# Antiferromagnetism in the $S=\frac{1}{2}$ antiferromagnetic Heisenberg model on a two-dimensional square lattice

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(Received 4 April 2000; revised manuscript received 12 June 2000).

We present a rigorous result and strong evidence to support existence of antiferromagnetic long-range order on a square lattice for the $S=\frac{1}{2}$ antiferromagnetic Heisenberg model.

Antiferromagnetism in the $S=\frac{1}{2}$ Heisenberg model on a square lattice has stood as a challenging subject for theoretical physicists for a very long time. Rigorous proof of the existence of antiferromagnetic (AF) long-range order (LRO) was given for $S\geqslant 1$ by Dyson, Lieb, and Simon.[1] It was generalized for $S=1/2$ on a cubic lattice[2] and for some $XXY$ models in two and three dimensions.[3,4] We now know that AFLRO exists in three dimensions for all spins and in two dimensions for $S>1/2$. Although there is no rigorous proof for $S=1/2$ on a square lattice, various numerical and analytical calculations[5] suggest that AFLRO exists in the ground state, which is destroyed by thermodynamic fluctuations at finite temperatures.[6] Another method to prove the existence of AFLRO was proposed by the author and his co-workers[7] for some asymmetric bipartite lattices. AFLRO exists even in some one-dimensional systems.[8] In this Brief Report, we present a rigorous example for AFLRO on a square lattice and a relation for the AF correlation function. Our result strongly supports the existence of AFLRO on a square lattice.

Our starting point is to introduce the model Hamiltonian on a square lattice,

$$H(\alpha)=J\sum_{i\in A,j\in B,D}\mathbf{S}_i\cdot\mathbf{S}_j+\alpha J\sum_{i\in C,j\in B,D}\mathbf{S}_i\cdot\mathbf{S}_j=H_A+\alpha H_C, \tag{1}$$

where $(i,j)$ are pairs of the nearest-neighbor sites. $\alpha\geqslant 0$ is the model parameter, and the model is reduced to the usual antiferromagnetic Heisenberg model which we are interested in when $\alpha=1$. Here $J$ is positive for the antiferromagnetic exchange coupling, and for convenience, we take $J=1$ as the unit of energy. We divide the square lattice into four sublattice as shown in Fig. 1. Denote the ground state of $H(\alpha)$ by $|\alpha\rangle$. To study AF long-range correlation in the state $|\alpha\rangle$, we introduce two correlation functions

$$F_{AF}(\alpha)=\langle\alpha|O^{\dagger}O|\alpha\rangle,$$

where

$$O=\frac{1}{\sqrt{N_\Lambda}}\sum_{i\in\Lambda}e^{i\mathbf{Q}\cdot\mathbf{r}_i}\mathbf{S}_i=\frac{1}{\sqrt{N_\Lambda}}(\mathbf{S}_A+\mathbf{S}_C-\mathbf{S}_B-\mathbf{S}_D)$$

and

$$F_{NNAF}(\alpha)=\frac{1}{N_\Lambda}\langle\alpha|\sum_{\langle i,j\rangle}e^{i\mathbf{Q}\cdot(\mathbf{r}_i-\mathbf{r}_j)}\mathbf{S}_i\cdot\mathbf{S}_j|\alpha\rangle,$$

where $\mathbf{Q}=(\pi,\pi)$, and $\langle i,j\rangle$ run over all possible pairs of nearest-neighbor sites. $N_\Lambda$ is the total number of lattice sites. $\mathbf{S}_X$ $(X=A,B,C,D)$ is the total spin on the sublattice $X$. Mathematically, if

$$F_{AF}(\alpha)=\gamma N_\Lambda$$

with $\gamma\neq 0$, we say that the state $|\alpha\rangle$ possesses AFLRO in the thermodynamic limit. $F_{NNAF}(\alpha)$ can be used to describe the nearest-neighbor antiferromagnetic (NNAF) correlation in the state $|\alpha\rangle$. As the model is defined on a square lattice, the correlation functions are invariant under the transformation $A\rightarrow C$, which we name the $AC$ symmetry.

The antiferromagnetic Heisenberg model was studied extensively over the last decades. Some rigorous results were established for a bipartite lattice by several authors. The bipartite lattice means that the lattice is divided into two sublattices: only spins on difference sublattice sites have AF exchange coupling. According to this definition, $A$ and $C$ belong to one sublattice, and $B$ and $D$ belong to another sublattice. Here we summarize: (1) The ground state of the model is nondegenerate apart from the trivial $(2S_{tot}+1)$-fold degeneracy caused by SU(2) symmetry. The total spin $S_{tot}$ is determined by the difference of the two sublattice site numbers $N_I$ and $N_{II}$, i.e.,[9,10]

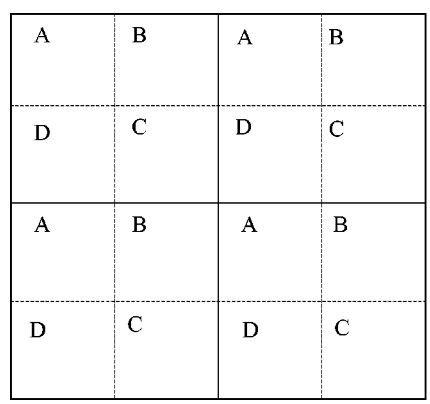


FIG. 1. The structure of four sublattices on a square lattice in Eq. (1). The solid line represents that the exchange coupling between spins on the two sites is 1, and the dashed line represents that the exchange coupling is $\alpha$. According to the definition of the bipartite lattice structure for the Lieb-Mattis theorem, $A$ and $C$ belong to one sublattice, and $B$ and $D$ belong to another sublattice.

 

$$S_{tot}=\frac{1}{2}|N_I-N_{II}|.$$

(2) On a chosen basis, the wave function of the ground state is positive definite, and the static spin-spin correlations satisfy[7,8]

$$e^{iQ\cdot(r_i-r_j)}\langle\alpha|\mathbf{S}_i\cdot\mathbf{S}_j|\alpha\rangle>0. \quad (2)$$

Proof of Eq. (2): According to the Lieb-Mattis theorem on Eq. (1), the ground state of Eq. (1) for any finite $\alpha$ is nondegenerate and positive definite on a chosen basis. Usually the $S=\frac{1}{2}$ operator can be expressed in terms of fermion operators $c_{i,\sigma}$ $(\sigma=\uparrow,\downarrow)$,

$$\mathbf{S}_i^+=c_{i,\uparrow}^\dagger c_{i,\downarrow};\quad \mathbf{S}_i^-=c_{i,\downarrow}^\dagger c_{i,\uparrow};\quad \mathbf{S}_i^z=(c_{i,\uparrow}^\dagger c_{i,\uparrow}-c_{i,\downarrow}^\dagger c_{i,\uparrow})/2.$$

The ground state for Eq. (1) can be expressed as

$$|\alpha\rangle=\sum_l C_l\mathbf{T}|\phi_l^\uparrow\rangle\otimes|\phi_l^\downarrow\rangle,$$

where

$$\mathbf{T}=\prod_{i\in I}(c_{i,\downarrow}^\dagger-c_{i,\downarrow})\prod_{i\in II}(c_{i,\downarrow}^\dagger+c_{i,\downarrow})$$

and $|\phi_l^\sigma\rangle$ is an orthogonal basis for $N=N_\Lambda/2$ for even $N_\Lambda$ [and $(N_\Lambda-1)/2$ for odd $N_\Lambda$] fermions with spin $\sigma$.[8] The Lieb-Mattis theorem tells us that the coefficients $C_l$ are positive for all possible configurations $l$ and unique. A simple evaluation shows that

$$e^{iQ\cdot(r_i-r_j)}\langle\alpha|\mathbf{S}_i^+\cdot\mathbf{S}_j^-|\alpha\rangle=\sum_{l,m}C_lC_m|(V_{ij})_{lm}|^2>0, \quad (3)$$

where

$$(V_{ij})_{lm}=\langle\phi_l^\sigma|c_{i,\sigma}^\dagger c_{j,\sigma}|\phi_m^\sigma\rangle.$$

On the other hand, since the ground state of Eq. (1) is a spin singlet for a square lattice, the isotropy of the ground state leads to

$$\langle\alpha|\mathbf{S}_i^x\cdot\mathbf{S}_j^x|\alpha\rangle=\langle\alpha|\mathbf{S}_i^y\cdot\mathbf{S}_j^y|\alpha\rangle=\langle\alpha|\mathbf{S}_i^z\cdot\mathbf{S}_j^z|\alpha\rangle. \quad (4)$$

Combination of Eqs. (3) and (4) leads to the inequality of Eq. (2).

Based on the two rigorous results, we have our first result of this paper:

$$\lim_{\alpha\to0}F_{AF}(\alpha)\geqslant\frac{N_\Lambda}{16}. \quad (5)$$

In other words, in the limit of $\alpha\to0$, it proves rigorously that AFLRO exists in the ground state of the model.

According to the Marshall-Lieb-Mattis theorem,[9,10] when $\alpha\to0$, the total spin on sublattices $A$, $B$, and $D$ is $S=N_\Lambda/8$, since sublattices $B$ and $D$ belong to the same sublattice, and sublattice $A$ belongs to another one, i.e.,

$$\langle\alpha|(\mathbf{S}_A+\mathbf{S}_B+\mathbf{S}_D)^2|\alpha\rangle=\frac{1}{8}N_\Lambda\left(\frac{1}{8}N_\Lambda+1\right),$$

when $\alpha\to0$. Strictly speaking, the ground state of Eq. (1) is highly degenerated when $\alpha=0$ as there are no interactions between spins on sublattice $C$ and other sublattices, and spins on sublattice $C$ can orient arbitrarily, which costs no energy. However, one of the states is semipositive definite and is spin singlet. The state can be regarded as the ground state of the limit of $\alpha\to0$ as the state is positive definite and nondegenerate for any finite $\alpha$. Thus, the total spin in the ground state for the whole square lattice is singlet,

$$\langle\alpha|(\mathbf{S}_A+\mathbf{S}_B+\mathbf{S}_C+\mathbf{S}_D)^2|\alpha\rangle=0. \quad (6)$$

According to the theory of angular momentum coupling, the total spin $\mathbf{S}_C$ must be also $S_C=N_\Lambda/8$, which is maximal. On the other hand, from Eq. (6), one obtains

$$-2\langle\alpha|\mathbf{S}_C\cdot(\mathbf{S}_B+\mathbf{S}_D)|\alpha\rangle=\langle\alpha|(\mathbf{S}_A+\mathbf{S}_B+\mathbf{S}_D)^2|\alpha\rangle+\langle\alpha|\mathbf{S}_C^2|\alpha\rangle+2\langle\alpha|\mathbf{S}_A\cdot\mathbf{S}_C|\alpha\rangle.$$

According to Eq. (2),

$$\langle\alpha|\mathbf{S}_X\cdot\mathbf{S}_Y|\alpha\rangle>0,$$

if $X$, $Y$ belong to $A$ and $C$ or $B$ and $D$:

$$\langle\alpha|\mathbf{S}_X\cdot\mathbf{S}_Y|\alpha\rangle<0,$$

if $X$ belongs to $A$ and $C$, and $Y$ belongs to $B$ and $D$. Combination of these two inequalities leads to

$$\langle\alpha|(\mathbf{S}_A-\mathbf{S}_B-\mathbf{S}_D)^2|\alpha\rangle>\langle\alpha|(\mathbf{S}_A+\mathbf{S}_B+\mathbf{S}_D)^2|\alpha\rangle.$$

From these relations, one obtains

$$\begin{aligned}\langle\alpha|(\mathbf{S}_A-\mathbf{S}_B+\mathbf{S}_C-\mathbf{S}_D)^2|\alpha\rangle&=\langle\alpha|(\mathbf{S}_A-\mathbf{S}_B-\mathbf{S}_D)^2|\alpha\rangle+\langle\alpha|\mathbf{S}_C^2|\alpha\rangle\\&\quad+2\langle\alpha|\mathbf{S}_A\cdot\mathbf{S}_C|\alpha\rangle-2\langle\alpha|\mathbf{S}_C\cdot(\mathbf{S}_B+\mathbf{S}_D)|\alpha\rangle\\&>2\langle\alpha|(\mathbf{S}_A+\mathbf{S}_B+\mathbf{S}_D)^2|\alpha\rangle+2\langle\alpha|\mathbf{S}_C^2|\alpha\rangle\\&=4\frac{N_\Lambda}{8}\left(\frac{N_\Lambda}{8}+1\right).\end{aligned}$$

Thus, in the limit of $\alpha\to0$, $F_{AF}(\alpha\to0)$ has order of $N_\Lambda$. Both $F_{AF}(\alpha)$ and $F_{NNAF}(\alpha)$ are continuous with respect to the parameter $\alpha$. This conclusion is drawn from the fact that the ground state of Eq. (1) is nondegenerate for any finite $\alpha$ as shown in Ref. 10. Any discontinuity of the functions must be related to the crossover of the ground state from one state to another with different good quantum numbers. The crossover can happen only at some point with degeneracy of the ground state. The nondegeneracy of the ground state has ruled out this possibility. Therefore we conclude that AFLRO exists in the ground state of $\alpha\to0$.

We have shown the existence of AFLRO at $\alpha\to0$. The previous results from numerical and analytical calculations strongly support that the correlation function $F_{AF}(\alpha)$ has order of $N_\Lambda$ for $\alpha=1$. From the continuity of $F_{AF}(\alpha)$ we anticipate that $F_{AF}(\alpha)$ has order of $N_\Lambda$ for small finite $\alpha$. However, we encounter some difficulty in generalizing the result in Eq. (5) to the case of finite $\alpha$. Instead of $F_{AF}(\alpha)$, we have a weaker conclusion on $F_{NNAF}(\alpha)$:

$$F_{NNAF}(\alpha)\ \text{ has its maximum at }\ \alpha=1.$$

The result tells us that the nearest-neighbor antiferromagnetic long-range correlation is strongest at $\alpha=1$, which is the case we are mostly interested in. This result strongly supports the existence of AFLRO at $\alpha=1$, as the nearest-neighbor correlation should become dominate for a system with the nearest-neighbor interaction.

Denote the ground state and ground-state energy of the Hamiltonian in Eq. (1) by $|\alpha\rangle$ and $E(\alpha)$, respectively. As the ground state is spin singlet and nondegenerate for any finite $\alpha$, $E(\alpha)$ must be continuous with respect to $\alpha$. Due to the $AC$ symmetry, when we exchange the position of $A$ and $C$ sublattice sites, the ground-state energy should remain unchanged. However, as

$$H_A+\alpha H_C=\alpha\left(\frac{1}{\alpha}H_A+H_C\right),$$

we obtain a relation

$$E(\alpha)=\alpha E\left(\frac{1}{\alpha}\right).$$

The Hamiltonian can be reorganized as

$$\left(\beta+\frac{1}{\beta}\right)(H_A+\alpha H_C)=\beta\left(H_A+\frac{\alpha}{\beta^2}H_C\right)+\frac{1}{\beta}(H_A+\alpha\beta^2H_C).$$

Multiplying the bra $\langle\alpha|$ from the left hand side and the ket $|\alpha\rangle$ from the right hand side, respectively,

$$\left(\beta+\frac{1}{\beta}\right)\langle\alpha|(H_A+\alpha H_C)|\alpha\rangle=\beta\langle\alpha|\left(H_A+\frac{\alpha}{\beta^2}H_C\right)|\alpha\rangle+\frac{1}{\beta}\langle\alpha|(H_A+\alpha\beta^2H_C)|\alpha\rangle.$$

Since $|\alpha\rangle$ may not be the ground state for the Hamiltonian $H_A+(\alpha/\beta^2)H_C$, from the variational principle, we have

$$\langle\alpha|\left(H_A+\frac{\alpha}{\beta^2}H_C\right)|\alpha\rangle\geqslant\left\langle\frac{\alpha}{\beta^2}\right|\left(H_A+\frac{\alpha}{\beta^2}H_C\right)\left|\frac{\alpha}{\beta^2}\right\rangle.$$

Therefore,

$$\left(\beta+\frac{1}{\beta}\right)E(\alpha)\geqslant\beta E\left(\frac{\alpha}{\beta^2}\right)+\frac{1}{\beta}E(\alpha\beta^2).$$

The energy $E(\alpha)$ is continuous with respect to $\alpha$. We expand $E(\alpha/\beta^2)$ and $E(\alpha\beta^2)$ near $\beta=1$, and obtain

$$\frac{d^2}{d\alpha^2}E(\alpha)\leqslant 0. \tag{7}$$

On the other hand, from the definition of $F_{NNAF}$, we obtain

$$F_{NNAF}(\alpha)=-\frac{1}{N_\Lambda}\langle\alpha|(H_A+H_C)|\alpha\rangle.$$

The differentiation of $\langle\alpha|(H_A+H_C)|\alpha\rangle$ with respect to $\alpha$ is

$$\begin{aligned}\frac{d}{d\alpha}\langle\alpha|(H_A+H_C)|\alpha\rangle &=\frac{d}{d\alpha}\langle\alpha|(H_A+\alpha H_C)|\alpha\rangle+\frac{d}{d\alpha}[(1-\alpha)\langle\alpha|H_C|\alpha\rangle]\\ &=\frac{d}{d\alpha}E(\alpha)-\langle\alpha|H_C|\alpha\rangle+(1-\alpha)\frac{d}{d\alpha}\langle\alpha|H_C|\alpha\rangle.\end{aligned} \tag{8}$$

Furthermore,

$$\frac{d}{d\alpha}E(\alpha)=\langle\alpha|\left[\frac{d}{d\alpha}(H_A+\alpha H_C)\right]|\alpha\rangle=\langle\alpha|H_C|\alpha\rangle. \tag{9}$$

The combination of Eqs. (9) and (8) leads to

$$\frac{d}{d\alpha}\langle\alpha|(H_A+H_C)|\alpha\rangle=(1-\alpha)\frac{d^2}{d\alpha^2}E(\alpha). \tag{10}$$

In other words, by using the inequality (7), one obtains

$$\frac{d}{d\alpha}F_{NNAF}(\alpha)=\begin{cases}\geqslant 0 & \text{for } \alpha<1,\\ =0 & \text{for } \alpha=1,\\ \leqslant 0 & \text{for } \alpha>1.\end{cases}$$

In fact, from the $AC$ symmetry,

$$F_{NNAF}(\alpha)=F_{NNAF}\left(\frac{1}{\alpha}\right).$$

Therefore we conclude that the nearest-neighbor antiferromagnetic correlation has its maximum at $\alpha=1$. Notice the fact that $F_{NNAF}(\alpha)$ is always positive. The maximal value of $F_{NNAF}(\alpha)$ indicates that the nearest-neighbor antiferromagnetic correlation is the strongest at $\alpha=1$. As long-range antiferromagnetism exists at the small $\alpha$ limit as we just proved in the preceding paragraphs, we anticipate that the stronger short-range antiferromagnetic correlation will enhance the long-range correlation, and the long-range correlation for $\alpha=1$ is stronger than that for small $\alpha$.

In short, we present a rigorous example with AFLRO on a square lattice for small $\alpha$. By utilizing the symmetry of the system and the variational principle, we show that the nearest-neighbor AF correlation becomes the strongest at $\alpha=1$; i.e., it is stronger than the correlation at small $\alpha$.

This work was supported by a RGC grant from Hong Kong.

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