dyson *et al.* for nonzero temperatures to prove the existence of a phase transition for $1 \geqslant r \geqslant 0.16$.) The case of spin 1/2 in two dimensions remains an open problem. Recently Gross *et al.*[7] have performed a quantum Monte Carlo simulation that shows that there is Néel order in the two-dimensional model. Of course one can argue that the two-point function does in fact decay to zero, but this decay is too slow to be seen in their simulation. We give a series of inequalities which involve the two-point function only at short distances, each of which by itself would imply Néel order.

This paper consists of two parts. In the first part we recall the basic inequality and strategy from ref. 3. We then show how to extend these methods to the case of spin 1/2 in three dimensions and to the model that interpolates between two and three dimensions. The second part of the paper provides a simple proof—directly adapted to the ground state—of the key inequality from ref. 3. This proof is included for the convenience of the reader. It can be skipped on a first reading of the paper.

To review the methods of Dyson *et al.* we consider a finite lattice Λ with an even number of sites in every direction and periodic boundary conditions. We define the Fourier transform of S_x^3,

$$S_q = |\Lambda|^{-1/2} \sum_{x \in \Lambda} e^{-iq \cdot x} S_x^3$$

Here q is in the reciprocal lattice. The Fourier transform of the two-point function in the ground state is then

$$g_q = \langle S_{-q} S_q \rangle \geqslant 0$$

where $\langle \cdot \rangle$ denotes expectation in the ground state. Note that the ground state is unique for the antiferromagnet.[12] Dyson *et al.* proved a pointwise upper bound on the analog of this function for nonzero temperatures. Their bound holds for all values of q except Q. By Q we denote either (π, π) or (π, π, π), depending on whether we are considering two or three dimensions. The zero-temperature limit of their inequality (as derived in ref. 10) in dimension d is

$$g_q \leqslant f_q, \qquad q \neq Q \tag{1}$$

where $f_q = (e_0 E_q / 6d E_{q-Q})^{1/2}$, $E_q = \sum_{i=1}^{d} (1 - \cos q_i)$, and $-e_0$ is the ground-state energy per site. Note that f_q depends on the spin S only through the dependence of e_0 on S. Inequality (1) is called an infrared bound, and a direct proof of it will be given later in this paper.

For an antiferromagnet the existence of Néel order corresponds to g_q containing a δ function at Q in the infinite-volume limit. Let m^2 be the coefficient of this delta function. If we integrate g_q (in the infinite-volume limit) over the Brillouin zone, we obtain the value of the two-point function at zero separation. The bound (1) then implies

$$m^2 + \int d^d q \, f_q \geqslant \int d^d q \, g_q = S(S+1)/3 \tag{2}$$

where

$$\int d^d q = (2\pi)^{-d} \int_0^{2\pi} dq_1 \cdots \int_0^{2\pi} dq_d$$

A simple argument by Anderson (reproduced in Appendix C of ref. 3) shows that $e_0 \leqslant S(dS + \frac{1}{2})$. Thus, inequality (2) forces m^2 to be nonzero if S

is large enough. Numerical evaluation of the resulting integrals shows that in both two and three dimensions $S=1$ is large enough.

To extend these methods, we make use of another piece of information about g_q, namely

$$\int d^d q \; g_q \cos q_i = \langle S_0^3 S_{\delta_i}^3 \rangle = -e_0/3d, \qquad i=1, 2, 3 \tag{3}$$

Here δ_i is the unit vector in the i direction. (The factor of $1/3d$ appears because there are d bonds per site in d dimensions and the expectation of $S_x^3 S_y^3$ is one-third of the expectation of $\mathbf{S}_x \cdot \mathbf{S}_y$.) If there is no Néel order, i.e., there is no δ-function at $q=Q$, then the upper bound (1) implies

$$e_0/3d \leqslant (e_0/6d)^{1/2} \int d^d q \; (E_q/E_{q-Q})^{1/2} \, d^{-1} \left(-\sum_{i=1}^{d} \cos q_i \right)_+ \tag{4}$$

where the positive part F_+ of a function F equals F when F is positive and is zero otherwise.

Turning now to $d=3$, we can evaluate the integral in (4) numerically and we find that the right side equals $0.0824(e_0)^{1/2}$. Thus, (4) implies that $e_0 \leqslant 0.550$. However, taking the Néel state as a variational state shows that $-e_0$ is less than $-3/4$ for $d=3$. This contradiction shows there must be Néel order when $d=3$ and $S=1/2$.

In two dimensions the above argument only shows that $e_0 \leqslant 1.064$. The numerical estimates[7–9,11,13] of e_0 are all around 0.67, so we cannot conclude from inequality (4) that there is Néel order when $S=1/2$.

The model that interpolates between two and three dimensions is obtained by considering a three-dimensional lattice with the Hamiltonian

$$H = \sum_{\{xy\}} J_{xy} \mathbf{S}_x \cdot \mathbf{S}_y \tag{5}$$

where the coupling constant J_{xy} equals 1 for bonds $\{xy\}$ in one of the first two coordinate directions and equals r for bonds in the third coordinate direction. We will prove that this model has Néel order if $1 \geqslant r \geqslant 0.16$ and $S=1/2$.

Letting g_q^r denote the Fourier transform of the two-point function for this model, we will show

$$0 \leqslant g_q^r \leqslant f_q^r, \qquad q \neq Q \tag{6}$$

where

$$\begin{aligned} f_q^r &= (e_0^r E_q^r / 12 E_{q-Q}^r)^{1/2} \\ E_q^r &= 2 - \cos q_1 - \cos q_2 + r(1 - \cos q_3) \end{aligned} \tag{7}$$

where $-e_0^r$ is the ground-state energy per site. We now consider the following mathematical problem. Assuming $m^2 = 0$, maximize $I = \int d^3q\, g_q$ over all functions g_q subject to both inequality (6) and to

$$\int d^3q\, g_q(\cos q_1 + \cos q_2 + r \cos q_3) = -e_0^r/3 \tag{8}$$

which is the analogue of (3) when $r \neq 1$. If the maximum of I is less than 1/4, then we have a contradiction, so m^2 must be nonzero, i.e., there must be Néel order.

We claim that the maximum of I is attained either by

$$g_q = f_q^r \chi(\cos q_1 + \cos q_2 + r \cos q_3 < \alpha) \tag{9a}$$

or

$$g_q = f_q^r \chi(\cos q_1 + \cos q_2 + r \cos q_3 > -\alpha) \tag{9b}$$

for some $\alpha \geqslant 0$. The characteristic function $\chi(\cdot)$ equals 1 if the expression inside $(\cdot)$ is true and 0 otherwise. Which of the two cases (9a) and (9b) we must choose and the value of the parameter α are determined by the constraint (8). For a given value of r, we determine α by numerically computing the integral in (8) using (9). With this α we then compute I. We do not know the exact value of e_0^r, so we carry out this calculation for several values of e_0 ranging from the Néel bound of $(2+r)/4$ to the Anderson bound of $(3+r)/4$. The critical value of r ranges from 0.16 when the Néel bound is used to 0.14 when the Anderson bound is used.

To show that the maximum is attained by (9), let g_q be a function which satisfies (6) and (8). Consider the two regions R_+ and R_- defined as follows:

$$R_\pm = \{q\colon \pm(\cos q_1 + \cos q_2 + r \cos q_3) > 0 \text{ and } g_q < f_q\}$$

Suppose *both* these regions have nonzero measure. Then we can increase g_q slightly in *both* regions in such a way that conditions (6) and (8) still hold. The new function has a larger I. Thus, we need only consider g_q such that *only one* of R_+ and R_- has positive measure.

Let us assume that R_+ has nonzero measure and R_- has zero measure. We shall show that this leads to (9a). [The other case, leading to (9b), is similar.] Suppose g_q is not given by (9a) for any α. Then there exists an $\alpha > 0$ such that both of the following sets have positive measure.

$$R_> = \{q\colon (\cos q_1 + \cos q_2 + r \cos q_3) > \alpha \text{ and } g_q > 0\}$$

$$R_< = \{q\colon (\cos q_1 + \cos q_2 + r \cos q_3) < \alpha \text{ and } g_q < f_q\}$$

We can then decrease g_q slightly in $R_>$ and increase it slightly in $R_<$ in such a way that (6) and (8) still hold. Since $\cos q_1 + \cos q_2 + r \cos q_3$ is greater on $R_>$ than on $R_<$, we must increase g_q more than we decrease it, i.e., $\int d^3q\, g_q$ must get larger. Thus, the maximizing g_q is given by (9a).

Although we cannot prove the existence of Néel order for spin 1/2 in two dimensions, we will show how to obtain sufficient conditions for the existence of Néel order which only involve the two-point function at relatively short distances. Define $\bar{g}(n)$ as follows:

$$\bar{g}(n) = \frac{1}{n+1} \sum_{m=0}^{n} (-1)^m \langle S_0^3 S_{m\delta_i}^3 \rangle \tag{10}$$

for $i = 1$ or 2. (Recall that δ_i is the unit vector in the i direction.) The two cases of $i = 1$ or 2 give the same result because of the invariance under rotations of the lattice by $\pi/2$. If there is no Néel order, then the infrared bound implies

$$\begin{aligned} \bar{g}(n) &= \int dq\, \frac{1}{2(n+1)} \sum_{m=0}^{n} (-1)^m [\cos(mq_1) + \cos(mq_2)]\, g_q \\ &\leqslant \int dq \left\{ \frac{1}{2(n+1)} \sum_{m=0}^{n} (-1)^m [\cos(mq_1) + \cos(mq_2)] \right\}_+ f_q \end{aligned} \tag{11}$$

The last integral is then computed numerically. Table I shows the resulting upper bound on $\bar{g}(n)$.

Table I. The Upper Bound on $\bar{g}(n)$ [See Eqs. (10) and (11)] Which Follows from the Infrared Bound (1) and the Assumption That There Is No Néel Order in the 2D, $S = 1/2$ Model, and the Value of $\bar{g}(n)$ Obtained Using the Numerical Results of Ref. 7[a]

n	Bound on $\bar{g}(n)$	$\bar{g}(n)$ using results of ref. 7
1	0.228	0.184
2	0.170	0.145
3	0.137	0.124
4	0.115	0.110
5	0.099	0.100
6	0.088	0.093
7	0.079	0.087
8	0.072	0.082

[a] Their numerical results were obtained using a Monte Carlo simulation on a 24×24 lattice and may require sizable corrections arising from the lack of manifest rotation invariance in the simulations. A contradiction for any one value of n implies that there must be Néel order.

Recently Gross *et al.*[7] have numerically computed the two-point function along a coordinate direction for distances up to 11. The numbers in the second column of Table I are the "raw" data from ref. 7 and should in principle be corrected for by extrapolating to zero temperature and infinite size, and for spin space isotropy. (We have simply assumed that the quoted $\langle S^z S^z \rangle$ correlations at distance n are estimates for one-third of the infinite-volume $\langle \mathbf{S} \cdot \mathbf{S} \rangle$ correlations. The authors of ref. 7. have alerted us to the possibility of sizable corrections originating from the lack of manifest rotation invariance in the simulations.)

We now give the proof of inequalities (1) and (6). Inequality (1) may be obtained by taking the zero-temperature limit of Dyson *et al.*'s bound on g_q. It is possible to prove inequality (1) directly in the ground state. Such a direct proof has not appeared in the literature as far as we know, so we provide it here. We start with the model defined on a finite lattice with periodic boundary conditions.

It is convenient to introduce the (positive) spectral weight function

$$R(\omega) = \frac{1}{2} \sum_n \left[|(\phi_n, S_q \phi_0)|^2 + |(\phi_n, S_{-q} \phi_0)|^2 \right] \delta(\omega - e_n + e_0)$$

where ϕ_n are the energy eigenstates, e_n are the corresponding eigenvalues, and ϕ_0 is the unique ground state. Then

$$g_q = \int_0^\infty d\omega \, R(\omega)$$

The susceptibility is

$$\chi_q = \int_0^\infty d\omega \, R(\omega) \, \omega^{-1}$$

By the Cauchy–Schwarz inequality,

$$\left[\int_0^\infty d\omega \, R(\omega) \right]^2 \leqslant \int_0^\infty d\omega \, R(\omega) \, \omega^{-1} \int_0^\infty d\omega \, R(\omega) \omega \tag{12}$$

The last integral is

$$\int_0^\infty d\omega \, R(\omega) \omega = \tfrac{1}{2} \langle [[S_q, H], S_{-q}] \rangle = 2 e_0 E_q / 3d \tag{13}$$

for the usual Heisenberg model after some computation.[3] We will show later that

$$\chi_q \leqslant \frac{1}{4} \frac{1}{E_{q-Q}}, \qquad q \neq Q \tag{14}$$

Combining (12)–(14) yields (1). Note that in this argument the Cauchy–Schwarz inequality plays the role played by the Falk–Bruch inequality[4] in the nonzero-temperature case.

For the model (5) which interpolates between two and three dimensions, the bound (14) holds with E_{q-Q} replaced by E^r_{q-Q}. The double commutator (13) equals

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

where ρ_1 and ρ_3 are the expectations of $\mathbf{S}_x\cdot\mathbf{S}_y$ for bonds $\{xy\}$ in the first and third lattice directions, respectively. We will show that $0\leqslant\rho_3\leqslant\rho_1$. This fact, together with $e^r_0=2\rho_1+r\rho_3$, implies that the double commutator is bounded above by $e^r_0E^r_q/3$. This, in turn, implies (6). First of all, $\rho_3\geqslant 0$, for if $\rho_3<0$, we would have that $-e^r_0>2\rho_1=\langle H^1+H^2\rangle$, where H^1 (resp. H^2) is the interaction in the 1 (resp. 2) direction in the lattice. We could then lower the energy, $-e^r_0$, by replacing the ground state ϕ_0 by the ground state for H^1+H^2. [This ground state is the product of the unique two-dimensional ground state for each (12) plane and has the property that $\rho_3=0$.] Now suppose that $\rho_3>\rho_1$ and assume that the lattice is cubic (i.e., the number of sites in each direction is the same). Then we can simply rotate the lattice about the 1 axis so that directions 2 and 3 are interchanged. The energy would then be $-\rho_1-r\rho_1-\rho_3$, which cannot be less than $-e^r_0=-2\rho_1-r\rho_3$. Thus, $\rho_3\leqslant\rho_1$.

We now turn to the bound on the susceptibility, inequality (14). The Heisenberg antiferromagnetic Hamiltonian is unitarily equivalent to the Hamiltonian

$$\sum_{\{xy\}}(-S^1_xS^1_y+S^2_xS^2_y-S^3_xS^3_y) \tag{15}$$

The unitary transformation is rotation by π about the 2 axis in the spin space at site x for all sites x with odd $|x|$. We work in the usual basis in which the matrices of S^1 and S^3 have only real entries, while S^2 has only purely imaginary entries. Define $T^1=S^1$, $T^2=iS^2$, $T^3=S^3$. Then the matrices T^i all have only real entries and the above Hamiltonian is

$$-\sum_{\langle xy\rangle}(T^1_xT^1_y+T^2_xT^2_y+T^3_xT^3_y) \tag{16}$$

Let $h=h_x$ be a real-valued function on the sites. We define an h-dependent Hamiltonian as follows:

$$H(h)=\frac{1}{2}\sum_{\{xy\}}[(T^1_x-T^1_y)^2+(T^2_x-T^2_y)^2+(T^3_x-T^3_y-h_x+h_y)^2] \tag{17}$$

When $h = 0$ this agrees with the above Hamiltonian except for a constant term. Let $E(h)$ be the ground-state energy of $H(h)$. We will show later that

$$E(h) \geqslant E(0), \qquad \forall h \tag{18}$$

Hence

$$\left. \frac{d^2}{d\lambda^2} E(\lambda h) \right|_{\lambda = 0} \geqslant 0 \tag{19}$$

We use perturbation theory to compute this derivative and take h_x to be $\cos q \cdot x$. The unitary transformation of rotation by π about the 2 axis changes S_x^3 to $(-1)^{|x|} S_x^3$, and so changes S_q to S_{q-Q}. The bound (14) then follows from (19).

Notice that (18) is equivalent to proving that $E(h)$ attains its minimum when h_x is a constant. Suppose $E(h)$ attains its minimum at a function $\bar{h}$, and there is a bond $\{x_0 y_0\}$ with $\bar{h}_{x_0} \neq \bar{h}_{y_0}$. The energy $E(h)$ may attain its minimum at more than one configuration, in which case we choose a minimizing configuration $\bar{h}$ with the least number of bonds $\{xy\}$ with $\bar{h}_x \neq \bar{h}_y$. We will then construct another function h' which is also a minimizer for E, but has fewer bonds with $h'_x \neq h'_y$. This contradiction will imply that $E(h)$ must attain its minimum at $h_x = \text{const}$.

We draw a plane through the midpoint of the bond $x_0 y_0$ and perpendicular to the bond. We also draw a second plane parallel to the first but shifted by $L/2$. (L is the number of sites in a single lattice direction, which we assume to be even.) These two planes, which will be denoted collectively by P, divide the lattice into two halves which we refer to as the right and left halves. (Remember that we are using periodic boundary conditions.)

We work in the usual real, orthonormal basis of S^3 eigenstates. Let ψ_α^L, ψ_β^R denote the basis vectors associated with the left and right half Hilbert spaces, respectively, so $\psi_\alpha^L \otimes \psi_\beta^R$ is a basis for the full Hilbert space. It is crucial to note that the Hamiltonian $H(\bar{h})$ has *real* matrix elements in this basis, so the ground state ψ can be written as

$$\psi = \sum_{\alpha, \beta} c_{\alpha\beta} \psi_\alpha^L \otimes \psi_\beta^R$$

for *real* numbers $c_{\alpha\beta}$. We will think of $c_{\alpha\beta}$ as the elements of a matrix which we denote by c.

There are three types of bonds. Bonds with both endpoints in the left half will be referred to as "left" bonds. Bonds with one endpoint in the left half and one in the right half will be referred to as "crossing." The "right" bonds are defined in the obvious way.

We denote the bonds crossing P by $\{x_i y_i\}$ with x_i in the left half and y_i in the right half. For these bonds we write

$$\begin{aligned}(T_x^1 - T_y^1)^2 + (T_x^2 - T_y^2)^2 + (T_x^3 - T_y^3 - \bar{h}_x + \bar{h}_y)^2 \\ = (T_x^1)^2 + (T_y^1)^2 - 2T_x^1 T_y^1 + (T_x^2)^2 + (T_y^2)^2 - 2T_x^2 T_y^2 \\ + (T_x^3 - \bar{h}_x)^2 + (T_y^3 - \bar{h}_y)^2 - 2(T_x^3 - \bar{h}_x)(T_y^3 - \bar{h}_y)\end{aligned} \tag{20}$$

Define H^L to be the sum of all the terms in $H(\bar{h})$ labeled by left bonds plus the terms $(T_x^1)^2 + (T_x^1)^2 + (T_x^3 - \bar{h}_x)^2$ from the crossing bonds. H^R is defined analogously. Then

$$H = H^L + H^R - 2\sum_i [T_{x_i}^1 T_{y_i}^1 + T_{x_i}^2 T_{y_i}^2 + (T_{x_i}^3 - \bar{h}_{x_i})(T_{y_i}^3 - \bar{h}_{y_i})] \tag{21}$$

Let

$$H_{\alpha\gamma}^L = (\psi_\alpha^L, H^L \psi_\gamma^L)$$

$$X_{\alpha\gamma}^{L,i} = (\psi_\alpha^L, T_{x_i}^1 \psi_\gamma^L), \qquad Y_{\alpha\gamma}^{L,i} = (\psi_\alpha^L, T_{x_i}^2 \psi_\gamma^L), \qquad Z_{\alpha\gamma}^{L,i} = (\psi_\alpha^L, (T_{x_i}^3 - \bar{h}_{x_i})\, \psi_\gamma^L)$$

and similarly for $H_{\alpha\gamma}^R$, $X_{\alpha\gamma}^{R,i}$, $Y_{\alpha\gamma}^{R,i}$, $Z_{\alpha\gamma}^{R,i}$ with x_i replaced by y_i. It is important to note that all these matrix elements are real. (It is here that the reality of all the vectors and operators is used.) We let $X^{L,i}$ denote the matrix whose (α, γ) element is $X_{\alpha\gamma}^{L,i}$. Then the transpose of $X^{L,i}$ is the same as the adjoint of $X^{L,i}$. The latter is denoted by $(X^{L,i})^\dagger$. The same notation and remark apply to the other quantities Y, Z, H.

Remembering that the $c_{\alpha\beta}$ are real, we obtain

$$\begin{aligned}E(\bar{h}) &= (\psi, H(\bar{h})\psi) \\ &= \sum_{\alpha\beta\gamma} c_{\alpha\beta} c_{\gamma\beta} H_{\alpha\gamma}^L + \sum_{\alpha\beta\gamma} c_{\alpha\beta} c_{\alpha\gamma} H_{\beta\gamma}^R \\ &\quad - 2\sum_i \sum_{\alpha\beta\gamma\delta} c_{\alpha\beta} c_{\gamma\delta} (X_{\alpha\gamma}^{L,i} X_{\beta\delta}^{R,i} + Y_{\alpha\gamma}^{L,i} Y_{\beta\delta}^{R,i} + Z_{\alpha\gamma}^{L,i} Z_{\beta\delta}^{R,i}) \\ &= \mathrm{Tr}\, cc^\dagger H^L + \mathrm{Tr}\, c^\dagger c H^R - 2\sum_i \mathrm{Tr}[c^\dagger X^{L,i} c (X^{R,i})^\dagger \\ &\quad + c^\dagger Y^{L,i} c (Y^{R,i})^\dagger + c^\dagger Z^{L,i} c (Z^{R,i})^\dagger]\end{aligned} \tag{22}$$

The next step is to prove a trace inequality. Let c, M, N be matrices, not necessarily real. Then we shall prove that

$$|\mathrm{Tr}\, c^\dagger M c N^\dagger|^2 \leqslant \mathrm{Tr}\, c_L M^\dagger c_L M\, \mathrm{Tr}\, c_R N c_R N^\dagger \tag{23}$$

where $c_L = (cc^\dagger)^{1/2}$ and $c_R = (c^\dagger c)^{1/2}$. Both c_L and c_R are Hermitian positive semidefinite and, by the polar decomposition theorem, there is a unitary matrix U such that $c = U c_R$ and $c^\dagger = c_R U^\dagger$. Thus, by the cyclicity of the trace

$$\mathrm{Tr}\, c^\dagger M c N^\dagger = \mathrm{Tr}\, AB$$

with

$$A = c_R^{1/2} U^\dagger M U c_R^{1/2}, \qquad B = c_R^{1/2} N^\dagger c_R^{1/2}$$

By the Schwarz inequality for traces

$$|\text{Tr } c^\dagger M c N^\dagger|^2 \leqslant \text{Tr } A^\dagger A \text{ Tr } B^\dagger B = \text{Tr } \alpha M^\dagger \alpha M \text{ Tr } c_R N c_R N^\dagger$$

with $\alpha = U c_R U^\dagger$. Since $\alpha^2 = U c_R^2 U^\dagger = cc^\dagger$, and since $cc^\dagger$ has a unique square root c_L, we have that $\alpha = c_L$. This proves (23).

To apply (23) to our case, consider $M = X^{L,i}$, $N = X^{R,i}$. Since $2ab \leqslant a^2 + b^2$, we have

$$2 \text{ Tr } c^\dagger X^{L,i} c (X^{R,i})^\dagger \leqslant \text{Tr } c_L X^{L,i} c_L (X^{L,i})^\dagger + c_R X^{R,i} c_R (X^{R,i})^\dagger \tag{24}$$

A similar inequality obviously holds with the X matrices replaced by Y or Z matrices.

The definitions of c_L and c_R and (24) imply

$$\begin{aligned} E(\bar{h}) \geqslant\ & \text{Tr } c_L^2 H^L + \text{Tr } c_R^2 H^R \\ & - \sum_i \text{Tr}[c_L X^{L,i} c_L (X^{L,i})^\dagger + c_L Y^{L,i} c_L (Y^{L,i})^\dagger + c_L Z^{L,i} c_L (Z^{L,i})^\dagger] \\ & - \sum_i \text{Tr}[c_R X^{R,i} c_R (X^{R,i})^\dagger + c_R Y^{R,i} c_R (Y^{R,i})^\dagger + c_R Z^{R,i} c_R (Z^{R,i})^\dagger] \end{aligned} \tag{25}$$

Let h_x^R denote the function which agrees with $\bar{h}_x$ on the right sites and on the left sites equals the reflection of $\bar{h}_x$ in the planes P. The h^L is defined analogously. Recall that $\bar{h}_x \neq \bar{h}_y$ for at least one crossing bond. Hence, at least one choice, h^R or h^L, has the property that it has strictly fewer bonds with $h_x \neq h_y$ than does the original $\bar{h}$.

Let

$$\psi^L = \sum_{\alpha,\beta} (c_L)_{\alpha\beta} \, \psi_\alpha^L \otimes \psi_\beta^R$$

with ψ^R defined analogously using $(c_R)_{\alpha\beta}$. (Note that $\|\psi^L\| = \|\psi^R\| = \|\psi\|$.) Then the right side of (25) equals

$$\tfrac{1}{2}(\psi^R, H(h^R)\, \psi^R) + (\psi^L, H(h^L)\, \psi^L) \geqslant \tfrac{1}{2} E(h^R) + \tfrac{1}{2} E(h^L)$$

We have chosen $\bar{h}$ so that $E(\bar{h})$ is a minimum, so this inequality implies that E also attains its minimum at both h^R and h^L. This contradicts the minimality of the number of bonds such that $\bar{h}_x \neq \bar{h}_y$, so (18) is proven. This concludes the proof of (14).

We have demonstrated the existence of Néel order in the ground state of the 3D spin-1/2 Heisenberg antiferromagnet. Although our methods do not work for the 2D model, they work surprisingly well for the model which interpolates between $d = 2$ and $d = 3$. The bound (1) on g_q and the value of the nearest neighbor correlation (3) are not by themselves sufficient to show the existence of Néel order in $d=2$ with $S=1/2$, so the obvious question is what additional information might show the existence of Néel order in this case. Rigorous lower bounds on the short-range correlations could prove the existence of Néel order (see Table I). Another possibility is to improve the bound on g_q. The two places where one could hope to improve this bound are to improve the bound on the susceptibility χ_q (14) or to improve inequality (12) resulting from the use of the Cauchy–Schwarz inequality. For the 1D spin-1/2 Heisenberg antiferromagnet the exact value[6,14] of χ_0 is $1/\pi^2$ while the bound (14) equals 1/8 at $q=0$. Thus, one cannot hope to improve the bound (14) by, for example, an overall factor of 2. If the Cauchy–Schwarz inequality (12) is close to being an equality, then $R(\omega)$ must be close to a δ-function at a single value of ω. Although this appears unlikely, we have not been able to improve inequality (12).

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