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Coexistence of the ferromagnetic and antiferromagnetic long-range orders in the generalized antiferromagnetic Heisenberg model on a bipartite lattice

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Abstract. The concept of ferrimagnetism was first proposed by Neel to explain why some materials have a macroscopic magnetization but no ferromagnetic long-range order, when the temperature T is lower than a phase transition temperature T_c. In this article, based on a theorem of Lieb and Mattis, we show in a mathematically rigorous way that the global ground states of the generalized antiferromagnetic Heisenberg model on a bipartite lattice with unequal sublattice points have both ferromagnetic and antiferromagnetic long-range orders with the latter being predominant. Our rigorous results conform to Neel's theory.

The magnetic properties of solids are of fundamental importance in the study of condensed matter physics. In addition to the well known ferromagnetism and antiferromagnetism, the existence of ferrimagnetism in some materials was proposed by Neel four decades ago [1]. A ferrimagnet represents an intermediate case between a ferromagnet of parallel spins and an antiferromagnet of equal antiparallel spins. According to Neel, a ferrimagnet is a magnetic material which exhibits a spontaneous magnetization below a phase transition temperature T_c. But, in contrast to ferromagnets, this magnetization arises from the unequal magnetic moments which are not parallel. One can find a comprehensive review on ferrimagnetism in [2].

To describe a ferrimagnet, one usually uses either the antiferromagnetic Heisenberg model or the positive-U Hubbard model. In the Heisenberg model, each magnetic spin is localized at a lattice point while, in the Hubbard model, electrons with a magnetic spin of $\frac{1}{2}$ are allowed to hop from one lattice point to another. The Hamiltonians of both models are defined on a bipartite lattice Λ, which has two sublattices, A and B, with unequal numbers of points. The main analytical techniques in studying these models were the mean-field theory and the spin-wave theory [2]. These are very intuitive and effective approximate methods. However, it is not easy to estimate the error in the final results obtained by them. Therefore, in this article, we would like to study these antiferromagnetic models in a mathematically rigorous way. By showing explicitly the existence of ferrimagnetism in the ground states of these models, we are able to achieve a better understanding on the interconnection between ferrimagnetism and the lattice structures.

To begin with, we shall first recall some established results, which will be used in the following.

In a seminal paper [3], Lieb and Mattis showed that the ground state of a generalized antiferromagnetic Heisenberg model on a bipartite lattice is non-degenerate apart from the trivial spin degeneracy. Furthermore, if all the localized spins have the same angular momentum s, then the total spin of the ground state is $L = s|N_A - N_B|$, where N_A and N_B are the numbers of the lattice points in sublattices A and B, respectively. Therefore, if the difference $|N_A - N_B|$ is a macroscopic quantity, the system has a spontaneous magnetization in its ground state. Recently, this result was also established for the positive-U Hubbard model at half-filling by Lieb [4]. However, *in both papers the existence of the magnetic* long-range orders (MLRO) in the ground states of these models was not addressed. For the antiferromagnetic Heisenberg model on the simple cubic lattice, this question has been studied by several authors [5–7]. They proved that, if the localized spin momentum $s \geqslant \frac{1}{2}$ and the lattice dimension $d \geqslant 3$, or $s \geqslant 1$ and $d = 2$, then the non-degenerate ground state of the antiferromagnetic Heisenberg model does have an antiferromagnetic long-range order. However, since the difference $|N_A - N_B| = 0$ for the simple cubic lattice, ferrimagnetism was not found in this case.

In a recent article [8], by using a theorem proved before [9], Shen *et al* showed that some of the $2L+1$ ground states of the positive-U Hubbard model on a bipartite lattice have *both transverse ferromagnetic and antiferromagnetic long-range orders when the lattice is* half-filled. It implies that ferrimagnetism does exist in a strongly correlated electron system for some specific filling fraction.

In this article, we shall first extend the result of [8] to the generalized antiferromagnetic Heisenberg model studied by Lieb and Mattis [3]. Namely, we show that some of the $2L+1$ degenerate ground states of the generalized antiferromagnetic Heisenberg model have both *transverse* ferromagnetic and antiferromagnetic long-range orders. Then, we shall show *how to extend these results to the longitudinal* MLRO *in the ground states of these models.* This extension is not quite straightforward, as one would think.

Take a finite lattice Λ with N_Λ lattice points. The Hamiltonian of the generalized antiferromagnetic Heisenberg model is of the following form:

$$H_\Lambda = \sum_{i,\, j\in\Lambda} J_{ij} s_i \cdot s_j \tag{1}$$

where $s_i = (s_{ix},\, s_{iy},\, s_{iz})$ are the spin operators localized at lattice point i and $J_{ij} \geqslant 0$ denotes the antiferromagnetic interaction between two spins at sites i and j, respectively. For simplicity, we shall assume that each localized spin has the same angular momentum $s \geqslant \frac{1}{2}$. The lattice is called bipartite with respect to Hamiltonian (1) if it can be divided into two separate sublattices, A and B, such that $J_{ij} \equiv 0$ when both lattice points i and j belong to the same sublattice A or B. Define the total spin and the total spin z-component operators by $S^2 = (\sum s_i)^2$ and $S_z = \sum s_{iz}$. We have

$$[H_\Lambda,\, S^2] = 0 \qquad [H_\Lambda,\, S_z] = 0\,. \tag{2}$$

Therefore, each eigenvector of H_Λ is also an eigenvector of S^2 and S_z.

For such a model, Lieb and Mattis proved the following theorem.

Theorem. (Lieb and Mattis): Let N_A and N_B be the numbers of lattice points in sublattice A and B, respectively. Let $L \equiv s|N_A - N_B|$. Then, the ground states of the antiferromagnetic Heisenberg model have the total spin $L(L+1)$. Furthermore, apart from the trivial $2L+1$ spin degeneracy, the ground state is non-degenerate.

By the Lieb and Mattis theorem, if the difference $|N_A - N_B| = \mathrm{O}(N_\Lambda)$, then the ground state of this generalized antiferromagnetic Heisenberg model has a spontaneous magnetization. However, this theorem tells us nothing about the existence of MLRO in these $2L+1$ degenerate ground states, which we shall address in the following. For this purpose, we shall now recall the definitions of the spin correlation functions and MLRO.

Let $\Psi_0(\Lambda)$ be the non-degenerate ground state of the generalized antiferromagnetic Heisenberg model. Let $s_{i+} \equiv s_{ix} + \mathrm{i}s_{iy}$ and $s_{i-} \equiv s_{ix} - \mathrm{i}s_{iy}$. When Λ is the simple cubic lattice, which is a special case of the bipartite lattices, we can simply define the *transverse* and *longitudinal* spin correlation functions by

$$g_{\mathrm{T}}(\boldsymbol{q}) \equiv \langle\Psi_0(\Lambda)|S_+(-\boldsymbol{q})S_-(\boldsymbol{q})|\Psi_0(\Lambda)\rangle \qquad g_{\mathrm{L}}(\boldsymbol{q}) \equiv \langle\Psi_0(\Lambda)|S_z(-\boldsymbol{q})S_z(\boldsymbol{q})|\Psi_0(\Lambda)\rangle \tag{3}$$

where

$$S_\alpha(\boldsymbol{q}) \equiv \frac{1}{\sqrt{N_\Lambda}}\sum_{\boldsymbol{i}\in\Lambda} s_{i\alpha}\exp\left(\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{i}\right) \qquad \alpha = +,\ -,\ z \tag{4}$$

and $\boldsymbol{q}$ is a reciprocal vector of the simple cubic lattice. If the inequality $g_{\mathrm{T}}(\boldsymbol{q}) \geqslant \beta N_\Lambda$ ($g_{\mathrm{L}}(\boldsymbol{q}) \geqslant \beta N_\Lambda$), where $\beta > 0$ is a constant independent of N_Λ, holds for some reciprocal vector $\boldsymbol{q}$, we say that $\Psi_0(\Lambda)$ has a momentum-$\boldsymbol{q}$ transverse (longitudinal) MLRO. In particular, the momentum-0 MLRO is the well known ferromagnetic long-range order and the momentum-$\boldsymbol{Q}$ ($\boldsymbol{Q} = (\pi,\ \pi, \ldots, \pi)$) MLRO represents the antiferromagnetic long-range order.

For an arbitrary bipartite lattice Λ, the above definitions may not be suitable. To extend the definitions of MLRO to the generalized antiferromagnetic Heisenberg model on such a lattice, we introduce the following definition.

Definition 1. A complex function $f(\boldsymbol{i})$ defined on lattice Λ is called admissible if $|f(\boldsymbol{i})| = 1$ for any $\boldsymbol{i} \in \Lambda$. For a specific admissible function $f(\boldsymbol{i})$, we define

$$g_{\mathrm{T}}(f) \equiv \langle\Psi_0(\Lambda)|S_+(\bar{f})S_-(f)|\Psi_0(\Lambda)\rangle \qquad g_{\mathrm{L}}(f) \equiv \langle\Psi_0(\Lambda)|S_z(\bar{f})S_z(f)|\Psi_0(\Lambda)\rangle \tag{5}$$

to be the transverse and longitudinal momentum-f spin correlation functions of $\Psi_0(\Lambda)$, respectively. In (5), $S_\alpha(f) \equiv (1/\sqrt{N_\Lambda})\sum_{\boldsymbol{i}\in\Lambda} f(\boldsymbol{i})s_{i\alpha}$, $\alpha = +,\ -,\ z$.

Obviously, the correlation functions defined above coincide with their conventional counterpart on the simple cubic lattice if we choose $f(\boldsymbol{i}) = \exp(\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{i})$. In particular, letting

$$\epsilon(\boldsymbol{i}) = \begin{cases} 1 & \text{if } \boldsymbol{i} \in A \\ -1 & \text{if } \boldsymbol{i} \in B \end{cases} \tag{6}$$

we see that the momentum-ϵ correlation functions, $g_{\mathrm{T}}(\epsilon)$ and $g_{\mathrm{L}}(\epsilon)$, are the transverse and longitudinal antiferromagnetic spin correlation functions of $\Psi_0(\Lambda)$. Similarly, the ferromagnetic correlation functions can be written as $g_{\mathrm{T}}(\nu)$ and $g_{\mathrm{L}}(\nu)$ with $\nu(\boldsymbol{i}) = 1$ for any $\boldsymbol{i} \in \Lambda$. With definition 1, the conditions for the existence of MLRO can be easily generalized to the ground states of the generalized antiferromagnetic Heisenberg model on an arbitrary bipartite lattice Λ.

Now, we are ready to show our new results. First, we prove the following theorem.

Theorem 1. Let Λ be a finite bipartite lattice with respect to Hamiltonian (1). Assume that $L = s|N_A - N_B| = \mathrm{O}(N_\Lambda)$. Then, a ground state $\Psi_0(M,\ \Lambda)$ ($-L \leqslant M \leqslant L$) of the generalized antiferromagnetic Heisenberg model on Λ has both transverse ferromagnetic and antiferromagnetic long-range orders, if M satisfies

$$L^2 - M^2 \geqslant \delta N_\Lambda^2 \tag{7}$$

where $\delta > 0$ is a constant independent of N_Λ.

Proof. We first perform a unitary transformation on H_Λ by letting

$$s_{ix} \to \epsilon(\boldsymbol{i})s_{ix} \qquad s_{iy} \to \epsilon(\boldsymbol{i})s_{iy} \qquad s_{iz} \to s_{iz}\,. \tag{8}$$

Formally, this unitary transformation can be achieved by operator $U_0 = \exp\left(i\pi \sum_{i\in B} s_{iz}\right)$. Under this transformation, the Hamiltonian H_Λ is mapped onto $\widetilde{H}_\Lambda$, which has the following form:

$$\widetilde{H}_\Lambda = \sum_{i,\, j\in\Lambda} \left[-J_{ij}\left(s_{ix}s_{jx} + s_{iy}s_{jy}\right) + J_{ij}s_{iz}s_{jz}\right]. \tag{9}$$

Consequently, H_Λ and $\widetilde{H}_\Lambda$ have the same spectrum. It is easy to see that $\left[\widetilde{H}_\Lambda,\, S_z\right] = 0$ still holds. Therefore, the Hilbert space of $\widetilde{H}_\Lambda$ can be divided into numerous subspaces. Each of them is characterized by a quantum number $S_z = M$. For a specific subspace V_M, we choose a basis of state vectors in the following manner.

$$\phi_\alpha = C\,(s_{1+})^{m_1}\,(s_{2+})^{m_2}\cdots\left(s_{N_\Lambda+}\right)^{m_{N_\Lambda}}\,\chi \tag{10}$$

where χ is the state in which $s_{iz} = -s$ and C is a positive normalization constant. Naturally, we require that $\left(m_1 + m_2 + \cdots + m_{N_\Lambda} - N_\Lambda\right)s = M$. In terms of this basis, we write $\widetilde{H}_\Lambda$ in a matrix. It is not difficult to see that all the off-diagonal elements of this matrix are non-positive, i.e. $\left(\widetilde{H}_\Lambda\right)_{mn} \leqslant 0$ if $m \neq n$. The diagonal elements of $\widetilde{H}_\Lambda$ are either positive or negative but all of them satisfy $|a_{mm}| \leqslant K$, where K is a positive constant. Furthermore, this matrix is irreducible. In other words, for any given pair of indices $(m,\, n)$, one can find a positive integer N such that $\left(\widetilde{H}_\Lambda^N\right)_{m,\,n} \neq 0$. For such a matrix, we have the well known Perron–Frobenius theorem [10]. It tells us that the lowest eigenvalue of $\widetilde{H}_\Lambda$ in V_M is non-degenerate and the ground state $\widetilde{\Psi}_0(M,\, \Lambda)$ is a linear combination of $\{\phi_\alpha\}$ with positive coefficients. Namely, we have

$$\widetilde{\Psi}_0(M,\, \Lambda) = \sum_\beta a_\beta \phi_\beta \qquad a_\beta > 0\,. \tag{11}$$

This positivity of coefficients leads to the following important consequence.

Let us take two arbitrary lattice points $(k,\, h)$ and consider the expectation value of operator $s_{k+}s_{h-}$ in $\widetilde{\Psi}_0(M,\, \Lambda)$. Since

$$\begin{aligned} s_{k+}|k,\, m\rangle &= \sqrt{s(s+1) - m(m+1)}\,|k,\, m+1\rangle \\ s_{h-}|h,\, m\rangle &= \sqrt{s(s+1) - m(m-1)}\,|h,\, m-1\rangle \end{aligned} \tag{12}$$

we have

$$\langle\widetilde{\Psi}_0(M,\, \Lambda)|s_{k+}s_{h-}|\widetilde{\Psi}_0(M,\, \Lambda)\rangle \geqslant 0 \tag{13}$$

by the positivity of coefficients.

We now perform the inverse unitary transformation U_0^{-1} on the subspace V_M. Obviously, V_M is invariant under U_0^{-1}. Also, $\widetilde{H}_\Lambda$ is mapped onto H_Λ and $\widetilde{\Psi}_0(M,\, \Lambda)$ onto $\Psi_0(M,\, \Lambda)$. However, inequality (13) now reads

$$\langle\Psi_0(M,\, \Lambda)|s_{k+}s_{h-}|\Psi_0(M,\, \Lambda)\rangle \begin{cases} \geqslant 0 & \text{if } k,\, h \in A \text{ or } B \\ \leqslant 0 & \text{otherwise}\,. \end{cases} \tag{14}$$

Therefore, the transverse spin correlation function of the non-degenerate ground state of H_Λ in each subspace V_M satisfies

$$g_{\mathrm{T}}(\epsilon) \geqslant g_{\mathrm{T}}(\nu)\,. \tag{15}$$

It implies that, if the ground state $\Psi_0(M,\, \Lambda)$ has the transverse ferromagnetic long-range order, it must also support the transverse antiferromagnetic long-range order.

On the other hand, by the Lieb and Mattis theorem, when $|N_A - N_B| \neq 0$, the global ground states of H_Λ have the total angular momentum $L = s|N_A - N_B|$. Therefore, the non-degenerate ground state $\Psi_0(M, \Lambda)$ in each subspace V_M subject to $-L \leqslant M \leqslant L$ is a global ground state of H_Λ. When L and M satisfy condition (7) of theorem 1, we have

$$\begin{aligned} g_{\rm T}(\nu) &= \langle \Psi_0(M, \Lambda)|S_+(\bar{\nu})S_-(\nu)|\Psi_0(M, \Lambda)\rangle \\ &= \frac{1}{N_\Lambda}\langle \Psi_0(M, \Lambda)|S_x^2 + S_y^2 + S_z|\Psi_0(M, \Lambda)\rangle \\ &= \frac{1}{N_\Lambda}\langle \Psi_0(M, \Lambda)|S^2 - S_z^2 + S_z|\Psi_0(M, \Lambda)\rangle \\ &\geqslant \frac{1}{N_\Lambda}\left[L^2 - M^2 + M\right] \geqslant \delta N_\Lambda . \end{aligned} \tag{16}$$

Therefore, $\Psi_0(M, \Lambda)$ has the transverse ferromagnetic long-range order. Consequently, by inequality (15), it also has the transverse antiferromagnetic long-range order. That ends our proof. □

Next, we shall extend theorem 1 to the longitudinal MLRO. At first glance, this extension seems straightforward since the Hamiltonian has the $SU(2)$ spin symmetry. However, as we show in the following, this problem demands more careful thinking due to the high degeneracy of the global ground states of H_Λ. To make our point more clear, let us consider a specific global ground state $\Psi_0(M = 0, \Lambda)$. Apparently, its quantum numbers S^2 and S_z satisfy the condition of theorem 1, if $|N_A - N_B| = O(N_\Lambda)$. Therefore, this state has both transverse ferromagnetic and antiferromagnetic long-range orders by theorem 1. However, a direct calculation reveals that it has no longitudinal ferromagnetic long-range order. Worse, one does not know how to prove the existence of the longitudinal antiferromagnetic long-range order in $\Psi_0(M = 0, \Lambda)$. As this example shows, the existence of the *transverse* MLRO in a global ground state of H_Λ does not imply the existence of the *longitudinal* MLRO in the same state when the global ground states are highly degenerate.

Remark 1. Indeed, the existence of the longitudinal antiferromagnetic long-range order in the ground state of the antiferromagnetic Heisenberg model on the simple cubic lattice has been proven by the authors of [6] and [7] in a completely different way. However, in their proofs, they relied heavily on the so-called reflection positivity, which is not enjoyed by the generalized antiferromagnetic Heisenberg model on an arbitrary bipartite lattice.

To begin with, we first prove the following lemma.

Lemma 1. Let $f(i)$ be an admissible function defined on Λ. Let $\Psi_0(M, \Lambda)$ be one of the $2L + 1$ global ground states of H_Λ. Then, the identity

$$g_{\rm T}(f) = 2\langle \Psi_0(M, \Lambda)|S_x(\bar{f})S_x(f)|\Psi_0(M, \Lambda)\rangle + \frac{M}{N_\Lambda} \tag{17}$$

holds.

Proof. By the definitions of $S_+(\bar{f})$ and $S_-(f)$, $g_{\rm T}(f)$ can be written as

$$\begin{aligned} g_{\rm T}(f) = \langle \Psi_0(M, \Lambda)|S_x(\bar{f})S_x(f) + S_y(\bar{f})S_y(f)|\Psi_0(M, \Lambda)\rangle \\ + \frac{\mathrm{i}}{N_\Lambda}\langle \Psi_0(M, \Lambda)\left| \sum_{k,h\in\Lambda} \bar{f}(k)f(h)[s_{ky}s_{hx} - s_{kx}s_{hx}] \right| \Psi_0(M, \Lambda)\rangle . \end{aligned} \tag{18}$$

We simplify the last sum on the right-hand side of (18) first. Take two distinct lattice points k and h. Obviously, we have $[s_{kx}, s_{hy}] = [s_{ky}, s_{hx}] = 0$. Therefore, $s_{ky}s_{hx} - s_{kx}s_{hy}$ is an Hermitian operator and hence its expectation value in any state is a real quantity. On the other hand, since H_Λ is a real matrix, its global ground state $\Psi_0(M, \Lambda)$ can be chosen as a real state vector. Consequently, the expectation value F of $s_{ky}s_{hx} - s_{kx}s_{hy}$ in $\Psi_0(M, \Lambda)$ must be a pure imaginary quantity because the operator is an imaginary matrix. This implies that $F \equiv 0$. Therefore, the sum on the right-hand side of (18) is reduced to $(\mathrm{i}/N_\Lambda)\langle\Psi_0(M, \Lambda)|\sum_{k\in\Lambda}\bar{f}(k)f(k)[s_{ky}s_{kx} - s_{kx}s_{ky}]|\Psi_0(M, \Lambda)\rangle$. Using the definition of the admissible functions and the spin-commutation relations, we find that this expectation is equal to M/N_Λ.

Next, we apply the unitary operator $U_1 = \exp\left((\mathrm{i}\pi/2)\sum_{i\in\Lambda}s_{iz}\right)$, which rotates each localized spin about the s_z axis by an angle $\pi/2$, to rewrite the expectation value of $S_y(\bar{f})S_y(f)$ in $\Psi_0(M, \Lambda)$. We obtain

$$
\begin{aligned}
&\langle\Psi_0(M, \Lambda)|S_y(\bar{f})S_y(f)|\Psi_0(M, \Lambda)\rangle \\
&\quad= \langle\Psi_0(M, \Lambda)|U_1^\dagger\left(U_1S_y(\bar{f})U_1^\dagger U_1S_y(f)U_1^\dagger\right)U_1|\Psi_0(M, \Lambda)\rangle \\
&\quad= \left\langle\Psi_0(M, \Lambda)\left|\exp\left(-\frac{\mathrm{i}\pi}{2}M\right)S_x(\bar{f})S_x(f)\exp\left(\frac{\mathrm{i}\pi}{2}M\right)\right|\Psi_0(M, \Lambda)\right\rangle \\
&\quad= \langle\Psi_0(M, \Lambda)|S_x(\bar{f})S_x(f)|\Psi_0(M, \Lambda)\rangle\,.
\end{aligned}
\tag{19}
$$

Substituting (19) into (18), lemma 1 is proved. □

Remark 2. In a previous paper [11], we have used the same technique as in the proof of lemma 1 to show that a strongly correlated hard-core Boson model has no energy gap in the thermodynamic limit.

After reading the proof of lemma 1, one would think that a similar identity $\langle\Psi_0(M, \Lambda)|S_x(\bar{f})S_x(f)|\Psi_0(M, \Lambda)\rangle = \langle\Psi_0(M, \Lambda)|S_z(\bar{f})S_z(f)|\Psi_0(M, \Lambda)\rangle$ can easily be proven by replacing U_1 with $U_2 = \exp\left((\mathrm{i}\pi/2)\sum_{i\in\Lambda}s_{iy}\right)$. Unfortunately, this is not true. Indeed, we do have $U_2S_x(\bar{f})U_2^\dagger U_2S_x(f)U_2^\dagger = S_z(\bar{f})S_z(f)$. However, since $U_2H_\Lambda U_2^\dagger = H_\Lambda$, the $2L+1$ global ground states of H_Λ, $\{\Psi_0(M, \Lambda)\}$, $-L \leqslant M \leqslant L$, will be transformed in terms of a $(2L+1)$-dimensional irreducible unitary representation of the $SU(2)$ group under U_2. In other words, $U_2|\Psi_0(M, \Lambda)\rangle$ is a very complicated linear combination of $\{\Psi_0(M, \Lambda)\}$. Although the coefficients of this linear combination can be determined by using group theory [12], one can hardly derive any useful information on the longitudinal MLRO in $\Psi_0(M, \Lambda)$ from this messy calculation. Therefore, one has to think more carefully.

We notice that, when the external fields are absent, the $2L+1$ degenerate global ground states of H_Λ have the same statistical mechanics weight. In other words, they are indistinguishable experimentally. Therefore, if one tries to detect MLRO in these states by some means (such as the neutron scattering technique), one can only obtain averaged data. This fact leads us to introduce the following definition.

Definition 2. Let $f(i)$ be an admissible function defined on lattice Λ and let $\{\Psi_0(M, \Lambda)\}$ be the global ground states of H_Λ. We define the averaged spin correlation functions by

$$
\begin{aligned}
G_{\mathrm{T}}(f) &\equiv \frac{1}{2L+1}\sum_{M=-L}^{L}\langle\Psi_0(M, \Lambda|S_+(\bar{f})S_-(f)|\Psi_0(M, \Lambda)\\
G_{\mathrm{L}}(f) &\equiv \frac{1}{2L+1}\sum_{M=-L}^{L}\langle\Psi_0(M, \Lambda)|S_z(\bar{f})S_z(f)|\Psi_0(M, \Lambda)\,.
\end{aligned}
\tag{20}
$$

Since lemma 1 holds for each $\Psi_0(M, \Lambda)$, we immediately obtain

$$
G_{\mathrm{T}}(f) = \frac{2}{2L+1}\sum_{M=-L}^{L}\langle\Psi_0(M, \Lambda)|S_x(\bar{f})S_x(f)|\Psi_0(M, \Lambda)\rangle\,. \tag{21}
$$

With definition 2, we now prove the following.

Theorem 2. Let Λ be a bipartite lattice with respect to H_Λ. If $|N_A - N_B| = O(N_\Lambda)$, then the global ground states of the generalized antiferromagnetic Heisenberg model on Λ have both *longitudinal* ferromagnetic and antiferromagnetic long-range orders.

Proof. First, we show that

$$G_{\mathrm{T}}(f) = 2G_{\mathrm{L}}(f) \tag{22}$$

holds for any admissible function $f(i)$. In fact, by (21), we need only show that the following identity

$$\sum_{M=-L}^{L} \langle \Psi_0(M,\ \Lambda)|S_x(\bar{f})S_x(f)|\Psi_0(M,\ \Lambda)\rangle = \sum_{M=-L}^{L} \langle \Psi_0(M,\ \Lambda)|S_z(\bar{f})S_z(f)|\Psi_0(M,\ \Lambda)\rangle \tag{23}$$

holds for any admissible function $f(i)$.

Applying the unitary operator $U_2 = \exp\left[(\mathrm{i}\pi/2)\sum_{i\in\Lambda} S_{iy}\right]$ to the left-hand side of (23), we have

$$\begin{aligned}
&\sum_{M=-L}^{L} \langle \Psi_0(M,\ \Lambda)|S_x(\bar{f})S_x(f)|\Psi_0(M,\ \Lambda)\rangle \\
&\quad= \sum_{M=-L}^{L} \langle \Psi_0(M,\ \Lambda)|U_2^\dagger \left(U_2 S_x(\bar{f})U_2^\dagger U_2 S_x(f)U_2^\dagger\right) U_2|\Psi_0(M,\ \Lambda)\rangle \\
&\quad= \sum_{M=-L}^{L}\sum_{M_1=-L}^{L}\sum_{M_2=-L}^{L} \bar{u}_{MM_1}u_{MM_2}\langle \Psi_0(M_1,\ \Lambda)|S_z(\bar{f})S_z(f)|\Psi_0(M_2,\ \Lambda)\rangle \\
&\quad= \sum_{M_1=-L}^{L}\sum_{M_2=-L}^{L} \delta_{M_1,\,M_2}\langle \Psi_0(M_1,\ \Lambda)|S_z(\bar{f})S_z(f)|\Psi_0(M_2,\ \Lambda)\rangle \\
&\quad= \sum_{M_1=-L}^{L} \langle \Psi_0(M_1,\ \Lambda)|S_z(\bar{f})S_z(f)|\Psi_0(M_1,\ \Lambda)\rangle\,.
\end{aligned} \tag{24}$$

In the above derivation, we used the fact that $U = (u_{mn})$ is a unitary matrix and hence

$$\sum_{M=-L}^{L} \bar{u}_{MM_1}u_{MM_2} = \delta_{M_1,\,M_2} \tag{25}$$

where $\delta_{M_1,\,M_2}$ is the well known Kronecker notation.

On the other hand, we notice that inequality (15) holds for each of the $2L+1$ global ground states. Consequently, it holds for $G_{\mathrm{T}}(f)$. Namely, we have $G_{\mathrm{T}}(\epsilon) \geqslant G_{\mathrm{T}}(\nu)$. Therefore, by identity (22), we obtain

$$G_{\mathrm{L}}(\epsilon) = \tfrac{1}{2}G_{\mathrm{T}}(\epsilon) \geqslant \tfrac{1}{2}G_{\mathrm{T}}(\nu) = G_{\mathrm{L}}(\nu)\,. \tag{26}$$

A direct calculation of $G_{\mathrm{L}}(\nu)$ yields

$$\begin{aligned}
G_{\mathrm{L}}(\nu) &= \frac{1}{(2L+1)N_\Lambda}\sum_{M=-L}^{L} \langle \Psi_0(M,\ \Lambda)|S_z S_z|\Psi_0(M,\ \Lambda)\rangle \\
&= \frac{2}{(2L+1)N_\Lambda}\left(L^2 + (L-1)^2 + \cdots + 1^2\right) \geqslant \frac{L^2}{3N_\Lambda}\,.
\end{aligned} \tag{27}$$

Therefore, when $L = s|N_A - N_B| = O(N_\Lambda)$, we have $G_L(\epsilon) \geqslant G_L(\nu) \geqslant \beta N_\Lambda$. It implies that the global ground states of the Heisenberg model on Λ have both longitudinal ferromagnetic and antiferromagnetic long-range orders. Therefore, the model represents a ferrimagnet.

Our proof is accomplished. □

Before finishing this article, we would like to make a remark.

Remark 3. Although we only proved lemma 1 and theorem 2 for the generalized antiferromagnetic Heisenberg model on a bipartite lattice, these results can easily be transplanted to the positive-U Hubbard model without further ado by using the following operator identities:

$$s_{i+} = c_{i\uparrow}^\dagger c_{i\downarrow} \qquad s_{i-} = c_{i\downarrow}^\dagger c_{i\uparrow} \qquad s_{iz} = \left(\tfrac{1}{2}\right)(n_{i\uparrow} - n_{i\downarrow}) . \tag{28}$$

In summary, we have shown in this article that the global ground states of the generalized antiferromagnetic Heisenberg model on a bipartite lattice Λ with $|N_A - N_B| = O(N_\Lambda)$ have both ferromagnetic and antiferromagnetic long-range orders. We have also shown that the antiferromagnetic long-range order is always predominant, as Neel proposed. Therefore, this model represents a ferrimagnet.

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