Bifurcation of ground states and ferrimagnetic long-range order in anisotropic mixed-spin systems

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In this paper, we study a generalized anisotropic mixed-spin ferrimagnetic Heisenberg model on an arbitrary bipartite lattice. We prove rigorously that, under some very general conditions, this model has a unique ground state with $S_z = 0$ in the XY regime and two degenerate ground states with nonzero magnetization in the Ising regime, respectively. Therefore, the isotropic point of this model is a bifurcation point for its ground states. Furthermore, we also show that, if magnetization of the ground states in the Ising regime is a macroscopic quantity in the thermodynamic limit, then these states have both ferromagnetic and antiferromagnetic long-range order. In other words, they are ferrimagnetically ordered. These conclusions confirm the previous results derived by numerical calculations on small one-dimensional mixed-spin chains.

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I. INTRODUCTION

Recently, the behaviors of quasi-one-dimensional quantum ferrimagnets attracted many physicists' interest.[1–25] Experimentally, such quasi-one-dimensional compounds have been successfully synthesized.[26,27] Most of them are molecular magnets containing two different transitional-metal magnetic ions, which are alternatively distributed on the lattice. The experimental results imply that the magnetic properties of these materials can be described by the quantum Heisenberg spin model with antiferromagnetic couplings between the localized spins of different values, such as $s_i = 1/2$ and $S_{i+1} = 1$.

Based on this understanding, further investigations showed clearly that the ground states of these systems are ferrimagnetic and support both ferromagnetic and antiferromagnetic long-range order.[3–6] Consequently, the elementary excitations have two branches: While the ferromagnetic excitations, which reduce magnetization of the system, are gapless, the antiferromagnetic excitations are gapped.[4–10] This structure of the excitation spectrum leads to $T^{1/2}$ and T^{-1} behaviors of the specific heat and the magnetic susceptibility at low temperature, respectively.[4,5,10–13]

Extension of this model to the anisotropic cases was made and studied by several groups.[1,9,14,15] In particular, by using exact numerical diagonalization on small samples and exploiting conformal invariance of the system in the continuum limit, Alcaraz and Malvezzi[1] found that, in the XY regime, the ground state of the system is nondegenerate and critical. On the other hand, in the Ising regime, the system has two degenerate ground states and each of them has a macroscopic magnetization.[1] Therefore, the isotropic point of the ferrimagnetic Heisenberg chain is, in fact, a bifurcation point of its ground states. These conclusions were further confirmed by Ono *et al.*[14] By applying the density-matrix renormalization-group technique,[28] they also found that, while each ground state of the model in the Ising regime is ferrimagnetically ordered, the longitudinal spin correlation in the unique ground state of the same system in the XY regime is short ranged.[14] In addition, Sakai and Yamamoto studied the magnetization plateau of the anisotropic ferrimagnetic Heisenberg chains in an external magnetic field.[9,15]

Then, a natural question arose as to whether these conclusions derived by numerical calculations on the one-dimensional mixed-spin chains can be rigorously reestablished for the ferrimagnetic Heisenberg model on an arbitrary bipartite lattice in higher dimensions. In the present paper, we would like to address this problem and show that, for a large class of the antiferromagnetic Heisenberg model on a higher-dimensional bipartite lattice, the above-mentioned results still hold true. In particular, their ground states in the Ising regime have both ferromagnetic and antiferromagnetic long-range order.

To begin, let us first recall several definitions and notation. We take a finite lattice Λ and let N_Λ be the number of lattice sites. The Hamiltonian of the ferrimagnetic Heisenberg model, which we shall study, is of the following form:

$$H = \sum_{\langle \mathbf{ij} \rangle} J_{\mathbf{ij}} (\tilde{S}_{\mathbf{i}x} \tilde{S}_{\mathbf{j}x} + \tilde{S}_{\mathbf{i}y} \tilde{S}_{\mathbf{j}y}) + \sum_{\langle \mathbf{ij} \rangle} J'_{\mathbf{ij}} \tilde{S}_{\mathbf{i}z} \tilde{S}_{\mathbf{j}z}, \tag{1}$$

where $\langle \mathbf{ij} \rangle$ denotes a pair of lattice sites and $\tilde{\mathbf{S}}_{\mathbf{i}}$ represents the localized spin operators at lattice site $\mathbf{i}$. *For a ferrimagnet, these spins may have different values at different lattice sites*. The parameters $J_{\mathbf{ij}} > 0$ and $J'_{\mathbf{ij}}$ are the antiferromagnetic couplings between the localized spins. We further assume that, in terms of Hamiltonian (1), lattice Λ is bipartite. In other words, it can be divided into two separate sublattices A and B such that $J_{\mathbf{ij}}$ and $J'_{\mathbf{ij}}$ only couple the spins at lattice sites $\mathbf{i}$ and $\mathbf{j}$, which belong to different sublattices. In the following, we shall use N_A and N_B to denote the numbers of lattice sites in A and B, respectively.

In fact, Hamiltonian (1) has been used to describe two categories of ferrimagnets in the literature. In the first case, sublattices A and B have the same number of sites, i.e., $N_A = N_B$. But the localized spins on two sublattices have different values. For example, we may have $|\tilde{S}_{\mathbf{i}}| = 1/2$ for $\mathbf{i} \in A$ and $|\tilde{S}_{\mathbf{i}}| = 1$ for $\mathbf{i} \in B$. The one-dimensional antiferromagnetic mixed-spin chains, which were studied in Refs. 1–25, belong to this category. In the second case, all the localized spins on either sublattice A or B have the same value S. However, sublattices A and B contain different numbers of sites, i.e., $N_A \neq N_B$ in this case. (Some examples can be found in Refs. 29–34.) In the following, without special notice, we shall treat both cases on the same footing.

By the definition of Hamiltonian (1), we notice that the total spin-z component operator $\hat{S}_z = \Sigma_{\mathbf{i}\in\Lambda}\tilde{S}_{\mathbf{i}z}$ commutes with the Hamiltonian. Consequently, the Hilbert space of H can be split into numerous subspaces $\{V(M)\}$. In each subspace $V(M)$, the quantum number $S_z = M$ is specified. In particular, at the isotropic point, $J_{\mathbf{ij}} = J'_{\mathbf{ij}}$, the total spin operator $\hat{S}^2$ is also a conserved quantity and hence, the well-known Lieb-Mattis theorem applies.[35] According to this theorem, the ground state of the isotropic ferrimagnetic Heisenberg Hamiltonian is highly degenerate and has spin $S = |N_A S_A - N_B S_B|$, where S_A and S_B are total spins on the A and B sublattices, respectively. As an application of this theorem, in Ref. 3, Tian further showed that the mixed-spin chain with different spins S_A and S_B being alternatively distributed along the lattice has both ferromagnetic and antiferromagnetic long-range order at the isotropic point. Therefore, it is a ferrimagnet. The same conclusion has been also proven for the second category of ferrimagnets with unequal numbers of sublattice sites.[30]

In the following, we investigate the degeneracy of the ground states and the possible existence of the magnetic long-range order in these states for the antiferromagnetic XXZ Hamiltonian (1) on an arbitrary bipartite lattice in higher dimensions. Two regions of parameters will be separately studied. The first one is the XY regime with $-J_{\mathbf{ij}} < J'_{\mathbf{ij}} < J_{\mathbf{ij}}$ being satisfied by any admissible pair of lattice-site indices $\mathbf{i}$ and $\mathbf{j}$. On the other hand, the Ising regime is characterized by the condition $J_{\mathbf{ij}} < J'_{\mathbf{ij}}$. In particular, for the anisotropic mixed-spin chain models considered in Refs. 1, 9, 14, and 15 the antiferromagnetic couplings are given by $J_{ij} = J\delta_{j,i+1}$ and $J'_{ij} = J'\delta_{j,i+1}$. Therefore, we have $-J < J' < J$ in the XY regime and $0 < J < J'$ in the Ising regime for spins at a pair of nearest-neighbor lattice sites. Our main results can be summarized in the following theorems.

Theorem 1. Let Λ be an arbitrary finite bipartite lattice on which Hamiltonian (1) is defined. For technical reasons, quantity $N_A S_A + N_B S_B$ is assumed to be an integer. Under these conditions, the ground state of Hamiltonian (1) in the XY regime is nondegenerate and has zero magnetization ($S_z = 0$). On the other hand, in the Ising regime, the degeneracy of the ground state becomes twofold and the total spin-z component of these ground states has values $S_z = \pm|N_A S_A - N_B S_B|$.

Theorem 2. Let $\Psi_0^{(1)}$ and $\Psi_0^{(2)}$ be the ground states of the anisotropic ferrimagnetic Heisenberg Hamiltonian H in the Ising regime with spin numbers $S_z = |N_A S_A - N_B S_B|$ and $S_z = -|N_A S_A - N_B S_B|$, respectively. If $|N_A S_A - N_B S_B|$ is a quantity of order $O(N_\Lambda)$ in the thermodynamic limit ($N_\Lambda \to \infty$), which is a condition satisfied by the mixed-spin model studied in Refs. 1–25, then both $\Psi_0^{(1)}$ and $\Psi_0^{(2)}$ have longitudinal ferromagnetic and antiferromagnetic long-range order. In other words, these ground states have ferrimagnetic long-range order.

In the following, we establish these theorems on a mathematically rigorous basis. To make our proofs more clear and readable, we organize the rest part of this paper as follows. In Sec. II, we prove theorem 1 in detail. In Sec. III, theorem 2 is proven. Finally, in Sec. IV, we offer some general remarks and then summarize our results.

II. THE PROOF OF THEOREM 1

To prove theorem 1, we shall apply a method introduced by Affleck and Lieb,[36] where they considered the standard one-dimensional antiferromagnetic XXZ model with equal spins distributing along the chain and found that the ground states of this model in both the XY regime and the Ising regime are nondegenerate. Therefore, bifurcation of the ground states is hidden in this case. Technically, Affleck and Lieb exploited the nondegeneracy of the ground state of the antiferromagnetic XXZ chain at the isotropic point to establish their theorem. However, for the antiferromagnetic XXZ Hamiltonian (1) on an arbitrary bipartite lattice, the ground states become highly degenerate at the isotropic point.[35] Therefore, we have to take a different approach to reestablish the nondegeneracy of the ground state of Hamiltonian (1) in the XY regime. As we shall show in the following, it can be achieved by introducing an auxiliary Hamiltonian.

Theorem 1 is based on the fact proven by Affleck and Lieb[36] that the ground states of Hamiltonian (1) are, at most, doubly degenerate in either the XY or the Ising regime. Let us first consider the Ising regime. In this case, condition $J_{\mathbf{ij}} < J'_{\mathbf{ij}}$ holds for any admissible pair of lattice-site indices $\mathbf{i}$ and $\mathbf{j}$. Following Ref. 36, we introduce a unitary transformation

$$\hat{U}_1 = \exp\left(i\frac{\pi}{2}\sum_{\mathbf{i}\in\Lambda}\tilde{S}_{\mathbf{i}y}\right), \tag{2}$$

which rotates each spin in Λ by an angle $\pi/2$ about the spin-y axis. Under this transformation, Hamiltonian (1) is mapped into the following equivalent form:

$$H_1 = \hat{U}_1^\dagger H \hat{U}_1 = \sum_{\langle \mathbf{ij}\rangle} (J'_{\mathbf{ij}}\tilde{S}_{\mathbf{i}x}\tilde{S}_{\mathbf{j}x} + J_{\mathbf{ij}}\tilde{S}_{\mathbf{i}y}\tilde{S}_{\mathbf{j}y}) + \sum_{\langle \mathbf{ij}\rangle} J_{\mathbf{ij}}\tilde{S}_{\mathbf{i}z}\tilde{S}_{\mathbf{j}z}. \tag{3}$$

To go further, we need to change the sign of the couplings in the first term of H_1. This can be achieved by applying another unitary transformation $\hat{U}_2 = \exp(i\pi\Sigma_{\mathbf{i}\in A}\tilde{S}_{\mathbf{i}z})$, which rotates each spin in sublattice A by an angle π about the spin-z axis and keeps the spins in sublattice B unchanged. Now, the twice transformed Hamiltonian reads

$$\begin{aligned} H_2 &= \hat{U}_2^\dagger H_1 \hat{U}_2 = (\hat{U}_1\hat{U}_2)^\dagger H (\hat{U}_1\hat{U}_2) \\ &= -\sum_{\langle \mathbf{ij}\rangle} (J'_{\mathbf{ij}}\tilde{S}_{\mathbf{i}x}\tilde{S}_{\mathbf{j}x} + J_{\mathbf{ij}}\tilde{S}_{\mathbf{i}y}\tilde{S}_{\mathbf{j}y}) + \sum_{\langle \mathbf{ij}\rangle} J_{\mathbf{ij}}\tilde{S}_{\mathbf{i}z}\tilde{S}_{\mathbf{j}z} \\ &= -\frac{1}{4}\sum_{\langle \mathbf{ij}\rangle} [(J'_{\mathbf{ij}} + J_{\mathbf{ij}})(\tilde{S}_{\mathbf{i}+}\tilde{S}_{\mathbf{j}-} + \tilde{S}_{\mathbf{i}-}\tilde{S}_{\mathbf{j}+}) \\ &\quad + (J'_{\mathbf{ij}} - J_{\mathbf{ij}})(\tilde{S}_{\mathbf{i}+}\tilde{S}_{\mathbf{j}+} + \tilde{S}_{\mathbf{i}-}\tilde{S}_{\mathbf{j}-})] + \sum_{\langle \mathbf{ij}\rangle} J_{\mathbf{ij}}\tilde{S}_{\mathbf{i}z}\tilde{S}_{\mathbf{j}z}. \end{aligned} \tag{4}$$

Notice that *all the couplings in the spin-flipping terms are negative, when* $J_{\mathbf{ij}} < J'_{\mathbf{ij}}$. Another important observation on H_2 is that its subspaces with $S_z =$ odd (or even) integers are connected by the second spin-flipping interaction in H_2, respectively. Consequently, the Hilbert space $\mathcal{V}$ of the Hamiltonian is decomposed into two disconnected sectors $\mathcal{V}_{\text{odd}}$ and $\mathcal{V}_{\text{even}}$. Each of them is a joint of the subspaces $V(M)$ with M being an odd or even integer. Here, we would like to emphasize that, *since H_2 is unitarily equivalent to the antiferromagnetic XXZ Hamiltonian (1) in the Ising regime, their global ground states should have the same degeneracy*.

For definiteness, we take $\mathcal{V}_{\text{even}} = \Sigma_{2m} \oplus V(2m)$, for example. Obviously, in each subspace $V(2m)$, a natural basis of vectors can be chosen as

$$\phi_\alpha(2m) = |S^A_{1z}, S^A_{2z}, \ldots, S^A_{N_A z}, S^B_{1z}, S^B_{2z}, \ldots, S^B_{N_B z}\rangle. \tag{5}$$

In Eq. (5), $S^A_{\mathbf{i}z}$ and $S^B_{\mathbf{j}z}$ are the z components of the spins at sites $\mathbf{i} \in A$ and $\mathbf{j} \in B$, respectively. Index α runs over all the possible spin configurations subject to the constraint condition

$$S^A_{1z} + \cdots + S^A_{N_A z} + S^B_{1z} + \cdots + S^B_{N_B z} = 2m. \tag{6}$$

Apparently, $\cup_{2m}\{\phi_\alpha(2m)\}$, the entire set of these vectors, spans the subspace $\mathcal{V}_{\text{even}}$. Similarly, a natural basis of $\mathcal{V}_{\text{odd}}$ can be also constructed in this way.

In terms of $\cup_{2m}\{\phi_\alpha(2m)\}$, we are able to rewrite Hamiltonian H_2 in $\mathcal{V}_{\text{even}}$ into a matrix $\mathcal{H}_{\text{even}}$, which has the following characteristics:

(i) The off-diagonal elements of $\mathcal{H}_{\text{even}}$ are nonpositive quantities. More precisely, they are either $-(J'_{\mathbf{ij}} + J_{\mathbf{ij}})/4$, $-(J'_{\mathbf{ij}} - J_{\mathbf{ij}})/4$, or zero.

(ii) $\mathcal{H}_{\text{even}}$ is irreducible in the sense that, for any pair of basis vectors $\phi_\alpha(2m_1)$ and $\phi_\beta(2m_2)$, there is a positive integer L such that

$$\langle \phi_\alpha(2m_1)|\mathcal{H}^L_{\text{even}}|\phi_\beta(2m_2)\rangle \neq 0. \tag{7}$$

This fact is based on the the connectivity of lattice Λ by the couplings $\{J_{\mathbf{ij}}\}$ and $\{J'_{\mathbf{ij}}\}$. As a result, any pair of vectors in $\cup_{2m}\{\phi_\alpha(2m)\}$ is also connected by an appropriate number of spin flippings.

To such a matrix, the well-known Perron-Fröbenius theorem in matrix theory applies.[37] This theorem tells us that the lowest eigenstate of $\mathcal{H}_{\text{even}}$ is nondegenerate. Furthermore, its ground-state wave function $\tilde{\Psi}_0(\text{even})$ satisfies Marshall's sign rule.[38] Namely, in the expansion of $\tilde{\Psi}_0(\text{even})$,

$$\tilde{\Psi}_0(\text{even}) = \sum_\alpha \sum_{2m} C_{\alpha m}\phi_\alpha(2m), \tag{8}$$

all the coefficients $C_{\alpha m}$ are real numbers and have the same sign. It is a fact that we shall exploit in the following.

By the same argument, one can also show that the ground state $\tilde{\Psi}_0(\text{odd})$ of Hamiltonian H_2 in the subspace $\mathcal{V}_{\text{odd}}$ is nondegenerate and satisfies Marshall's sign rule. Therefore, the global ground states of H_2 are, at most, doubly degenerate. By the unitary equivalence between H_2 and Hamiltonian (1) in the Ising regime, this conclusion implies that the degeneracy of the global ground state of the antiferromagnetic XXZ Hamiltonian (1) in the Ising regime is, at most, twofold.

Similarly, for the antiferromagnetic XXZ Hamiltonian in the XY regime, we introduce a different unitary transformation $\hat{U}_3 = \exp(i\pi/2\Sigma_{\mathbf{i}\in\Lambda}\tilde{S}_{\mathbf{i}x})$, which rotates each spin in lattice Λ by an angle $\pi/2$ about the spin-x axis. After applying both $\hat{U}_3$ and $\hat{U}_2$ to the Hamiltonian H, we obtain

$$\begin{aligned} H_3 &= (\hat{U}_3\hat{U}_2)^\dagger H(\hat{U}_3\hat{U}_2) \\ &= -\sum_{\langle \mathbf{ij}\rangle} (J_{\mathbf{ij}}\tilde{S}_{\mathbf{i}x}\tilde{S}_{\mathbf{j}x} + J'_{\mathbf{ij}}\tilde{S}_{\mathbf{i}y}\tilde{S}_{\mathbf{j}y}) + \sum_{\langle \mathbf{ij}\rangle} J_{\mathbf{ij}}\tilde{S}_{\mathbf{i}z}\tilde{S}_{\mathbf{j}z} \\ &= -\frac{1}{4}\sum_{\langle \mathbf{ij}\rangle} [(J_{\mathbf{ij}} + J'_{\mathbf{ij}})(\tilde{S}_{\mathbf{i}+}\tilde{S}_{\mathbf{j}-} + \tilde{S}_{\mathbf{i}-}\tilde{S}_{\mathbf{j}+}) + (J_{\mathbf{ij}} - J'_{\mathbf{ij}}) \\ &\quad \times (\tilde{S}_{\mathbf{i}+}\tilde{S}_{\mathbf{j}+} + \tilde{S}_{\mathbf{i}-}\tilde{S}_{\mathbf{j}-})] + \sum_{\langle \mathbf{ij}\rangle} J_{\mathbf{ij}}\tilde{S}_{\mathbf{i}z}\tilde{S}_{\mathbf{j}z}. \end{aligned} \tag{9}$$

In the XY regime, $J_{\mathbf{ij}} > J'_{\mathbf{ij}}$ for any admissible pair of lattice-site indices and hence, all the spin-flipping interactions in H_2 have negative signs. By repeating the above proof for the Ising case, one can easily see that ground states of H_3 as well as of the original Hamiltonian (1) in the XY regime are also, at most, doubly degenerate. With this knowledge, we are ready to prove theorem 1.

Since the ground states of Hamiltonian (1) in subspaces $V(M)$ and $V(-M)$ are trivially doubly degenerate, i.e., $E_0(S_z = M) = E_0(S_z = -M)$, the conclusion established above implies that, in both the XY and the Ising regimes, a level crossing between the ground states and the excited states is forbidden. In fact, if this statement is not true and such a level crossing occurs at some specific points $\{J_{\mathbf{ij}}\} = \{J^c_{\mathbf{ij}}\}$ and $\{J'_{\mathbf{ij}}\} = \{J'^c_{\mathbf{ij}}\}$, say, in the XY regime, then the ground states of Hamiltonian (1) must be, at least, threefold degenerate there. It is a possibility that has been excluded. As a direct consequence of the absence of level crossing between the ground states and the excited states, S_z, the total spin-z component of the ground states should be a continuous function of the parameters $\{J_{\mathbf{ij}}\}$ and $\{J'_{\mathbf{ij}}\}$ varying in both the XY and the Ising regions. On the other hand, because S_z is integer valued, we conclude that its value is constant in each regime.

Now, we let $\{J_{\mathbf{ij}}\}$ tend to zero in the Ising regime. In this limit, Hamiltonian (1) is reduced to the Ising Hamiltonian, whose ground states are trivially degenerate and have spin numbers $S_z = \pm|N_A S_A - N_B S_B|$. Therefore, the ground states of the antiferromagnetic XXZ Hamiltonian (1) in the Ising regime are also doubly degenerate and have the same spin numbers, even if $\{J_{\mathbf{ij}}\} \neq 0$.

Next, we consider Hamiltonian (1) in the XY regime. By letting all the couplings $J'_{\mathbf{ij}}$ tend to zero, we obtain an antiferromagnetic XY Hamiltonian. By applying the unitary transformation $\hat{U}_2$, it can be mapped into a ferromagnetic XY Hamiltonian $H_F(XY)$ on the same lattice. For our purpose, we notice that each subspace $V(S_z=M)$ is still mapped into itself under this transformation. Therefore, the global ground states of the antiferromagnetic and the ferromagnetic XY models have the same spin value S_z. To determine it, we introduce an auxiliary Hamiltonian,

$$\begin{aligned} H_{\rm aux} &= -\sum_{\mathbf{i}\in\Lambda}\sum_{\mathbf{j}\in\Lambda}(\tilde{S}_{\mathbf{i}x}\tilde{S}_{\mathbf{j}x}+\tilde{S}_{\mathbf{i}y}\tilde{S}_{\mathbf{j}y}) \\ &= -\left(\sum_{\mathbf{i}\in\Lambda}\tilde{S}_{\mathbf{i}x}\right)\left(\sum_{\mathbf{j}\in\Lambda}\tilde{S}_{\mathbf{j}x}\right)-\left(\sum_{\mathbf{i}\in\Lambda}\tilde{S}_{\mathbf{i}y}\right)\left(\sum_{\mathbf{j}\in\Lambda}\tilde{S}_{\mathbf{j}y}\right) \\ &= -\left(\sum_{\mathbf{i}\in\Lambda}\tilde{\mathbf{S}}_{\mathbf{i}}\right)\cdot\left(\sum_{\mathbf{j}\in\Lambda}\tilde{\mathbf{S}}_{\mathbf{j}}\right)+\left(\sum_{\mathbf{i}\in\Lambda}\tilde{S}_{\mathbf{i}z}\right)\left(\sum_{\mathbf{j}\in\Lambda}\tilde{S}_{\mathbf{j}z}\right) \end{aligned} \quad (10)$$

on the same lattice with the same distribution of the spin operators as $H_F(XY)$. Apparently, by its definition, $H_{\rm aux}$ has equal ferromagnetic coupling between any pair of the localized spins. Its usefulness relies on the fact that *it is connected to $H_F(XY)$ by continuously changing the ferromagnetic couplings among the spins without inducing a level crossing between the ground states and the excited states*. [The proof of this statement can be easily achieved by repeating the arguments in proving the absence of such a level crossing for the antiferromagnetic XXZ Hamiltonian (1) in the XY regime.] Therefore, we are able to read spin numbers S_z of the global ground states of both $H_F(XY)$ and Hamiltonian (1) in the XY regime by inspecting the ground state of $H_{\rm aux}$.

Obviously, $H_{\rm aux}$ commutes with both the total spin operators $\hat{S}^2_{\rm tot}$ and $\hat{S}_z$. Furthermore, by its definition, the energy spectrum of $H_{\rm aux}$ is simply given by

$$E(S_{\rm tot},\ S_z)=-S_{\rm tot}(S_{\rm tot}+1)+S_z^2. \quad (11)$$

Therefore, the global ground state of $H_{\rm aux}$ always has spin number $S_z=0$, if $S_{\rm tot}$ is an integer. (That is the reason we assume that quantity $|N_AS_A+N_BS_B|$ is an integer in theorem 1.) Consequently, the global ground state of Hamiltonian (1) in the XY regime has $S_z=0$ and hence, is nondegenerate. Our proof is accomplished. Q.E.D.

Theorem 1 tells us that a bifurcation of the global ground states occurs at the isotropic point of the ferrimagnetic Heisenberg model. Furthermore, the ground states of Hamiltonian (1) in the Ising regime have macroscopic magnetization if $|N_AS_A-N_BS_B|$ is a quantity of order $O(N_\Lambda)$ in the thermodynamic limit. In theorem 2, this result is further strengthened. It states that, in fact, these ground states have also both ferromagnetic and antiferromagnetic long-range order.

III. PROOF OF THEOREM 2

To establish theorem 2, we shall apply a technique similar to one that we developed in a previous paper to prove the existence of the ferrimagnetic long-range order in the ferrimagnetic mixed-spin chain.[3] Naturally, due to the absence of spin rotation symmetry in the antiferromagnetic XXZ model, some technical subtleties have to be dealt with care in the present case.

For definiteness, let us take $\Psi_0^{(1)}$, for example. As shown above, under the transformation $\hat{U}_1\hat{U}_2$, Hamiltonian (1) in the Ising regime is mapped onto H_2. Since this transformation is unitary, $\Psi_0^{(1)}$ is also mapped to a global ground state $\tilde{\Psi}_0$ of H_2. In general, $\tilde{\Psi}_0$ is a linear combination of $\tilde{\Psi}_0(\text{odd})$ and $\tilde{\Psi}_0(\text{even})$, i.e.,

$$\tilde{\Psi}_0=a\tilde{\Psi}_0(\text{odd})+b\tilde{\Psi}_0(\text{even}), \quad (12)$$

where a and b are complex constants.

Now, we show that the spin-correlation function of $\tilde{S}_x$ in $\tilde{\Psi}_0$ satisfies inequality

$$\langle\tilde{\Psi}_0|\tilde{S}_{\mathbf{h}x}\tilde{S}_{\mathbf{k}x}|\tilde{\Psi}_0\rangle\geq 0, \quad (13)$$

for any pair of lattice sites **h** and **k**. In fact, by substituting $\tilde{S}_x=(1/2)(\tilde{S}_++\tilde{S}_-)$ into the left-hand side of Eq. (13), we obtain

$$\begin{aligned} &\langle\tilde{\Psi}_0|\tilde{S}_{\mathbf{h}x}\tilde{S}_{\mathbf{k}x}|\tilde{\Psi}_0\rangle \\ &=\frac{1}{4}\langle\tilde{\Psi}_0|\tilde{S}_{\mathbf{h}+}\tilde{S}_{\mathbf{k}+}|\tilde{\Psi}_0\rangle+\frac{1}{4}\langle\tilde{\Psi}_0|\tilde{S}_{\mathbf{h}-}\tilde{S}_{\mathbf{k}-}|\tilde{\Psi}_0\rangle \\ &+\frac{1}{4}\langle\tilde{\Psi}_0|\tilde{S}_{\mathbf{h}+}\tilde{S}_{\mathbf{k}-}|\tilde{\Psi}_0\rangle+\frac{1}{4}\langle\tilde{\Psi}_0|\tilde{S}_{\mathbf{h}-}\tilde{S}_{\mathbf{k}+}|\tilde{\Psi}_0\rangle. \end{aligned} \quad (14)$$

Therefore, if each term on the right-hand side of Eq. (14) is non-negative, inequality (13) holds true. For example, we have

$$\begin{aligned} \langle\tilde{\Psi}_0|\tilde{S}_{\mathbf{h}+}\tilde{S}_{\mathbf{k}+}|\tilde{\Psi}_0\rangle &= |a|^2\langle\tilde{\Psi}_0(\text{odd})|\tilde{S}_{\mathbf{h}+}\tilde{S}_{\mathbf{k}+}|\tilde{\Psi}_0(\text{odd})\rangle \\ &+|b|^2\langle\tilde{\Psi}_0(\text{even})|\tilde{S}_{\mathbf{h}+}\tilde{S}_{\mathbf{k}+}|\tilde{\Psi}_0(\text{even})\rangle. \end{aligned} \quad (15)$$

In Eq. (15), the mixing matrix elements between $\tilde{\Psi}_0(\text{odd})$ and $\tilde{\Psi}_0(\text{even})$ are absent because operator $\tilde{S}_{\mathbf{h}+}\tilde{S}_{\mathbf{k}+}$ connects only the spin configurations in the same sector.

Next, we use the fact that the expansion coefficients of both $\tilde{\Psi}_0(\text{odd})$ and $\tilde{\Psi}_0(\text{even})$ in terms of the basis vectors $\cup_{2m+1}\{\phi_\alpha(2m+1)\}$ and $\cup_{2m}\{\phi_\alpha(2m)\}$ satisfy Marshall's sign rule. By this rule, in the expectation

$$\begin{aligned} &\langle\tilde{\Psi}_0(\text{odd or even})|\tilde{S}_{\mathbf{h}+}\tilde{S}_{\mathbf{k}+}|\tilde{\Psi}_0(\text{odd or even})\rangle \\ &=\sum_{(n,\ \alpha)}C_{\alpha_1n_1}C_{\alpha_2n_2}\langle\phi_{\alpha_1}(n_1)|\tilde{S}_{\mathbf{h}+}\tilde{S}_{\mathbf{k}+}|\phi_{\alpha_2}(n_2)\rangle, \end{aligned} \quad (16)$$

product $C_{\alpha_1n_1}C_{\alpha_2n_2}$ is non-negative for any pair of indices $(\alpha_1,\ n_1)$ and $(\alpha_2,\ n_2)$. Therefore, the right-hand side of Eq. (16) is a positive quantity, if each matrix element

$\langle \phi_{\alpha_1 n_1} | \tilde{S}_{\mathbf{h}+} \tilde{S}_{\mathbf{k}-} | \phi_{\alpha_2 n_2} \rangle$ is non-negative. In fact, this condition is trivially satisfied for any pair of basis vectors $\phi_{\alpha_1}(n_1)$ and $\phi_{\alpha_2}(n_2)$ because the action of $\tilde{S}_{\mathbf{h}+}$ and $\tilde{S}_{\mathbf{k}+}$ on a basis vector $\phi_\alpha(n)$ is determined by the rule

$$\tilde{S}_{\mathbf{i}+} | S_{1z}^A, \ldots, S_{\mathbf{i}z}^A, \ldots, S_{N_A z}^A, \; S_{1z}^B, \ldots, S_{N_B z}^B \rangle = \sqrt{S_{\mathbf{i}}^A (S_{\mathbf{i}}^A + 1) - S_{\mathbf{i}z}^A (S_{\mathbf{i}z}^A + 1)} \quad | \ldots, S_{\mathbf{i}z}^A + 1, \ldots \rangle, \tag{17}$$

assuming $\mathbf{i} \in A$. Similarly, one can easily show that the rest terms in Eq. (15) are also non-negative and hence, inequality (13) holds true.

Finally, we apply the inverse of the unitary transformation $\hat{U}_1 \hat{U}_2$ to Eq. (13). Under this transformation, $\tilde{\Psi}_0$ is mapped back onto $\Psi_0^{(1)}$ and the spin operators are changed by

$$[(\hat{U}_1 \hat{U}_2)^{-1}]^\dagger \tilde{S}_{\mathbf{i}x} [(\hat{U}_1 \hat{U}_2)^{-1}] = \epsilon(\mathbf{i}) \tilde{S}_{\mathbf{i}z}, \tag{18}$$

where function $\epsilon(\mathbf{i})$ is defined by $\epsilon(\mathbf{i}) = -1$ if $\mathbf{i} \in A$ and $\epsilon(\mathbf{i}) = 1$ if $\mathbf{i} \in B$. Therefore, under the unitary transformation, inequality (13) now reads

$$\epsilon(\mathbf{h}) \epsilon(\mathbf{k}) \langle \Psi_0^{(1)} | \tilde{S}_{\mathbf{h}z} \tilde{S}_{\mathbf{k}z} | \Psi_0^{(1)} \rangle \geqslant 0. \tag{19}$$

In other words, the longitudinal spin correlation in $\Psi_0^{(1)}$ is antiferromagnetic. Equation (19) also implies the following relation:

$$\epsilon(\mathbf{h}) \epsilon(\mathbf{k}) \langle \Psi_0^{(1)} | \tilde{S}_{\mathbf{h}z} \tilde{S}_{\mathbf{k}z} | \Psi_0^{(1)} \rangle \geqslant \langle \Psi_0^{(1)} | \tilde{S}_{\mathbf{h}z} \tilde{S}_{\mathbf{k}z} | \Psi_0^{(1)} \rangle. \tag{20}$$

By summing up both sides of Eq. (20) over $\mathbf{h}$ and $\mathbf{k}$, we obtain

$$\langle \Psi_0^{(1)} | \left(\sum_{\mathbf{i} \in \Lambda} \epsilon(\mathbf{i}) \tilde{S}_{\mathbf{i}z} \right) \left(\sum_{\mathbf{j} \in \Lambda} \epsilon(\mathbf{j}) \tilde{S}_{\mathbf{j}z} \right) | \Psi_0^{(1)} \rangle \geqslant \langle \Psi_0^{(1)} | \left(\sum_{\mathbf{i} \in \Lambda} \tilde{S}_{\mathbf{i}z} \right) \left(\sum_{\mathbf{j} \in \Lambda} \tilde{S}_{\mathbf{j}z} \right) | \Psi_0^{(1)} \rangle = |N_A S_A - N_B S_B|^2. \tag{21}$$

Therefore, if $|N_A S_A - N_B S_B|$ is a quantity of order $O(N_\Lambda)$ as $N_\Lambda \to \infty$, then $\Psi_0^{(1)}$ has both longitudinal ferromagnetic and antiferromagnetic long-range order. The same conclusion holds also for $\Psi_0^{(2)}$. Theorem 2 is proven. Q.E.D.

IV. REMARKS AND CONCLUSIONS

In theorem 1, we show that the ground state of the ferromagnetic XY model on a bipartite lattice is nondegenerate and has spin number $S_z = 0$. In fact, by following this proof, one can easily see that the same conclusion also holds for the ferromagnetic XY model on an arbitrary lattice, even if Λ is not at all bipartite. Naturally, in the general case, the ferromagnetic XY Hamiltonian $H_F(XY)$ is no longer equivalent to the antiferromagnetic XY Hamiltonian, as they are on a bipartite lattice.

In proving theorem 2, we first established inequality (13) on the spin correlation of $\tilde{S}_x$ in the ground state $\tilde{\Psi}_0$ of H_2 and then, mapped it into an inequality satisfied by the longitudinal spin-correlation function in $\Psi_0^{(i)}$, the ground states of the original antiferromagnetic XXZ Hamiltonian in the Ising regime. Naturally, one expects that this strategy should also apply to establish the existence of magnetic long-range order for the same model in the XY regime. However, the approach actually does not work in this case. The main problem is caused by the negative sign in the spin operator identity $\tilde{S}_y = (\tilde{S}_+ - \tilde{S}_-)/2i$ and the anisotropy in Hamiltonian (1). Consequently, we could not even establish an inequality such as Eq. (13) for the correlation function of $\tilde{S}_y$ in the nondegenerate ground state of H_3, which is equivalent to Hamiltonian (1) in the XY regime. Besides, even if we were successful in proving such a inequality, which could then be mapped by the inverse of $\hat{U}_3 \hat{U}_2$ into Eq. (19) with $\Psi_0^{(1)}$ being replaced with the unique ground state of Hamiltonian (1) in the XY regime, this method still fails. That is due to the fact that the total spin-z component of the nondegenerate ground state of Hamiltonian (1) in the XY regime is zero. Consequently, Eq. (21) cannot tell us anything about the possible existence of magnetic long-range order in the XY regime. It is still open as to whether such an order exists at all in the XY regime of the Hamiltonian. We shall address this problem in the future.

In summary, in this paper, we studied a generalized anisotropic ferrimagnetic Heisenberg model on a bipartite lattice. We proved that, when the maximal spin $N_A S_A + N_B S_B$ of the system is an integer, the model has a unique ground state with $S_z = 0$ in the XY regime and two degenerate ground states with $S_z = \pm |N_A S_A - N_B S_B|$ in the Ising regime, respectively. Therefore, the isotropic point of this model is a bifurcation point for its ground states. Furthermore, we also showed that if the magnetization of the ground states in the Ising regime is macroscopic in the thermodynamic limit, then the ground states have both ferromagnetic and antiferromagnetic long-range order. Therefore, they are ferrimagnetic. Our conclusions confirm and generalize the previous results derived by numerical calculations on small samples of one-dimensional mixed-spin chains.

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