Phase transition and ferrimagnetic long-range order in the mixed-spin Heisenberg model with single-ion anisotropy

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In the present paper, we study the quantum phase transition in the mixed-spin Heisenberg model with the single-ion anisotropy on a bipartite lattice. We prove rigorously that, when the single-ion anisotropy energy D is positive, the model has a unique ground state with the total spin-z component $S_z=0$. On the other hand, when the single-ion anisotropy energy is negative and favors the longitudinal spin direction, the global ground state of the system becomes doubly degenerate. Therefore, $D=0$ is the bifurcation point for the global ground state of the system. Furthermore, we show also that, in the latter case, the global ground state of the mixed-spin Heisenberg chain has the ferrimagnetic long-range order. Our conclusions confirm and generalize the previous results derived by numerical calculations on small size samples.

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I. INTRODUCTION

Low-dimensional antiferromagnetic quantum spin systems remain at the forefront of research on condensed matter physics for many years. For these systems, the Hamiltonians involved are relatively simple and the low dimensionality often allows very accurate numerical treatments. In particular, the quasi-one-dimensional quantum ferrimagnets, which have been successfully synthesized in experiments,[1–3] attracted many physicists' interest.[4–30] These materials are molecular magnets containing two different transitional-metal magnetic ions, which are alternatively distributed on the chain. 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, the theoretical investigations on these systems show clearly that their ground states have both the ferromagnetic and the antiferromagnetic long-range orders.[6–10] In other words, they are ferrimagnets. Consequently, the elementary excitations have two branches: While the ferromagnetic excitations, which reduce magnetization of the system, are gapless, the antiferromagnetic excitations are gapped. 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.[11–14]

Naturally, in the real materials, anisotropy caused by the crystalline field plays also an important role in determining the properties of magnetic systems.[31] To take the anisotropic effects into consideration, the simplest approach is to let the super-exchange couplings in the transverse and longitudinal spin directions be different. It gives the antiferromagnetic *XXZ*-model. As is well known, the phase diagram of this model consists of two regions: When the transverse interaction between spins is stronger, the system is in the *XY* regime. On the other hand, if the longitudinal spin interaction is dominant, the system behaves like an Ising antiferromagnet. In particular, by using exact numerical diagonalization on small size samples and exploiting conformal invariance of the one-dimensional *XXZ* Hamiltonian in continuum limit, Alcaraz and Malvezzi studied the phase diagram of the quasi-one-dimensional ferrimagnetic *XXZ* chain in detail.[4] They found that, in the *XY* regime, the ground state of the system is nondegenerate and critical. But, in the Ising regime, it has two degenerate ground states and each of them has an extensive spin number S_z. Therefore, the isotropic Heisenberg point is, in fact, a bifurcation point for the ground state of the ferrimagnetic *XXZ* chain. These conclusions were further confirmed by Ono *et al.*[17] By the density-matrix renormalization group calculation, they concluded that each ground state of the model in the Ising regime is ferrimagnetically ordered. Recently, by applying a method introduced by Affleck and Lieb,[32] we were able to rigorously re-establish these results for the ferrimagnetic *XXZ* model on any higher dimensional bipartite lattice.[33]

Another type of anisotropy, which is widely studied in literature, can be described by the so-called single-ion energy $D\Sigma_{\mathbf{i}}(S_{\mathbf{i}}^z)^2$ for the quantum spin systems with $S\geqslant 1$.[31] Theoretically, the properties of the anisotropic Heisenberg antiferromagnet with the single-ion term have been investigated by either the spin-wave theories or numerical calculations on small size samples.[34–37] For instance, by exact diagonalization calculation, it was found that the ground state phase diagram of the anisotropic Heisenberg chain with uniform spin $S=1$ has three regions: As the intensity of the single-ion anisotropy energy changes from $-\infty$ to ∞, the system undergoes first a transition from the Neel phase into the Haldane phase and then, another transition into the large-D phase.[37] On the other hand, for the mixed-spin ferrimagnetic chain with $(S_i,S_{i+1})=(1/2,1)$, Sakai and Okamoto considered recently the effect of the single-ion term on the phase diagram and the magnetization plateaus of the model.[38] By using the same numerical technique, they showed that, unlike the anisotropic Heisenberg chain with uniform spins, the Haldane phase is absent in the mixed-spin chain and the Neel phase is now long-range ordered.

In this article, we would like to study the properties of the anisotropic mixed-spin model with the single-ion energy term by an independent and mathematically rigorous approach. We shall prove that $D=0$ is indeed the bifurcation point for the ground state of this model, by applying a method due to Affleck and Lieb[32] and some results established in our previous paper.[33] More precisely, we show that, when $D>0$, the ground state of the model is nondegenerate and has $S_z=0$. On the other hand, when $D<0$, the ground state becomes doubly degenerate and each state is antiferromagnetically ordered. To be more general, in this paper, we do not impose any restrictions on dimension of the bipartite lattice and values of the unequal quantum spins, which are alternatively distributed on the lattice. In addition, our results cover both the anisotropic mixed-spin ferrimagnets and the so-called AB_2-type ferrimagnets, which have uniform spins distributed on a bipartite lattice with unequal numbers of sublattice sites per unit cell.[39–44]

To begin with, let us first recall several definitions and notation.

Take a finite lattice Λ and let N_Λ be the number of lattice sites. The Hamiltonian of the anisotropic antiferromagnetic Heisenberg model with the single-ion anisotropy is of the following form:

$$H=\sum_{\langle\mathbf{ij}\rangle} J_{\mathbf{ij}}\hat{\mathbf{S}}_{\mathbf{i}}\cdot\hat{\mathbf{S}}_{\mathbf{j}}+D\sum_{\mathbf{i}\in\Lambda}(\hat{S}_{\mathbf{i}z})^2, \tag{1}$$

where $\langle\mathbf{ij}\rangle$ denotes a pair of lattice sites and $\hat{\mathbf{S}}_{\mathbf{i}}$ represents the localized spin operator at lattice site $\mathbf{i}$. The parameter $J_{\mathbf{ij}}>0$ is the antiferromagnetic coupling between the localized spins at sites $\mathbf{i}$ and $\mathbf{j}$ and $-\infty<D<\infty$ denotes the strength of the single-ion anisotropy in the system. 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, $J_{\mathbf{ij}}$ only couples the spins at lattice sites, which belong to different sublattices. In the following, we shall use N_A and N_B for the number of sites in sublattices A and B, respectively.

In literature, two categories of ferrimagnets are widely studied. In the first category, sublattices A and B of the model have the same number of sites, i.e., $N_A=N_B$. But, the localized spins on these sublattices have different values S_A and S_B, say $S_A=\frac{1}{2}$ and $S_B=1$. Obviously, the one-dimensional antiferromagnetic mixed-spin chain, which we discussed above, belongs to this category. In the second case, all the spins of the system have the same value S on both the sublattices. However, these sublattices have different numbers of sites, n_A and n_B, in each unit cell, such as the AB_2 chains studied in Refs. 39–44. In the following, we shall treat both categories of ferrimagnets on the same footing.

Obviously, when $D=0$, Eq. (1) is reduced to the Hamiltonian of the isotropic ferrimagnetic Heisenberg model, whose properties have been thoroughly studied. In particular, the total spin $\hat{S}^2$ is a conserved quantity in this system. As shown by Lieb and Mattis,[45] the global ground state of the model on a bipartite lattice has the total spin $S=|N_AS_A-N_BS_B|$ and hence, is highly degenerate. Furthermore, in Refs. 6–10 and 39–44, it has been shown that these ground states support both the ferromagnetic and the antiferromagnetic long-range orders. Therefore, the system is ferrimagnetically ordered. In this paper, we shall prove that the single-ion anisotropy destroys the high spin-degeneracy. However, the ferrimagnetic long-range order is, at least, preserved in the regime of $D<0$.

With the above preparations, we can now summarize our main results in the following theorems.

Theorem 1: Let Λ be an arbitrary finite bipartite lattice on which Hamiltonian (1) is defined. Assume that quantity $N_AS_A+N_BS_B$ is an integer. Then, the global ground state of Hamiltonian (1) is nondegenerate and has the total spin-z component $S_z=0$ when $D>0$. On the other hand, for $D<0$, its global ground state becomes doubly degenerate and has $S_z=\pm|N_AS_A-N_BS_B|$.

In Theorem 1, we impose the condition $N_AS_A+N_BS_B$ $=$integer on the system to avoid the trivial spin degeneracy caused by a half-integer spin number S_z. When this condition is satisfied, S_z of any eigenstate of the system will be an integer. In particular, the global ground state of Hamiltonian (1) in the region of $D>0$ has $S_z=0$ rather than $S_z=\pm 1/2$, as stated in Theorem 1. A detailed discussion on this issue for the XXZ model can be found in Sec. II of Ref. 33.

Theorem 2: Let $\Psi_0^{(1)}$ and $\Psi_0^{(2)}$ be the global ground states of the anisotropic ferrimagnetic Heisenberg Hamiltonian H with $D<0$. If their spin number $S_z=\pm|N_AS_A-N_BS_B|$ are of order $O(N_\Lambda)$ in the thermodynamic limit, then both $\Psi_0^{(1)}$ and $\Psi_0^{(2)}$ have the longitudinal ferromagnetic and antiferromagnetic long-range orders, i.e., they are ferrimagnetically ordered.

In a previous paper,[33] we proved similar results for the ferrimagnetic XXZ Hamiltonian. More precisely, we found that its global ground state is nondegenerate in the XY regime and is doubly degenerate in the Ising regime. Furthermore, when the condition of Theorem 2 is satisfied, the XXZ model is ferrimagnetically ordered in the Ising regime. With these facts in mind, we are able to understand qualitatively the above theorems by the following argument: When $D>0$, each spin on the lattice Λ is forced down into the XY plane by the single-ion energy. Consequently, the system should behave more or less like the XXZ model in the XY regime. Therefore, one expects that its global ground state is nondegenerate as the one of the XY model does. On the other hand, for $D<0$, the longitudinal spin direction is favored by the single-ion term and hence, the system should be akin to the XXZ model in the Ising regime. Consequently, $D=0$ should be the bifurcation point of its global ground state. In the following, we shall justify this argument by proving rigorously Theorems 1 and 2.

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 established. Finally, in Sec. IV, we make some general remarks and then, summarize our results.

II. THE PROOF OF THEOREM 1

To prove Theorem 1, we shall employ a method introduced by Affleck and Lieb and use some of our previous results. By following Affleck and Lieb,[32] we are able to show that, in both regions of $D>0$ and $D<0$, the global ground state of Hamiltonian (1) is, at most, twofold degenerate. However, in order to determine the exact degeneracy of the ground state in each regime and show the existence of the ferrimagnetic long-range order, we need to introduce an auxiliary *XXZ* Hamiltonian, whose phase transition we have studied in Ref. 33.

Proof of Theorem 1: Let us first consider the case of $D>0$. We introduce the following auxiliary Hamiltonian:

$$H_{\mathrm{aux}} = \sum_{\langle \mathbf{ij}\rangle} J_{\mathbf{ij}}(\hat{S}_{\mathbf{i}x}\hat{S}_{\mathbf{j}x} + \hat{S}_{\mathbf{i}y}\hat{S}_{\mathbf{j}y}) + \sum_{\langle \mathbf{ij}\rangle} J'_{\mathbf{ij}}\hat{S}_{\mathbf{i}z}\hat{S}_{\mathbf{j}z} + D\sum_{\mathbf{i}\in\Lambda}(\hat{S}_{\mathbf{i}z})^2 \tag{2}$$

on the same lattice and require $0 \leqslant J'_{\mathbf{ij}} \leqslant J_{\mathbf{ij}}$. It represents the antiferromagnetic *XXZ* Hamiltonian with the single-ion anisotropy. Obviously, when $J'_{\mathbf{ij}}=J_{\mathbf{ij}}$, H_{aux} is reduced to Hamiltonian (1).

For Hamiltonian (2), the total spin-z component $\hat{S}_z$ is a good quantum number. Therefore, its Hilbert space can be split into numerous subspaces $\{V(S_z=M)\}$. In each subspace, the Hamiltonian has a ground state $\Psi_0(M)$. Following the proof of Lieb-Mattis theorem,[45] one can easily show that $\Psi_0(M)$ is nondegenerate in any admissible subspace $V(M)$. However, the global ground state of Hamiltonian (2) in the whole Hilbert space $V=\cup_M \oplus V(M)$ could be highly degenerate. Here, we want to show that, in fact, the degeneracy of the global ground state of Hamiltonian (2) cannot be larger than 2.

For this purpose, we apply a unitary transformation

$$\hat{U}_1 = \exp\left(i\frac{\pi}{2}\sum_{\mathbf{i}\in\Lambda}\hat{S}_{\mathbf{i}x}\right), \tag{3}$$

which rotates each spin in the lattice by an angle $\pi/2$ about spin-x axis, to the Hamiltonian. Under this transformation, the spin operator $\hat{S}_{\mathbf{i}z}$ and $\hat{S}_{\mathbf{i}y}$ are mapped into $-\hat{S}_{\mathbf{i}y}$ and $\hat{S}_{\mathbf{i}z}$, respectively. Consequently, the transformed Hamiltonian now reads

$$\begin{aligned}\tilde{H}_{\mathrm{aux}} &= \hat{U}_1^{\dagger}H_{\mathrm{aux}}\hat{U}_1\\ &= \sum_{\langle \mathbf{ij}\rangle}(J_{\mathbf{ij}}\hat{S}_{\mathbf{i}x}\hat{S}_{\mathbf{j}x} + J'_{\mathbf{ij}}\hat{S}_{\mathbf{i}y}\hat{S}_{\mathbf{j}y}) + \sum_{\langle \mathbf{ij}\rangle} J_{\mathbf{ij}}\hat{S}_{\mathbf{i}z}\hat{S}_{\mathbf{j}z} + D\sum_{\mathbf{i}\in\Lambda}(\hat{S}_{\mathbf{i}y})^2.\end{aligned} \tag{4}$$

To go further, we need to change sign of the coupling constants in the first summation of $\tilde{H}_{\mathrm{aux}}$. It can be achieved by applying another unitary transformation $\hat{U}_2=\exp(i\pi\Sigma_{\mathbf{i}\in A}\hat{S}_{\mathbf{i}z})$, which rotates each spin in sublattice A by an angle π about spin-z axis and keeps the spins in sublattice B unchanged. Under this transformation, we have

$$\hat{U}_2^{\dagger}\hat{S}_{\mathbf{i}x}\hat{U}_2 = \epsilon(\mathbf{i})\hat{S}_{\mathbf{i}x}, \quad \hat{U}_2^{\dagger}\hat{S}_{\mathbf{i}y}\hat{U}_2 = \epsilon(\mathbf{i})\hat{S}_{\mathbf{i}y}, \quad \hat{U}_2^{\dagger}\hat{S}_{\mathbf{i}z}\hat{U}_2 = \hat{S}_{\mathbf{i}z}, \tag{5}$$

where $\epsilon(\mathbf{i})=-1$ for $\mathbf{i}\in A$ and $\epsilon(\mathbf{i})=1$ for $\mathbf{i}\in B$. Consequently, we obtain the following twice transformed Hamiltonian:

$$\begin{aligned}\tilde{\tilde{H}}_{\mathrm{aux}} &= \hat{U}_2^{\dagger}\tilde{H}_{\mathrm{aux}}\hat{U}_2\\ &= (\hat{U}_1\hat{U}_2)^{\dagger}H_{\mathrm{aux}}(\hat{U}_1\hat{U}_2)\\ &= -\sum_{\langle \mathbf{ij}\rangle}(J_{\mathbf{ij}}\hat{S}_{\mathbf{i}x}\hat{S}_{\mathbf{j}x} + J'_{\mathbf{ij}}\hat{S}_{\mathbf{i}y}\hat{S}_{\mathbf{j}y})\\ &\quad + \sum_{\langle \mathbf{ij}\rangle} J_{\mathbf{ij}}\hat{S}_{\mathbf{i}z}\hat{S}_{\mathbf{j}z} - \frac{D}{4}\sum_{\mathbf{i}\in\Lambda}(\hat{S}_{\mathbf{i}+} - \hat{S}_{\mathbf{i}-})^2\\ &= -\frac{1}{4}\sum_{\langle \mathbf{ij}\rangle}[(J_{\mathbf{ij}} + J'_{\mathbf{ij}})(\hat{S}_{\mathbf{i}+}\hat{S}_{\mathbf{j}-} + \hat{S}_{\mathbf{i}-}\hat{S}_{\mathbf{j}+})\\ &\quad + (J_{\mathbf{ij}} - J'_{\mathbf{ij}})(\hat{S}_{\mathbf{i}+}\hat{S}_{\mathbf{j}+} + \hat{S}_{\mathbf{i}-}\hat{S}_{\mathbf{j}-})] + \sum_{\langle \mathbf{ij}\rangle} J_{\mathbf{ij}}\hat{S}_{\mathbf{i}z}\hat{S}_{\mathbf{j}z}\\ &\quad - \frac{|D|}{4}\sum_{\mathbf{i}\in\Lambda}(\hat{S}_{\mathbf{i}+}^2 + \hat{S}_{\mathbf{i}-}^2 - \hat{S}_{\mathbf{i}+}\hat{S}_{\mathbf{i}-} - \hat{S}_{\mathbf{i}-}\hat{S}_{\mathbf{i}+}),\end{aligned} \tag{6}$$

where $\hat{S}_{\mathbf{i}+}=\hat{S}_{\mathbf{i}x}+i\hat{S}_{\mathbf{i}y}$ and $\hat{S}_{\mathbf{i}-}=\hat{S}_{\mathbf{i}+}^{\dagger}$. We would like to emphasize that *all the coefficients of the spin-flipping interactions in Hamiltonian* $\tilde{\tilde{H}}_{\mathrm{aux}}$ *are negative for* $J'_{\mathbf{ij}} \leqslant J_{\mathbf{ij}}$ *and* $D>0$, except the on-site spin-flipping terms $\hat{S}_{\mathbf{i}+}\hat{S}_{\mathbf{i}-}$ and $\hat{S}_{\mathbf{i}-}\hat{S}_{\mathbf{i}+}$ in the last line of Eq. (6). They have positive coefficient $D/4$. Fortunately, in constructing the matrix of Hamiltonian (6), these terms only contribute to its diagonal elements since they leave each spin configuration unchanged. Therefore, it does not cause any problem in proving Theorem 1. On the other hand, the subspaces with $S_z=$odd and even integers are separately connected by these interactions. Consequently, the Hilbert space of $\tilde{\tilde{H}}_{\mathrm{aux}}$ is decomposed into two disconnected sectors $\mathcal{V}_{\mathrm{odd}}$ and $\mathcal{V}_{\mathrm{even}}$. Each of them is a joint set of the subspaces $\{V(M)\}$ with M being an odd or even integer.

Next, for a natural basis of $V(M)$, we choose vectors

$$\phi_{\alpha}(M) = |S_{1z}^{A}, S_{2z}^{A}, \ldots, S_{N_A z}^{A}, S_{1z}^{B}, S_{2z}^{B}, \ldots, S_{N_B z}^{B}\rangle, \tag{7}$$

where $S_{\mathbf{i}z}^{A}$ and $S_{\mathbf{j}z}^{B}$ are the z-component of the spins at sites $\mathbf{i}\in A$ and $\mathbf{j}\in B$, respectively. Since $\phi_{\alpha}(M)$ is a vector in subspace $V(M)$, we impose the following condition:

$$S_{1z}^{A} + \cdots + S_{N_A z}^{A} + S_{1z}^{B} + \cdots + S_{N_B z}^{B} = M \tag{8}$$

on it and let index α run over all the admissible spin configurations. Obviously, each set of vectors $\cup_n\{\phi_{\alpha}(2n)\}$ and $\cup_n\{\phi_{\alpha}(2n+1)\}$ spans the corresponding subspace $\mathcal{V}_{\mathrm{even}}$ and $\mathcal{V}_{\mathrm{odd}}$, respectively.

For definiteness, let us take the subspace $\mathcal{V}_{\mathrm{even}}$ for example. In terms of the basis $\cup_n\{\phi_{\alpha}(2n)\}$, the transformed Hamiltonian $\tilde{\tilde{H}}_{\mathrm{aux}}$ can be written into a matrix $\tilde{\tilde{\mathcal{H}}}_{\mathrm{aux}}$. It has the following characteristics:

(i) The off-diagonal elements of the matrix are nonpositive quantities. More precisely, they are either zero or negative quantities $-(J_{\mathbf{ij}}-J'_{\mathbf{ij}})/4$, $-(J_{\mathbf{ij}}+J'_{\mathbf{ij}})/4$, and $-D/4$ multiplied by some positive factors of form $\sqrt{S(S+1)-S_z(S_z+1)}$.

(ii) $\tilde{\tilde{\mathcal{H}}}_{\mathrm{aux}}$ is irreducible in the sense that, for any pair of basis vectors $\phi_{\alpha}(2n_1)$ and $\phi_{\beta}(2n_2)$, there is a positive integer L such that

$$\langle \phi_\alpha(2n_1)|\mathcal{H}^L_{\text{aux}}|\phi_\beta(2n_2)\rangle \neq 0. \tag{9}$$

It is due to the fact that lattice Λ is connected by the spin-flipping interactions $\hat{S}_{\mathbf{i}+}\hat{S}_{\mathbf{j}-}$ and each subspace $V(2n)$ is connected to $V(2n\pm 2)$ by either operators $\hat{S}_{\mathbf{i}+}\hat{S}_{\mathbf{j}+}+\hat{S}_{\mathbf{i}-}\hat{S}_{\mathbf{j}-}$ or $\hat{S}^2_{\mathbf{i}+}+\hat{S}^2_{\mathbf{i}-}$.

To such a matrix, the well-known Perron-Fröbenius theorem in matrix theory applies.[46] This theorem tells us that the ground-state wave function $\tilde{\tilde{\Psi}}^{\text{aux}}_0$ (even) of $\tilde{\tilde{\mathcal{H}}}_{\text{aux}}$ in the subspace $\mathcal{V}_{\text{even}}$ satisfies Marshall's sign rule.[47] Namely, in the expansion

$$\tilde{\tilde{\Psi}}^{\text{aux}}_0(\text{even}) = \sum_n \sum_\alpha C_{n\alpha}\phi_\alpha(2n), \tag{10}$$

all the coefficients $C_{n\alpha}$ can be chosen real and positive. Therefore, the ground state is nondegenerate.

Similarly, we can show that the ground state of $\tilde{\tilde{H}}_{\text{aux}}$ in $\mathcal{V}_{\text{odd}}$ is also nondegenerate. Therefore, its global ground state can be, at most, doubly degenerate. On the other hand, since the transformed $\tilde{\tilde{H}}_{\text{aux}}$ is unitarily equivalent to the auxiliary Hamiltonian in Eq. (2) when $D>0$ and $0\leqslant J'_{\mathbf{ij}}\leqslant J_{\mathbf{ij}}$, we immediately conclude that the global ground state of the latter Hamiltonian must have the same degeneracy, which is not larger than 2.

This conclusion implies that, in the parameter region of $D>0$ and $0\leqslant J'_{\mathbf{ij}}\leqslant J_{\mathbf{ij}}$, a level crossing between the ground state and the excited states of the auxiliary Hamiltonian is forbidden. In fact, if this statement is not true and such a level crossing does occur at some point in the region, then the global ground state of the auxiliary Hamiltonian must be, at least, threefold degenerate there. This is due to the fact that, although the ground state of the auxiliary Hamiltonian in each subspace $V(M)$ is nondegenerate, its ground states in subspaces $V(-M)$ and $V(M)$ are obviously degenerate. Therefore, the occurrence of such a level crossing requires that the ground states of H_{aux} in four subspaces $V(\pm M_1)$ and $V(\pm M_2)$ (or three subspaces if $M_1=0$) are degenerate at the crossing point. However, this possibility has been excluded.

Obviously, the absence of level-crossing between the global ground state and the excited states of the Hamiltonian indicates that S_z of the global ground state should be an integer-valued continuous function of parameters D and $J'_{\mathbf{ij}}$ in the region. Therefore, it must be a constant. As a result, we can determine the total spin-z component of the global ground state of Hamiltonian (1) as follows: First, we choose a value of $J'_{\mathbf{ij}}$, which is strictly less than $J_{\mathbf{ij}}$, and let D tend to zero. In this limit, Hamiltonian (2) is reduced to the antiferromagnetic XXZ Hamiltonian in the XY regime. For this Hamiltonian, in Ref. 33, we proved that its global ground state is nondegenerate and has $S_z=0$. (Because the proof is rather lengthy, we shall not repeat it here.) Therefore, by the continuity argument, the global ground state of Hamiltonian (2) in the specified parameter region must be also nondegenerate and has the same total spin-z component. Then, we set $J'_{\mathbf{ij}}=J_{\mathbf{ij}}$, which represents the boundary of the parameter region. By the same continuity argument, we reach the conclusion of Theorem 1 for the case of $D>0$.

Next, we consider the case of $D<0$. As done above, we study first the global ground state of the auxiliary Hamiltonian in Eq. (2). However, in this case, we assume that the coupling constants $J'_{\mathbf{ij}}$ in the longitudinal spin direction are larger than or equal to $J_{\mathbf{ij}}$. Correspondingly, we apply a different unitary transformation $\hat{U}_3=\exp(i\pi/2\Sigma_{\mathbf{i}\in\Lambda}\hat{S}_{\mathbf{i}y})$, which rotates each spin in lattice Λ by an angle $\pi/2$ about spin-y axis, and then, $\hat{U}_2$ again to H_{aux}. Under these transformations, we obtain

$$\begin{aligned}
H'_{\text{aux}} &= (\hat{U}_3\hat{U}_2)^\dagger H_{\text{aux}}(\hat{U}_3\hat{U}_2)\\
&= -\sum_{\langle\mathbf{ij}\rangle}(J'_{\mathbf{ij}}\hat{S}_{\mathbf{i}x}\hat{S}_{\mathbf{j}x}+J_{\mathbf{ij}}\hat{S}_{\mathbf{i}y}\hat{S}_{\mathbf{j}y})+\sum_{\langle\mathbf{ij}\rangle}J_{\mathbf{ij}}\hat{S}_{\mathbf{i}z}\hat{S}_{\mathbf{j}z}-|D|\sum_{\mathbf{i}\in\Lambda}(\hat{S}_{\mathbf{i}x})^2\\
&= -\frac{1}{4}\sum_{\langle\mathbf{ij}\rangle}[(J'_{\mathbf{ij}}+J_{\mathbf{ij}})(\hat{S}_{\mathbf{i}+}\hat{S}_{\mathbf{j}-}+\hat{S}_{\mathbf{i}-}\hat{S}_{\mathbf{j}+})\\
&\quad +(J'_{\mathbf{ij}}-J_{\mathbf{ij}})(\hat{S}_{\mathbf{i}+}\hat{S}_{\mathbf{j}+}+\hat{S}_{\mathbf{i}-}\hat{S}_{\mathbf{j}-})]+\sum_{\langle\mathbf{ij}\rangle}J_{\mathbf{ij}}\hat{S}_{\mathbf{i}z}\hat{S}_{\mathbf{j}z}\\
&\quad -\frac{|D|}{4}\sum_{\mathbf{i}\in\Lambda}(\hat{S}^2_{\mathbf{i}+}+\hat{S}^2_{\mathbf{i}+}+\hat{S}_{\mathbf{i}+}\hat{S}_{\mathbf{i}-}+\hat{S}_{\mathbf{i}-}\hat{S}_{\mathbf{i}+}).
\end{aligned} \tag{11}$$

Now, by repeating the above proof, it can be easily shown that the global ground states of H'_{aux} as well as the auxiliary Hamiltonian in the parameter region of $D<0$ and $J'_{\mathbf{ij}}\geqslant J_{\mathbf{ij}}$ are also, at most, doubly degenerate. It implies that a level-crossing between the global ground state and the excited states of the auxiliary Hamiltonian cannot take place in the region.

To determine the exact degeneracy of the global ground state and its total spin-z component, we apply again the continuity argument. Take a specific value of $J'_{\mathbf{ij}}$, which is strictly larger than $J_{\mathbf{ij}}$, and let $|D|$ tend to zero. Then, H_{aux} is reduced to the XXZ Hamiltonian in the Ising regime. Since level-crossing between the global ground state and the excited states of the auxiliary Hamiltonian is absent in this limit, both the global ground states of H_{aux} and the XXZ Hamiltonian in the Ising regime should have the same S_z. Again, in Ref. 33, we showed that the global ground state of the latter Hamiltonian is doubly degenerate and has spin numbers $S_z=\pm|N_AS_A-N_BS_B|$. Therefore, by the continuity argument, we conclude that, when $J'_{\mathbf{ij}}=J_{\mathbf{ij}}$, the global ground state of Hamiltonian (1) is doubly degenerate and has the total spin-z component $S_z=\pm|N_AS_A-N_BS_B|$, when $|D|\neq 0$.

Our proof of Theorem 1 is accomplished. QED

Theorem 1 tells us that $D=0$ represents the bifurcation point for the global ground state of the ferrimagnetic Heisenberg Hamiltonian (1). However, as we know, the global ground state of the same Hamiltonian at $D=0$ has total spin $S=|N_AS_A-N_BS_B|$ and hence, is highly degenerate.[45] Therefore, this theorem gives us the following picture on the evolution of the global ground state of Hamiltonian (1) as the parameter D varies: When D is less than zero, the global ground state has two degenerate members. One of them takes on the lowest S_z and the other has the highest one, which are allowed by the total spin $S=|N_AS_A-N_BS_B|$. Then, as D tends to zero, these two states are eventually merged with other members of the global ground state at the isotropic point. As

D further increases and becomes positive, the degeneracy of the global ground state is destroyed by the quantum fluctuations. One of the $2S+1$ members is singled out for the global ground state of the system and it has $S_z=0$. This is a typical example of the so-called "order from disorder" phenomenon considered in the study of quantum phase transition.

Next, we turn to the proof of Theorem 2.

III. PROOF OF THEOREM 2

Since the global ground state of Hamiltonian (1) in the region of $D<0$ has the total spin-z component $S_z=\pm|N_AS_A-N_BS_B|$, one expects that the system has the ferrimagnetic long-range order, if S_z is a quantity of order $O(N_\Lambda)$ in the thermodynamic limit. Theorem 2 tells us that, indeed, this speculation is correct.

To prove this theorem, we apply a technique developed previously by us in Refs. 9 and 40 for establishing the existence of the magnetic long-range order in the isotropic Heisenberg ferrimagnets. In the current case, since the spin rotation symmetry is broken by the anisotropic single-ion terms, we need to deal with some technical subtleties with care.

Proof of Theorem 2: For definiteness, let us take $\Psi_0^{(1)}$, one of the degenerate global ground states of Hamiltonian (1) in the region of $D<0$ for example. As shown above, under the transformation $\hat{U}_3\hat{U}_2$, the Hamiltonian is mapped onto H'_{aux} with $J'_{\mathbf{ij}}=J_{\mathbf{ij}}$. In the meantime, $\Psi_0^{(1)}$ is also mapped to a ground state Ψ'_0 of the transformed Hamiltonian. In general, this state is a linear combination of $\Psi'_0(\text{odd})$ and $\Psi'_0(\text{even})$, which are the nondegenerate global ground states of H'_{aux} in the subspaces $\mathcal{V}_{\text{odd}}$ and $\mathcal{V}_{\text{even}}$, respectively. Explicitly, we have

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

where a and b are complex constants.

Let us now consider the spin correlation function of $\hat{S}_x$ in Ψ'_0. We would like to show that

$$\langle\Psi'_0|\hat{S}_{\mathbf{i}x}\hat{S}_{\mathbf{j}x}|\Psi'_0\rangle \geqslant 0 \tag{13}$$

holds for any pair of lattice sites $\mathbf{i}$ and $\mathbf{j}$. To prove inequality (13), we substitute identity $\hat{S}_{\mathbf{i}x}=(1/2)(\hat{S}_{\mathbf{i}+}+\hat{S}_{\mathbf{i}-})$ into its left-hand side and rewrite the correlator as

$$\begin{aligned}\langle\Psi'_0|\hat{S}_{\mathbf{i}x}\hat{S}_{\mathbf{j}x}|\Psi'_0\rangle &= \tfrac{1}{4}\langle\Psi'_0|\hat{S}_{\mathbf{i}+}\hat{S}_{\mathbf{j}+}|\Psi'_0\rangle + \tfrac{1}{4}\langle\Psi'_0|\hat{S}_{\mathbf{i}-}\hat{S}_{\mathbf{j}-}|\Psi'_0\rangle \\ &\quad + \tfrac{1}{4}\langle\Psi'_0|\hat{S}_{\mathbf{i}+}\hat{S}_{\mathbf{j}-}|\Psi'_0\rangle + \tfrac{1}{4}\langle\Psi'_0|\hat{S}_{\mathbf{i}-}\hat{S}_{\mathbf{j}+}|\Psi'_0\rangle.\end{aligned} \tag{14}$$

Therefore, if each term on the right-hand side of Eq. (14) is non-negative, then inequality (13) is certainly true.

Take the first term on the right-hand side of Eq. (14) for example. We have

$$\begin{aligned}\langle\Psi'_0|\hat{S}_{\mathbf{i}+}\hat{S}_{\mathbf{j}+}|\Psi'_0\rangle &= |a|^2\langle\Psi'_0(\text{odd})|\hat{S}_{\mathbf{i}+}\hat{S}_{\mathbf{j}+}|\Psi'_0(\text{odd})\rangle \\ &\quad + |b|^2\langle\Psi'_0(\text{even})|\hat{S}_{\mathbf{i}+}\hat{S}_{\mathbf{j}+}|\Psi'_0(\text{even})\rangle.\end{aligned} \tag{15}$$

In Eq. (15), the mixing matrix elements between $\Psi'_0(\text{odd})$ and $\Psi'_0(\text{even})$ are absent. That is due to the fact that the operators $\hat{S}_{\mathbf{i}+}\hat{S}_{\mathbf{j}+}$ connect only the spin configurations in the same sector $\mathcal{V}_{\text{odd}}$ or $\mathcal{V}_{\text{even}}$, respectively. Now, we recall that the expansion coefficients $\{C_{n\alpha}\}$ of the wave functions $\Psi'_0(\text{odd})$ $(\Psi'_0(\text{even}))$ in terms of the basis vectors $\cup_n\{\phi_\alpha(2n+1)\}$ $(\cup_m\{\phi_\beta(2n)\})$ satisfy Marshall's sign rule, i.e., they are real and positive. Moreover, it is easy to show that, for any pair of spin configurations $\phi_{\alpha_1}(n_1)$ and $\phi_{\alpha_2}(n_2)$, the matrix element $\langle\phi_{\alpha_1}(n_1)|\hat{S}_{\mathbf{i}+}\hat{S}_{\mathbf{j}+}|\phi_{\alpha_2}(n_2)\rangle$ is either zero or a positive quantity because the action of $\hat{S}_{\mathbf{i}+}$ or $\hat{S}_{\mathbf{j}+}$ on any basis vector produces only zero or positive factors of form $\sqrt{S(S+1)-S_z(S_z+1)}$. Therefore, we have

$$\begin{aligned}&\langle\Psi'_0(\text{odd or even})|\hat{S}_{\mathbf{i}+}\hat{S}_{\mathbf{j}+}|\Psi'_0(\text{odd or even})\rangle \\ &\quad = \sum_{(n_1,\alpha_1)}\sum_{(n_2,\alpha_2)} C_{n_1\alpha_1}C_{n_1\alpha_2}\langle\phi_{\alpha_1}(n_1)|\hat{S}_{\mathbf{i}+}\hat{S}_{\mathbf{j}+}|\phi_{\alpha_2}(n_2)\rangle \geqslant 0.\end{aligned} \tag{16}$$

Similarly, we can show that the rest terms on the right-hand side of Eq. (14) are also non-negative. That yields inequality (13).

Inequality (13) implies actually that the longitudinal spin correlation in the global ground state $\Psi_0^{(1)}$ is antiferromagnetic. To see that, we apply the inverse of the unitary transformation $\hat{U}_3\hat{U}_2$ to Eq. (13). Under this transformation, the ground state Ψ'_0 of H'_{aux} is mapped back onto $\Psi_0^{(1)}$ and the spin operators are changed by

$$[(\hat{U}_3\hat{U}_2)^{-1}]^\dagger\hat{S}_{\mathbf{i}x}[(\hat{U}_3\hat{U}_2)^{-1}] = \epsilon(\mathbf{i})\hat{S}_{\mathbf{i}z}. \tag{17}$$

Therefore, inequality (13) is equivalent to

$$\epsilon(\mathbf{i})\epsilon(\mathbf{j})\langle\Psi_0^{(1)}|\hat{S}_{\mathbf{i}z}\hat{S}_{\mathbf{j}z}|\Psi_0^{(1)}\rangle \geqslant 0. \tag{18}$$

It tells us that the longitudinal spin correlator is positive for sites $\mathbf{i}$ and $\mathbf{j}$ belonging to the same sublattice and negative otherwise. Consequently, we have

$$\begin{aligned}\epsilon(\mathbf{i})\epsilon(\mathbf{j})\langle\Psi_0^{(1)}|\hat{S}_{\mathbf{i}z}\hat{S}_{\mathbf{j}z}|\Psi_0^{(1)}\rangle &= |\langle\Psi_0^{(1)}|\hat{S}_{\mathbf{i}z}\hat{S}_{\mathbf{j}z}|\Psi_0^{(1)}\rangle| \\ &\geqslant \langle\Psi_0^{(1)}|\hat{S}_{\mathbf{i}z}\hat{S}_{\mathbf{j}z}|\Psi_0^{(1)}\rangle.\end{aligned} \tag{19}$$

Now, we sum up both sides of Eq. (19) over $\mathbf{i}$ and $\mathbf{j}$. It yields

$$\begin{aligned}&\left\langle\Psi_0^{(1)}\right|\left(\sum_{\mathbf{i}\in\Lambda}\epsilon(\mathbf{i})\hat{S}_{\mathbf{i}z}\right)\left(\sum_{\mathbf{j}\in\Lambda}\epsilon(\mathbf{j})\hat{S}_{\mathbf{j}z}\right)\left|\Psi_0^{(1)}\right\rangle \\ &\quad \geqslant \left\langle\Psi_0^{(1)}\right|\left(\sum_{\mathbf{i}\in\Lambda}\hat{S}_{\mathbf{i}z}\right)\left(\sum_{\mathbf{j}\in\Lambda}\hat{S}_{\mathbf{j}z}\right)\left|\Psi_0^{(1)}\right\rangle = |N_AS_A-N_BS_B|^2.\end{aligned} \tag{20}$$

Therefore, if $|N_AS_A-N_BS_B|$ is a quantity of order $O(N_\Lambda)$ as $N_\Lambda\to\infty$, the right-hand side of the above inequality is proportional to N_Λ^2. It indicates that $\Psi_0^{(1)}$ has both the longitudinal ferromagnetic and the antiferromagnetic long-range orders.

By following the above proof, we can easily show that $\Psi_0^{(2)}$ has also long-range order under the conditions of Theorem 2. That ends our proof of the theorem. QED

IV. SOME REMARKS AND CONCLUSIONS

Some remarks are in order.

Remark 1: In the proof of Theorem 2, we establish first inequality (13) for the transverse spin correlation in the ground state Ψ_0' of the transformed Hamiltonian H'_{aux}. Then, we map it into an inequality satisfied by the longitudinal spin correlation in the global ground state of the original Hamiltonian with $D<0$. Naturally, one will expect that the same strategy should be also applicable to establish the existence of the magnetic long-range order in the model for the case of $D>0$. Unfortunately, such a direct approach actually fails. The problem is caused by the negative sign in the spin operator identity $\hat{S}_{\mathbf{i}y}=(\hat{S}_{\mathbf{i}+}-\hat{S}_{\mathbf{i}-})/2i$. Consequently, it is even very difficult to show whether inequality (13) holds for the spin correlator $\langle\hat{S}_{\mathbf{i}y}\hat{S}_{\mathbf{j}y}\rangle$ of the transformed Hamiltonian $\tilde{\tilde{H}}_{\text{aux}}$, let alone the existence of the magnetic ordering in the anisotropic Heisenberg model with $D>0$. It remains an interesting open problem to prove the existence of ferrimagnetic long-range order in this case.

Remark 2: In Sec. II, we actually showed that Theorem 1 still holds true even if both the anisotropies, which are respectively caused by the single-ion anisotropy and the unequal superexchange couplings in different spin directions, coexist in the system, as long as they do not frustrate each other. Naturally, one would like to ask what happens if these anisotropies are not compatible in a given parameter region, say the one of $D>0$ and $J'_{\mathbf{ij}}>J_{\mathbf{ij}}$. Based on the previous results derived by numerical calculation on small size chains, we expect the bifurcation point for the global ground state of the system should be changed. For instance, in Ref. 37, the authors calculated the phase diagram of the antiferromagnetic *XXZ* chain with uniform spins $(S=1)$ by exact diagonalization. They found that the phase transition point between the *XY* phase and the Haldane phase, which is replaced by the Ising phase in the ferrimagnetic Heisenberg models, is shifted from $J'_{\mathbf{ij}}=J_{\mathbf{ij}}$ for $D=0$ to a larger value $J'_{\mathbf{ij}}(D)$ for $D>0$. However, since the method of Affleck and Lieb does not apply in this case, we cannot prove these results on a rigorous basis. Apparently, some new techniques have to be developed to tackle it. We shall pursue this project in the future.

In summary, in this paper, we study the quantum phase transition in the mixed-spin Heisenberg model with the single-ion anisotropy on a bipartite lattice. We prove rigorously that, when the single-ion energy D is positive, the model has a unique ground state with $S_z=0$. On the other hand, when the single-ion energy is negative and favors the longitudinal spin direction, the global ground state becomes doubly degenerate and has the total spin-z component $S_z=\pm|N_AS_A-N_BS_B|$. Therefore, $D=0$ is actually a bifurcation point for its global ground state. Furthermore, we also show that the global ground state of the model has both the ferromagnetic and the antiferromagnetic long-range orders when $D<0$, if $|N_AS_A-N_BS_B|$ is a quantity of order $O(N_\Lambda)$ in the thermodynamic limit. In other words, the system is a ferrimagnet. Our conclusions confirm and generalize the previous results on the one-dimensional mixed-spin chains by numerical calculations.

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