Quantum phase transition in the one-dimensional compass model using the pseudospin approach

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In the present paper, we investigate quantum phase transition in the one-dimensional compass model introduced by Brzezicki *et al.* [Phys. Rev. B **75**, 134415 (2007)]. Unlike the previous approach based on the Jordan-Wigner transformation, we use directly the standard pseudospin representation in our investigation. Therefore, our method can be potentially applied to study rigorously the properties of the same model in higher dimensions. By applying the reflection positivity technique, we are able to determine degeneracy of the global ground state and the quantum phase-transition point of this model. We find also that the transition is of the first order. These results are consistent with the previous conclusions. However, some differences are also uncovered.

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I. INTRODUCTION

During the past five decades, through extensive experimental and theoretical works, the important role played by the orbital degree of freedom in determining the magnetic and transport properties of transition-metal oxide (TMO) materials has been widely recognized.^{1–6} It is the complex interplay among the charge, spin, orbital, and lattice degrees of freedom existing in these systems which makes their phase diagrams extremely rich and induces various fascinating physical phenomena. For instance, the experimentally observed *A*-type antiferromagnetic spin order with electronic spins being aligned parallel in the *x*-*y* plane and antiparallel along the *z* axis⁷ is stabilized by the more robust orbital ordering.^{8–13}

In the TMO compounds, there exist two possible mechanisms which can lead to orbital ordering. One of them is due to the virtual hopping of electron, which causes the superexchange interaction between orbital degrees of freedoms at different lattice sites under the strong on-site electronelectron repulsion.^{8–11} Another is based on the cooperative Jahn-Teller (JT) effect,¹⁴ by which the lattice distortion lifts the electronic orbital degeneracy in the system.^{15,16} In this case, it is the virtual-phonon exchange which produces the effective orbital interaction. However, for the half-filled transition-metal compounds, both mechanisms give almost the same type of effective Hamiltonian, which can be written as¹⁷

$$\begin{split} \hat{H}_{\text{eff}} &= J_{\parallel} \sum_{\mathbf{i} \in \Lambda} \left(\frac{1}{2} \hat{T}_{\mathbf{i}}^{z} + \frac{\sqrt{3}}{2} \hat{T}_{\mathbf{i}}^{x} \right) \left(\frac{1}{2} \hat{T}_{\mathbf{i}+\mathbf{e}_{x}}^{z} + \frac{\sqrt{3}}{2} \hat{T}_{\mathbf{i}+\mathbf{e}_{x}}^{x} \right) \\ &+ J_{\parallel} \sum_{\mathbf{i} \in \Lambda} \left(\frac{1}{2} \hat{T}_{\mathbf{i}}^{z} - \frac{\sqrt{3}}{2} \hat{T}_{\mathbf{i}}^{x} \right) \left(\frac{1}{2} \hat{T}_{\mathbf{i}+\mathbf{e}_{y}}^{z} - \frac{\sqrt{3}}{2} \hat{T}_{\mathbf{i}+\mathbf{e}_{y}}^{x} \right) \\ &+ J_{\perp} \sum_{\mathbf{i} \in \Lambda} \hat{T}_{\mathbf{i}}^{z} \hat{T}_{\mathbf{i}+\mathbf{e}_{z}}^{z}, \end{split}$$
(1)

where \mathbf{e}_x , \mathbf{e}_y , and \mathbf{e}_z are unit vectors in x, y, and z directions, respectively. In Eq. (1), \hat{T}_i^x , \hat{T}_j^y , and \hat{T}_i^z are the pseudospin operators which represent the orbital degree of freedom in the system. They satisfy the conventional commutation rela-

tions of spin operators. In particular, the two eigenstates of \hat{T}^{τ} correspond to the atomic $|3z^2 - r^2\rangle$ and $|x^2 - y^2\rangle$ orbitals in a transition-metal ion, respectively.

In literature, Eq. (1) is called the Hamiltonian of 120° model.¹⁷ We would like to emphasize that, although Hamiltonian (1) looks similar to the conventional antiferromagnetic Heisenberg model, there exists actually a qualitative difference between them. While the Heisenberg model on the simple-cubic lattice is free of frustration, the 120° model has a built-in competition among orbital superexchange interactions and is, hence, intrinsically frustrated. In fact, from Hamiltonian (1), one can easily see that the superexchange interaction along the *z* axis of lattice favors alternating $d_{3z^2-r^2}$ and $d_{x^2-y^2}$ orbital order. However, the other interaction terms tend to stabilize "antiferromagnetic" orbital ordering of $(d_{3x^2-r^2}, d_{y^2-z^2})$ and $(d_{3y^2-r^2}, d_{z^2-x^2})$ in either *x*- or *y*-axis direction, respectively.

Furthermore, the Hamiltonian lacks also the continuous SU(2) pseudospin symmetry. Therefore, the well-known Mermin-Wagner theorem¹⁸ does not apply. As a result, the quantum fluctuations in one- or two-dimensional compass model are not sufficiently strong, and hence orbital orders may survive in these cases. Taking these facts into consideration, one would naturally ask whether the intrinsic frustration in the 120° model destroys completely long-range orbital orders. It is a difficult problem and has been vigorously studied by many physicists in the past decade.¹⁹⁻²⁴ For instance, the authors of Ref. 20 calculated the orbital excitation spectrum of the 120° model in two dimensions by the spinwave theory. They found that its orbital-wave dispersion is gapless and an orbital ordering exists at zero temperature. In particular, Biskup et al.²⁵ established recently the existence of orbital phase transitions for the classical version of this model. More precisely, by treating the pseudospins in Hamiltonian (1) as classical entities and employing a spin-wave argument, they showed that, when temperature T is sufficiently low, this model has six distinct thermodynamically stable states and each of them supports a long-range orbital order. Very recently, by applying the reflection positivity method,²⁶ we were able to prove rigorously that the ground state of a simplified 120° model, whose Hamiltonian is given by setting $J_{\perp}=0$ in Hamiltonian (1), supports a transverse antiferromagnetic orbital ordering.²⁷ However, due to technical complexities, we were not able to determine whether long-range orbital orders exist in the ground state of the three-dimensional 120° model itself, although recent analysis on a related Hubbard-type Hamiltonian found that such an ordering cannot be stabilized in three dimensions.²⁸

To make further progress, some authors considered also the so-called compass model.^{8,17} In terms of the pseudospin operators, its Hamiltonian is of the following form:

$$\hat{H} = \sum_{\mathbf{i} \in \Lambda} \left(J_x \hat{T}_{\mathbf{i}}^x \hat{T}_{\mathbf{i}+\mathbf{e}_x}^x + J_y \hat{T}_{\mathbf{i}}^y \hat{T}_{\mathbf{i}+\mathbf{e}_y}^y + J_z \hat{T}_{\mathbf{i}}^z \hat{T}_{\mathbf{i}+\mathbf{e}_z}^z \right).$$
(2)

Here, $J_x > 0$, $J_y > 0$, and $J_z > 0$ denote the superexchange interactions between pseudospin operators located at site **i** and one of its nearest-neighbor sites in *x*, *y*, and *z* axis, respectively. Similar to the 120° model, there exist obviously intrinsic competitions among orbital orderings in different directions of lattice too. While the first term of Hamiltonian (2) favors an Ising type of antiferromagnetic ordering along *x* direction, the other interactions stabilize the similar type of ordering in either *y* or *z* direction. In a sense, this model is merely a simplified version of the 120° model. Therefore, it is also called the 90° model in literature.

Naturally, the main interest in this model is focused on the possible existence of long-range orbital orders and quantum phase transitions in it.²⁹⁻³⁴ In particular, for the classical compass model on two- or three-dimensional simple-cubic lattices, it is easy to see that the ground state of the model is infinitely degenerate. However, this "accidental" degeneracy can be lifted with either thermodynamic or quantum fluctuations. In fact, by mapping the classical Hamiltonian of the compass model to a four-state Potts model and applying the multicanonical Monte Carlo simulation, Mishra et al.²⁹ showed that such "order from disorder" mechanism indeed works. It leads to the appearance of directional ordering of fluctuations at low but finite temperature, although the conventional long-range orders are absent in two dimensions. This interesting conclusion was further confirmed by later investigations on either classical or quantum-mechanical two-dimensional compass models.31,32,34

Recently, it has been also proposed that the compass model could be used to generate protected cubits, and hence it may have potential application in the quantum information techniques.^{35,36} For this purpose, the ground-state degeneracy of the quantum-mechanical compass model and the existence of a possible nonvanishing gap in its spectrum are the main concerned issues.

Here, we would like to emphasize that most of the abovementioned conclusions were derived by either numerical calculations or approximate methods such as the mean-field theories. Therefore, it is certainly desirable if some exact results can be established for the compass model. Recently, Brzezicki *et al.*³⁷ studied a one-dimensional version of this model. By applying the Jordan-Wigner transformation to the pseudospin operators, they were able to map it into a spinless fermion model, whose spectrum can be exactly determined. Consequently, these authors achieved it in drawing its phase diagram. They showed that the quantum phase transition in this one-dimensional model is of the first order.

These conclusions are certainly very illuminating and provide us with deeper insights into the intrinsic frustration effects in the system. On the other hand, one would also like to see if these results still hold in higher dimensions. However, as is well known, the Jordan-Wigner transformation can be hardly applied to two- or three-dimensional systems. Therefore, in order to address this question, new techniques must be developed.

In the present paper, we shall reconsider the onedimensional compass model. Different from the previous work, we employ directly the pseudospin representation in our investigation. By applying the reflection positivity technique introduced by Dyson *et al.*,²⁶ we are able to determine degeneracy of its global ground state and the quantum phasetransition point in the system. Moreover, we find that the transition is of the first order. Our main results are consistent with the previous ones derived in Ref. 37. However, we uncover also some interesting differences. More importantly, our method provides a different approach to study rigorously the properties of the compass model in higher dimensions—a task which cannot be accomplished by the previous technique. We shall carry out this investigation in our future work.

This paper is organized as follows. In Sec. II, we shall introduce the one-dimensional compass model and discuss some important properties of it. In Sec. III, we determine degeneracy of its global ground state and study the quantum phase transition in the system. In Sec. IV, we summarize up the main conclusions of this work. Finally, in the Appendix of this paper, we establish an important inequality which is used in Sec. III.

II. ONE-DIMENSIONAL COMPASS MODEL

To begin with, we introduce Hamiltonian of the onedimensional compass model studied in Ref. 37. Take a finite one-dimensional chain Λ with L sites. In terms of the pseudospin operators, the Hamiltonian can be written as

$$\hat{H} = \sum_{i=1}^{L/2} \left(\hat{T}_{2i}^{\varepsilon} \hat{T}_{2i+1}^{\varepsilon} + J_x \hat{T}_{2i-1}^x \hat{T}_{2i}^x + J_z \hat{T}_{2i-1}^{\varepsilon} \hat{T}_{2i}^z \right).$$
(3)

In the following, we shall choose L=4m with m being a positive integer (The reason for such choice will be explained in Sec. III.) We impose also the periodic boundary conditions on the lattice.

Notice that our notation is slightly different from the one used in Ref. 37. In the previous paper, these authors introduced a parameter α for the ratio of $J_x/(J_x+J_z)$. However, we would like to consider the more general cases in which the coupling constants J_x and J_z are allowed to take on arbitrary values. As shown in Sec. III, such generalization causes only minor technical problems.

Obviously, Hamiltonian (3) lacks the SU(2) (pseudo)spin symmetry enjoyed by the conventional Heisenberg model. However, it does have a hidden internal symmetry, which is important for our investigation. Let

$$\hat{H}_{1} = \sum_{i=1}^{L/2} \left(\hat{T}_{2i}^{\varepsilon} \hat{T}_{2i+1}^{\varepsilon} + J_{x} \hat{T}_{2i-1}^{x} \hat{T}_{2i}^{x} \right), \quad \hat{H}_{2} = J_{z} \sum_{i=1}^{L/2} \hat{T}_{2i-1}^{\varepsilon} \hat{T}_{2i}^{\varepsilon}.$$
(4)

Then, we can rewrite Hamiltonian (3) as

$$\hat{H} = \hat{H}_1 + \hat{H}_2.$$
 (5)

Now, by using the anticommutation relations satisfied by the Pauli matrices, it is easy to check that \hat{H}_1 commutes with \hat{H}_2 ; i.e., $[\hat{H}_1, \hat{H}_2]=0$ holds. As a result, the spectrum of Hamiltonian (3) is simply given by the sum of eigenvalues of \hat{H}_1 and \hat{H}_2 .

Another important property of the one-dimensional compass model is that its Hilbert space has a very peculiar structure. To make this point clearer, we choose the conventional pseudospin representation, in which operator \hat{T}_i^{ϵ} is diagonal at each lattice site. Consequently, a natural basis of vectors for Hamiltonian (3) is given by

$$|\Psi_{\alpha}\rangle = |T_1^{\varsigma} = s_1, T_2^{\varsigma} = s_2, \dots, T_L^{\varsigma} = s_L\rangle$$
(6)

with $s_i = 1/2$ or -1/2. Obviously, these vectors are orthonormal and the total number of them is 2^L .

With definition (6), one can easily see that when a longitudinal interaction term, such as $\hat{T}_{2i}^{\varepsilon}\hat{T}_{2i+1}^{\varepsilon}$ or $J_z\hat{T}_{2i-1}^{\varepsilon}\hat{T}_{2i}^{\varepsilon}$, acts on $|\Psi_{\alpha}\rangle$ the vector is unchanged. However, it will be mapped to a different vector $|\Psi_{\beta}\rangle$ by any pseudospin flipping term $J_x\hat{T}_{2i-1}^{x}\hat{T}_{2i}^{x}$. In fact, such a term can be rewritten as

$$J_{x}\hat{T}_{2i-1}^{x}\hat{T}_{2i}^{x} = \frac{J_{x}}{4}(\hat{T}_{2i-1}^{+} + \hat{T}_{2i-1}^{-})(\hat{T}_{2i}^{+} + \hat{T}_{2i}^{-})$$

$$= \frac{J_{x}}{4}(\hat{T}_{2i-1}^{+}\hat{T}_{2i}^{+} + \hat{T}_{2i-1}^{+}\hat{T}_{2i}^{-} + \hat{T}_{2i-1}^{-}\hat{T}_{2i}^{+} + \hat{T}_{2i-1}^{-}\hat{T}_{2i}^{-}),$$
(7)

where $\hat{T}_{2i}^{+}=\hat{T}_{2i}^{x}+i\hat{T}_{2i}^{y}$ and \hat{T}_{2i}^{-} is its Hermitian conjugate. Therefore, it changes the total pseudospin-*z* component of each configuration by either 0 or ± 2 . Moreover, we notice that this interaction acts only on a pair of pseudospins at the end sites of bond (2i-1,2i). Consequently, the four possible configurations of these pseudospins can be divided into two separate groups

$$\mathcal{H}_{2i}^{(1)} = \left\{ \psi_{i}^{(1,1)} = \left(T_{2i-1}^{\varepsilon} = \frac{1}{2}, T_{2i}^{\varepsilon} = \frac{1}{2} \right) ,$$

$$\psi_{i}^{(1,2)} = \left(T_{2i-1}^{\varepsilon} = -\frac{1}{2}, T_{2i}^{\varepsilon} = -\frac{1}{2} \right) \right\},$$

$$\mathcal{H}_{2i}^{(2)} = \left\{ \psi_{i}^{(2,1)} = \left(T_{2i-1}^{\varepsilon} = \frac{1}{2}, T_{2i}^{\varepsilon} = -\frac{1}{2} \right) ,$$

$$\psi_{i}^{(2,2)} = \left(T_{2i-1}^{\varepsilon} = -\frac{1}{2}, T_{2i}^{\varepsilon} = \frac{1}{2} \right) \right\},$$
(8)

and the pseudospin flipping interaction does not mix them up.



FIG. 1. (Color online) Diagram for $\tilde{\Psi}_{\alpha}$. Here, 1 (0) denotes the up (down) pseudospin.

Keeping these facts in mind, it is now easy to see that the Hilbert space of Hamiltonian (3) can be decomposed as

$$\mathcal{H} = \sum_{i=1}^{L/2} \sum_{k_1, k_2, \dots, k_{L/2}} \oplus \mathcal{H}_{2i}^{(k_i)}$$
$$= \sum_{k_1, k_2, \dots, k_{L/2}} \oplus (\mathcal{H}_2^{(k_1)} \oplus \mathcal{H}_4^{(k_2)} \oplus \cdots \oplus \mathcal{H}_{2i}^{(k_i)} \oplus \cdots \oplus \mathcal{H}_{2i}^{(k_{L/2})}), \tag{9}$$

where k_i takes on values of 1 or 2. Since each direct sum in the parentheses on the right-hand side of Eq. (9) is invariant under the action of Hamiltonian (3), it is a subspace of the system. Correspondingly, we define sequence $(k_1, k_2, ..., k_i, ..., k_{L/2})$ to be its characterizing sequence.

Obviously, a more suitable basis of vectors for this subspace is given by

$$\widetilde{\Psi}_{\alpha} = \phi_{2}^{(k_{1},\mu_{1})} \otimes \phi_{4}^{(k_{2},\mu_{2})} \otimes \cdots \otimes \phi_{2i}^{(k_{i},\mu_{i})} \otimes \cdots \otimes \phi_{L}^{(k_{L/2},\mu_{L/2})}$$
(10)

with $\phi_{2i}^{(k_i,\mu_i)}$ being one of the two configurations in sector $\mathcal{H}_{2i}^{(k_i)}$. Graphically, such a vector can be depicted as in Fig. 1.

III. QUANTUM PHASE TRANSITION IN THE ONE-DIMENSIONAL COMPASS MODEL

With the above preparations, we are ready to state our main results. First, let us consider the ground state of Hamiltonian (3) in each subspace. We have the following theorem:

Theorem 1. When $J_x \neq 0$, for any specific characterizing sequence $(k_1, k_2, \ldots, k_{L/2})$, the ground state of Hamiltonian (3) in the subspace

$$\mathcal{H}(k_1, k_2, \dots, k_{L/2}) \equiv \mathcal{H}_2^{(k_1)} \oplus \mathcal{H}_4^{(k_2)} \oplus \dots \oplus \mathcal{H}_{2i}^{(k_i)} \oplus \dots \oplus \mathcal{H}_L^{(k_{L/2})}$$
(11)

is nondegenerate.

Proof 1. For definiteness, let us assume that $J_x < 0$. Otherwise, we introduce a transformation

$$\hat{U}_1 = \prod_{l=1}^{L/2} \exp(i\pi \hat{T}_{2l}^z), \qquad (12)$$

which rotates the pseudospin operators at each even lattice site 2i by an angle π about the \hat{T}^z axis. Under this transformation, the pseudospin flipping terms will change sign while other terms are invariant. Therefore, the sign of J_x is irrelevant as far as the ground-state degeneracy is concerned.

Next, in terms of the basis vectors given in Eq. (10), we write Hamiltonian (3) into a matrix $H(k_1, k_2, ..., k_{L/2})$. It has the following properties:

(i) All the off-diagonal elements of this matrix are nonpositive. More precisely, they are equal to either zero or J_x .

(ii) $H(k_1, k_2, ..., k_{L/2})$ is irreducible in the subspace $\mathcal{H}(k_1, k_2, ..., k_{L/2})$. In other words, for any pair of row and column indices *m* and *n*, one can find a positive integer *K* such that

$$[H^{K}(k_{1},k_{2},\ldots,k_{L/2})]_{mn} \neq 0.$$
(13)

It is due to the fact that the subspace $\mathcal{H}(k_1, k_2, \dots, k_{L/2})$ is connected by the pseudospin flipping interactions; i.e., any basis vector Ψ_β in the subspace $\mathcal{H}(k_1, k_2, \dots, k_{L/2})$ can be reached from an initial state Ψ_α in the same subspace by a finite number of pseudospin flipping.

For such a matrix, the Perron-Fröbenius theorem in matrix theory applies.³⁸ It tells us that the lowest eigenvalue of $H(k_1, k_2, \ldots, k_{L/2})$ is unique. In other words, the ground state of Hamiltonian (3) in the subspace $\mathcal{H}(k_1, k_2, \ldots, k_{L/2})$ is non-degenerate. QED.

A direct corollary of Theorem 1 is:

Corollary 1. The global ground state of Hamiltonian (3) is, at most, $2^{L/2}$ -fold degenerate.

In fact, by Eq. (9), the Hilbert space of the system is decomposed as a direct sum of subspaces $\{\mathcal{H}(k_1, k_2, \ldots, k_{L/2})\}$, which are characterized by sequences $\{(k_1, k_2, \ldots, k_{L/2})\}$ with $k_i=1$ or 2. Obviously, the total number of these sequences is $2^{L/2}$. On the other hand, by Theorem 1, the ground state of Hamiltonian (3) in each subspace is nondegenerate. Therefore, degeneracy of the global ground state of the system cannot be larger than $2^{L/2}$.

Corollary 1 can be further improved. For this purpose, one needs to exploit the internal symmetries of the compass model in a more sophisticated way. Let us first consider the special case of $J_z=0$. Under this condition, Hamiltonian (3) is reduced to \hat{H}_1 defined in Eq. (4). For this Hamiltonian, we have:

Theorem 2. When $J_z=0$, the ground states of Hamiltonian \hat{H}_1 in subspaces $\mathcal{H}^{(1)}=\mathcal{H}(k_1=k_2=\cdots=k_{L/2}=1)$ and $\mathcal{H}^{(2)}=\mathcal{H}(k_1=k_2=\cdots=k_{L/2}=2)$ have the lowest energy. In other words, they are the global ground state of the system. Furthermore, the ground state in each subspace, which is created from $\mathcal{H}^{(1)}$ ($\mathcal{H}^{(2)}$) by replacing an even number of indices $\{k_i=1\}$ ($\{k_i=2\}$) with integer $k_i=2$ ($k_i=1$), has also the lowest energy. Therefore, the global ground state is actually $2^{L/2-1}$ -fold degenerate in this case.

In our investigation, the above conclusions were initially derived by numerical calculation on the one-dimensional compass model. However, our data are different from the previous results. In Ref. 37, the authors found that degeneracy of the global ground state is $2 \times 2^{L/2}$ when $\alpha = 1$, which is equivalent to setting $J_z=0$ and $J_x=1$. This discrepancy kindles our interest in this seemingly simple but highly frustrated model.

Proof 2. To make our proof of Theorem 2 more readable, we introduce some useful definitions. For obvious reason, we call both subspaces $\mathcal{H}^{(1)}$ and $\mathcal{H}^{(2)}$ homogeneous. Therefore, any subspace, which is created from $\mathcal{H}^{(1)}$ by replacing some indices $k_i=1$ with 2, or from $\mathcal{H}^{(2)}$ by replacing some indices $k_i=2$ with 1, is called unhomogeneous. By this definition,

there must exist, at least, one pair of neighboring indices k_j and k_{j+1} which have different values, say $k_j=1$ and $k_{j+1}=2$, in the characterizing sequence of an unhomogeneous subspace. In this case, we call the lattice bond (2j, 2j+1), which is saddled between these two indices, a "bad" one. Therefore, one subspace $\mathcal{H}^{(\mu)}$ is more unhomogeneous than another subspace $\mathcal{H}^{(\nu)}$ if the former has more bad bonds.

With these definitions, we are able to prove

Lemma 1. Let $\Psi_0^{(\alpha)}$ be the nondegenerate ground state of Hamiltonian \hat{H}_1 in an unhomogeneous subspace $\mathcal{H}^{(\alpha)}$. Assume that it is also a global ground state. Then, there exists a more homogeneous subspace $\mathcal{H}^{(\beta)}$, in which the ground state of \hat{H}_1 coincides with its global ground state too.

To establish this lemma, we shall apply the reflection positivity method developed in Ref. 26. However, since the proof is quite lengthy, we shall postpone it to the Appendix of this paper.

A direct corollary of Lemma 1 is that one of the ground states of \hat{H}_1 in the two homogeneous subspaces must be a global ground state. On the other hand, it is easy to see that there is a one-to-one mapping between the basis vectors of subspaces $\mathcal{H}^{(1)}$ and $\mathcal{H}^{(2)}$. Under this mapping, H(1, 1, ..., 1), the Hamiltonian matrix in subspace $\mathcal{H}^{(1)}$ is unitarily equivalent to its counterpart in subspace $\mathcal{H}^{(2)}$. Consequently, both the ground states $\Psi_0^{(1)}$ and $\Psi_0^{(2)}$ in these homogeneous subspaces are global ground states.

Next, we study the nondegenerate ground state of H_1 in an unhomogeneous subspace $\mathcal{H}^{(\alpha)}$. We find that if the subspace is created from one of the homogeneous subspaces $\mathcal{H}^{(1)}$ and $\mathcal{H}^{(2)}$ by an even number of index replacements, then the corresponding Hamiltonian matrix $H(\alpha)$ in this subspace can be always brought into the form of either $H(1,1,\ldots,1)$ or $H(2,2,\ldots,2)$ by exchanging properly its rows and columns. As is well known, this operation is equivalent to constructing a unitary mapping between the basis vectors of $\mathcal{H}^{(\alpha)}$ and the homogeneous subspace. [For a concrete example, one may study such a mapping between subspaces $\mathcal{H}(1,2,2,1)$ and $\mathcal{H}(2,2,2,2)$ for a ring with L=8 sites.] Consequently, these matrices must have the same spectrum. In particular, their ground-state energies must be equal. Therefore, $\Psi_0^{(\alpha)}$ is also a global ground state.

On the other hand, if an unhomogeneous subspace $\mathcal{H}^{(\beta)}$ is created from either $\mathcal{H}^{(1)}$ or $\mathcal{H}^{(2)}$ by an odd number of index replacements, no such unitary mapping can be found. As a result, the spectrum of $H(\beta)$ is different from the one of matrices H(1, 1, ..., 1) and H(2, 2, ..., 2). As explained in a remark at the end of Appendix, it implies that the ground state $\Psi_0^{(\beta)}$ of \hat{H}_1 in subspace $\mathcal{H}^{(\beta)}$ has a higher energy than its counterparts $\Psi_0^{(1)}$ and $\Psi_0^{(2)}$ in the homogeneous subspaces. Therefore, it cannot be a global ground state of the system.

Summarizing these results, we conclude that, when $J_z=0$, the global ground state of the one-dimensional compass model coincides with its ground states in such subspaces, which are created from a homogeneous subspace by an even number of index replacements. Since the total number of these subspaces is $2^{L/2-1}$, the global ground state of the system is also $2^{L/2-1}$ -fold degenerate.

Our proof of Theorem 2 is accomplished. QED.

Finally, we study the case of $J_z \neq 0$. Interestingly, the high ground-state degeneracy of the system is completely lifted

by this perturbation. More precisely, we have:

Theorem 3. When $J_z \neq 0$, the global ground state of Hamiltonian (3) is nondegenerate. More precisely, for J_z < 0, the global ground state Ψ_0 coincides with the one in the homogeneous subspace $\mathcal{H}^{(1)}$. For $J_z > 0$, it is given by the ground state of the system in $\mathcal{H}^{(2)}$.

Proof 3. When $J_z \neq 0$, Hamiltonian (3) is completely recovered. However, as we emphasized in Sec. II, the newly added Hamiltonian \hat{H}_2 commutes with \hat{H}_1 , which is the Hamiltonian of the system for $J_z=0$. Therefore, they should have a common set of eigenvectors. In fact, a direct inspection reveals that the eigenvalue of \hat{H}_2 in each subspace $\mathcal{H}(k_1, k_2, \dots, k_i, \dots, k_{L/2})$ is actually a constant.

Intuitively, by comparing Hamiltonian (3) with the wellknown Heisenberg model in an external magnetic field, one can think of \hat{H}_2 as an "external field" perturbation in addition to the "unperturbated" Hamiltonian \hat{H}_1 . Therefore, the ground state of \hat{H}_1 in each subspace $\mathcal{H}^{(\alpha)}$ is also the ground state of Hamiltonian (3) in the same subspace. However, the high ground-state degeneracy of \hat{H}_1 is completely lifted by this perturbation. Since \hat{H}_2 has its minimum in either subspace $\mathcal{H}^{(1)}$ for $J_z < 0$ or $\mathcal{H}^{(2)}$ for $J_z > 0$, so does Hamiltonian (3). It determines in which subspace the global ground state of the system should be. QED.

As a direct application of Theorems 2 and 3, we reach immediately the following conclusions:

Corollary 2. $J_z=0$ is the quantum phase-transition point of the one-dimensional compass model. Moreover, the corresponding transition is of the first order.

Proof 4. The first statement is trivial. To see why the transition is of the first order, we notice that the global ground state is in different subspaces $\mathcal{H}^{(1)}$ and $\mathcal{H}^{(2)}$ on the left- and right-hand sides of the transition point. Therefore, a ground-state level crossing occurs at $J_z=0$. It indicates that the transition must be of the first-order. QED.

As a final remark, we would like to point out that the similar phenomenon of ground-state bifurcation was also observed in some ferrimagnets with anisotropic interactions.³⁹

IV. SUMMARY

In Secs. I and III, we investigate the quantum phase transition in the one-dimensional compass model previously introduced by Brzezicki *et al.*³⁷ Our main purpose is to develop a different rigorous approach in frame of the conventional pseudospin representation to study such a complicated system with built-in frustrations.

By applying the reflection positivity technique²⁶ and exploiting internal symmetry of the system, we find that, at $J_z=0$, the global ground state of Hamiltonian (3) is highly degenerate. However, the degeneracy of ground state is completely lifted on both sides of this point. In fact, for either $J_z<0$ or $J_z>0$, the global ground state becomes nondegenerate and appears in different subspaces. In other words, a ground-state level crossing occurs at $J_z=0$. It implies that $J_z=0$ is the quantum phase-transition point of the one-dimensional compass model and the transition is of the first

order. These results confirm the previous conclusions derived from Ref. 37. However, we also find difference on some issues such as degeneracy of the global ground state at $J_z = 0$.

More importantly, unlike the previous approach based on the Jordan-Wigner transformation, our method can be potentially applied to study rigorously the compass model in higher dimensions. It is a more interesting system which may have application to quantum information techniques. We shall carry out such investigation in our future work.

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APPENDIX: PROOF OF LEMMA 1

To prove Lemma 1, we shall apply the reflection positivity technique developed by Dyson *et al.*²⁶ First, we introduce a set \mathcal{N} . It consists of all the subspaces $\mathcal{H}^{(\alpha)}$ in which the ground states of \hat{H}_1 coincide with its global ground state. We assume that neither homogeneous subspace $\mathcal{H}^{(1)}$ nor $\mathcal{H}^{(2)}$ is in this set. Otherwise, the lemma becomes trivial. Under this assumption, \mathcal{N} must contain one subspace, say $\mathcal{H}^{(\beta)}$, which is the least unhomogeneous; i.e., it has the minimal number of bad bonds. Obviously, integer N_{\min} should be finite but nonzero. However, we shall show that such an integer does not exist. Therefore, Lemma 1 must be true.

To start with, we consider the characterizing sequence $(k_1^{(\beta)}, k_2^{(\beta)}, \dots, k_j^{(\beta)}, k_{j+1}^{(\beta)}, \dots, k_{L/2}^{(\beta)})$ of $\mathcal{H}^{(\beta)}$. By its definition, this sequence must have, at least, a pair of neighboring indices $k_l^{(\beta)}$ and $k_{l+1}^{(\beta)}$ such that they take on different values (say $k_l^{(\beta)} = 1$ and $k_{l+1}^{(\beta)} = 2$). Therefore, the bond (2l, 2l+1), on which only the interaction term $\hat{T}_{2l}^{\epsilon} \hat{T}_{2l+1}^{\epsilon}$ acts, is a bad bond.

To go further, let us choose an arbitrary bad bond, say (2j,2j+1), and draw a perpendicular plane *P* through its middle. Since the one-dimensional lattice forms a ring of *L* = 4*m* sites under the periodic boundary condition, this plane must also cut through the middle of another bond (2j', 2j' + 1), which is on the opposite side of the specific bad bond and has only the interaction term $\hat{T}_{2j'}^{\varepsilon} \hat{T}_{2j'+1}^{\varepsilon}$ acting on it. We would like to emphasize that this bond may be either bad or not. It does not affect our following argument. As a result, the one-dimensional lattice ring Λ is divided into two equal halves Λ_L and Λ_R , which we refer to as the left and right sublattices, respectively.

In terms of this division of lattice, Hamiltonian \hat{H}_1 can be rewritten as

$$\begin{aligned} \hat{H}_{1} &= \sum_{i=1}^{L/2} \left(\hat{T}_{2i}^{\varepsilon} \hat{T}_{2i+1}^{\varepsilon} + J_{x} \hat{T}_{2i-1}^{x} \hat{T}_{2i}^{x} \right) \\ &= \hat{H}_{L} + \hat{H}_{R} + \hat{T}_{2j}^{\varepsilon} \hat{T}_{2j+1}^{\varepsilon} + \hat{T}_{2j'}^{\varepsilon} \hat{T}_{2j'+1}^{\varepsilon}. \end{aligned} \tag{A1}$$

In Eq. (A1), \hat{H}_L and \hat{H}_R represent the interactions which are

solely defined on sublattices Λ_L and Λ_R , respectively. The rest of the terms denotes the pseudospin interactions on the bonds (2j, 2j+1) and (2j', 2j'+1), which are cut by the plane *P*.

However, the reflection positivity method cannot be directly applied to Hamiltonian (A1) since signs of the last two terms in it are positive. To remedy this problem, we introduce a unitary transformation

$$\hat{U}_2 = \prod_{l \in \Lambda_L} \exp(i\pi \hat{T}_l^y), \tag{A2}$$

which rotates each pseudospin on the left sublattice by an angle π about the \hat{T}^y axis and does not affect the pseudospin operators on the right sublattice. Under this transformation, both \hat{H}_L and \hat{H}_R are invariant but the last two terms of Eq. (A1) change their signs. More importantly, both the subspace $\mathcal{H}^{(\beta)}$ and its characterizing sequence are also invariant.

In the following, for simplicity, we shall use the same notation \hat{H}_1 for the transformed Hamiltonian, whose last two terms in Eq. (A1) have now negative signs. To it, we can apply the reflection positivity method.

We choose two complete sets of pseudospin configurations $\{\psi_{\mu}^{L}\}$ and $\{\phi_{\nu}^{R}\}$ as the basis vectors for the Hilbert spaces on the left and right sublattices, respectively. Obviously, the set of their direct products $\{\psi_{\mu}^{L} \otimes \phi_{\nu}^{R}\}$ gives a basis for the total Hilbert space of the system. In particular, in terms of this basis, the ground-state wave function in subspace $\mathcal{H}^{(\beta)}$ can be written as

$$\Psi_0^{(\beta)} = \sum_{\mu,\nu} W_{\mu\nu}^{(\beta)} \psi_{\mu}^L \otimes \phi_{\nu}^R.$$
 (A3)

Here, $W_{\mu\nu}^{(\beta)}$ are the expansion coefficients. By taking μ for the row index and ν for the column index, we can write these coefficients into a matrix $W^{(\beta)}$. Consequently, the energy of $\Psi_0^{(\beta)}$, which is also a global ground state of \hat{H}_1 , is given by

$$E_{0} = \langle \Psi_{0}^{(\beta)} | \hat{H}_{1} | \Psi_{0}^{(\beta)} \rangle = \sum_{\mu_{1},\mu_{2},\nu} \overline{W}_{\mu_{1}\nu}^{(\beta)} W_{\mu_{2}\nu}^{(\beta)} \langle \psi_{\mu_{1}}^{L} | \hat{H}_{L} | \psi_{\mu_{2}}^{L} \rangle + \sum_{\mu,\nu_{1},\nu_{2}} \overline{W}_{\mu\nu_{1}}^{(\beta)} W_{\mu\nu_{2}}^{(\beta)} \langle \psi_{\nu_{1}}^{R} | \hat{H}_{R} | \psi_{\nu_{2}}^{R} \rangle \\ - \sum_{\mu_{1},\mu_{2},\nu_{1},\nu_{2}} \overline{W}_{\mu_{1}\nu_{1}}^{(\beta)} W_{\mu_{2}\nu_{2}}^{(\beta)} \langle \psi_{\mu_{1}}^{L} | \hat{T}_{2j}^{\varepsilon} | \psi_{\mu_{2}}^{L} \rangle \langle \psi_{\nu_{1}}^{R} | \hat{T}_{2j+1}^{\varepsilon} | \psi_{\nu_{2}}^{R} \rangle - \sum_{\mu_{1},\mu_{2},\nu_{1},\nu_{2}} \overline{W}_{\mu_{1}\nu_{1}}^{(\beta)} W_{\mu_{2}\nu_{2}}^{(\beta)} \langle \psi_{\mu_{1}}^{L} | \hat{T}_{2j'+1}^{\varepsilon} | \psi_{\mu_{2}}^{L} \rangle \langle \psi_{\nu_{1}}^{R} | \hat{T}_{2j'}^{\varepsilon} | \psi_{\nu_{2}}^{R} \rangle \\ = \operatorname{Tr}[H_{L} \mathcal{W}^{(\beta)}(\mathcal{W}^{(\beta)})^{\dagger}] + \operatorname{Tr}[H_{R}(\mathcal{W}^{(\beta)})^{\dagger} \mathcal{W}^{(\beta)}] - \operatorname{Tr}[(\mathcal{W}^{(\beta)})^{\dagger} T_{2j}^{\varepsilon} \mathcal{W}^{(\beta)} T_{2j+1}^{\varepsilon}] - \operatorname{Tr}[\mathcal{W}^{(\beta)} T_{2j'}^{\varepsilon} (\mathcal{W}^{(\beta)})^{\dagger} T_{2j'+1}^{\varepsilon}].$$
(A4)

In the last two terms of the third equality of this equation, $T_{2j}^{\varepsilon}, T_{2j+1}^{\varepsilon}, T_{2j'}^{\varepsilon}, T_{2j'+1}^{\varepsilon}$ are the matrices of the corresponding operators $\hat{T}_{2j}^{\varepsilon}, \hat{T}_{2j+1}^{\varepsilon}, \hat{T}_{2j'}^{\varepsilon}, \hat{T}_{2j'+1}^{\varepsilon}$, respectively. However, in general, matrix $\mathcal{W}^{(\beta)}$ may not be Hermitian.

However, in general, matrix $\mathcal{W}^{(\beta)}$ may not be Hermitian. In the worst case, it could be even not square. Fortunately, for such a singular matrix, we still have the following lemma:

Lemma 2. Let \mathcal{W} be an $m \times n$ matrix. Assume that m > n for definiteness. Then, there exist an $n \times n$ unitary matrix $U_{\mathcal{W}}$, an $n \times n$ diagonal matrix $\Lambda_{\mathcal{W}}$, and an $m \times n$ orthogonal matrix $V_{\mathcal{W}}$, whose columns are orthonormal vectors such that the identity

$$\mathcal{W} = V_{\mathcal{W}} \Lambda_{\mathcal{W}} U_{\mathcal{W}} \tag{A5}$$

holds. Moreover, all the elements $\{\lambda_l\}$ of Λ_W are nonnegative, i.e., $\lambda_l \ge 0$.

In literature, this lemma is called the singular decomposition theorem. Its proof can be found in a standard textbook on matrix theory.⁴⁰

By applying the singular decomposition theorem to the ground state $\Psi_0^{(\beta)}$, we obtain

$$\Psi_{0}^{(\beta)} = \sum_{\mu,\nu} W_{\mu\nu}^{(\beta)} \psi_{\mu}^{L} \otimes \phi_{\nu}^{R} = \sum_{l} \lambda_{l}(\beta) \xi_{l}^{L}(\beta) \otimes \chi_{l}^{R}(\beta),$$
(A6)

where the basis vectors are defined by

$$\xi_l^L(\beta) = \sum_{\mu} (V_{\mathcal{W}^{(\beta)}})_{\mu l} \psi_{\mu}^L, \quad \chi_l^R(\beta) = \sum_{\nu} (U_{\mathcal{W}^{(\beta)}})_{l\nu} \psi_{\nu}^R.$$
(A7)

Since matrix $U_{\mathcal{W}^{(\beta)}}$ is unitary and $V_{\mathcal{W}^{(\beta)}}$ is orthogonal, these vectors, which are defined on different sublattices, are also orthonormal.

As a result, Eq. (A4) can be rewritten as

$$E_{0} = \sum_{l} \lambda_{l}^{2}(\beta) \left(\langle \xi_{l}^{L}(\beta) | \hat{H}_{L} | \xi_{l}^{L}(\beta) \rangle + \langle \chi_{l}^{R}(\beta) | \hat{H}_{R} | \chi_{l}^{R}(\beta) \rangle \right)$$
$$- \sum_{l_{1},l_{2}} \lambda_{l_{1}}(\beta) \lambda_{l_{2}}(\beta) \langle \xi_{l_{2}}^{L} | \hat{T}_{2j}^{\varepsilon} | \xi_{l_{1}}^{L} \rangle \langle \chi_{l_{2}}^{R}(\beta) | \hat{T}_{2j+1}^{\varepsilon} | \chi_{l_{1}}^{R}(\beta) \rangle$$
$$- \sum_{l_{1},l_{2}} \lambda_{l_{1}}(\beta) \lambda_{l_{2}}(\beta) \langle \xi_{l_{2}}^{L}(\beta) | \hat{T}_{2j'+1}^{\varepsilon} | \xi_{l_{1}}^{L}(\beta) \rangle$$
$$\times \langle \chi_{l_{2}}^{R}(\beta) | \hat{T}_{2j'}^{\varepsilon} | \chi_{l_{1}}^{R}(\beta) \rangle, \qquad (A8)$$

and the nonnegative quantities $\{\lambda_l(\beta)\}\$ are subjected to the condition

$$\langle \Psi_0^{(\beta)} | \Psi_0^{(\beta)} \rangle = \operatorname{Tr}[(\mathcal{W}^{(\beta)})^{\dagger} \mathcal{W}^{(\beta)}] = \sum_l \lambda_l^2(\beta) = 1.$$
(A9)

In the following, without causing confusion, we shall drop superscripts L and R as well as lattice-site indices 2j, 2j + 1, 2j', 2j' + 1 in Eq. (A8) for convenience.

Finally, by applying inequality $|ab| \le 1/2(|a|^2 + |b|^2)$ to each term in the last two summations of Eq. (A8), we are able to write it into the following inequality:

$$\begin{split} E_{0} &\geq \frac{1}{2} \sum_{l} \lambda_{l}^{2}(\beta) (\langle \xi_{l}(\beta) | \hat{H}_{L} | \xi_{l}(\beta) \rangle + \langle \xi_{l}(\beta) | \hat{H}_{L} | \xi_{l}(\beta) \rangle) \\ &+ \frac{1}{2} \sum_{l} \lambda_{l}^{2}(\beta) (\langle \chi_{l}(\beta) | \hat{H}_{R} | \chi_{l}(\beta) \rangle + \langle \chi_{l}(\beta) | \hat{H}_{R} | \chi_{l}(\beta) \rangle) \\ &- \frac{1}{2} \sum_{l_{1},l_{2}} \lambda_{l_{1}}(\beta) \lambda_{l_{2}}(\beta) \langle \xi_{l_{2}}(\beta) | \hat{T}^{\varepsilon} | \xi_{l_{1}}(\beta) \rangle \overline{\langle \xi_{l_{2}}(\beta) | \hat{T}^{\varepsilon} | \xi_{l_{1}}(\beta) \rangle} \\ &- \frac{1}{2} \sum_{l_{1},l_{2}} \lambda_{l_{1}}(\beta) \lambda_{l_{2}}(\beta) \langle \chi_{l_{2}}(\beta) | \hat{T}^{\varepsilon} | \chi_{l_{1}}(\beta) \rangle \overline{\langle \chi_{l_{2}}(\beta) | \hat{T}^{\varepsilon} | \chi_{l_{1}}(\beta) \rangle} \\ &- \frac{1}{2} \sum_{l_{1},l_{2}} \lambda_{l_{1}}(\beta) \lambda_{l_{2}}(\beta) \langle \xi_{l_{2}}(\beta) | \hat{T}^{\varepsilon} | \xi_{l_{1}}(\beta) \rangle \overline{\langle \xi_{l_{2}}(\beta) | \hat{T}^{\varepsilon} | \xi_{l_{1}}(\beta) \rangle} \\ &- \frac{1}{2} \sum_{l_{1},l_{2}} \lambda_{l_{1}}(\beta) \lambda_{l_{2}}(\beta) \langle \chi_{l_{2}}(\beta) | \hat{T}^{\varepsilon} | \chi_{l_{1}}(\beta) \rangle \overline{\langle \chi_{l_{2}}(\beta) | \hat{T}^{\varepsilon} | \chi_{l_{1}}(\beta) \rangle}. \end{split}$$

$$(A10)$$

Although it looks quite complicated, one can bring this inequality into a more compact form by introducing wave functions

$$\Psi_1 = \sum_l \lambda_l(\beta) \xi_l^L(\beta) \otimes \overline{\xi}_l^R(\beta), \quad \Psi_2 = \sum_l \lambda_l(\beta) \chi_l^L(\beta) \otimes \overline{\chi}_l^R(\beta),$$
(A11)

where $\bar{\xi}_l(\beta)$ and $\bar{\phi}_l(\beta)$ are the complex conjugates of $\xi_l(\beta)$ and $\bar{\phi}_l(\beta)$, respectively. Since Hamiltonians \hat{H}_L and \hat{H}_R have exactly the same form, the right-hand side of the above inequality can be further rewritten as $1/2(\langle \Psi_1 | \hat{H}_1 | \Psi_1 \rangle$ $+ \langle \Psi_2 | \hat{H}_1 | \Psi_2 \rangle$. Therefore, inequality (A10) actually reads

$$E_{0} \geq \frac{1}{2} \langle \Psi_{1} | \hat{H}_{1} | \Psi_{1} \rangle + \frac{1}{2} \langle \Psi_{2} | \hat{H}_{1} | \Psi_{2} \rangle.$$
 (A12)

We would like to point out that, by its definition, the wave function Ψ_1 belongs to a subspace $\mathcal{H}^{(\gamma)}$, which is, in general, different from the original unhomogeneous subspace $\mathcal{H}^{(\beta)}$. So does Ψ_2 , which is in another subspace $\mathcal{H}^{(\delta)}$. An important observation is that, at least, one of these subspaces, say $\mathcal{H}^{(\gamma)}$, is strictly less unhomogeneous than the original subspace $\mathcal{H}^{(\beta)}$. To make this point clearer, let us study more carefully the characterizing sequence of $\mathcal{H}^{(\gamma)}$. By construction of wave function Ψ_1 , this sequence is determined by the following rule. If the subsequences of $(k_1^{(\beta)}, k_2^{(\beta)}, \ldots, k_{L/2}^{(\beta)})$ on the left and right sublattices are, respectively, given by $(k_{j'-1}^{(\beta)}, k_{j'-2}^{(\beta)}, \ldots, k_{j-1}^{(\beta)})$ and $(k_{j'}^{(\beta)}, k_{j'+1}^{(\beta)}, \ldots, k_j^{(\beta)})$, then the characterizing sequence of $\mathcal{H}^{(\gamma)}$ is given by

$$K^{(\gamma)} = [k_{j'-1}^{(\gamma)} = k_{j'-1}^{(\beta)}, \dots, k_{j-1}^{(\gamma)} = k_{j-1}^{(\beta)}, k_j^{(\gamma)} = R(k_{j-1}^{(\beta)}), \dots, k_{j'}^{(\gamma)} = R(k_{j'-1}^{(\beta)})], \quad (A13)$$

where $R(k_i^{(\beta)})$ stands for the mapping of integer $k_i^{(\beta)}$ by reflection in plane *P*. For instance, we have $k_i^{(\gamma)} = R(k_{i-1}^{(\beta)})$

 $=k_{j-1}^{(\beta)}$. That is due to the fact that the wave function Ψ_1 , which is in the subspace $\mathcal{H}^{(\gamma)}$, is an expansion of basis vectors $\{\xi_l^L(\beta) \otimes \overline{\xi}_l^R(\beta)\}$. Therefore, a basis of $\mathcal{H}^{(\gamma)}$ is actually given by all the direct products of a configuration $\xi_l^L(\beta)$ on the left sublattice and the complex conjugate of its reflected image by plane *P* on the right sublattice.

Similarly, the characterizing sequence of subspace $\mathcal{H}^{(\delta)}$ is of the form $K^{(\delta)} = [R(k_j^{(\beta)}), \dots, R(k_{j'+1}^{(\beta)}), R(k_{j'}^{(\beta)}), k_{j'}^{(\beta)}, k_{j'+1}^{(\beta)}, \dots, k_j^{(\beta)}]$. Naturally, by the above construction, bonds (2j, 2j+1) and (2j', 2j'+1) are no longer bad in either $K^{(\gamma)}$ or $K^{(\delta)}$. Therefore, one of subspaces $\mathcal{H}^{(\gamma)}$ and $\mathcal{H}^{(\delta)}$ must be strictly less unhomogeneous than $\mathcal{H}^{(\beta)}$.

Keeping these facts in mind, we can further strengthen inequality (A12) as

$$E_0 \ge \frac{1}{2} E_0(\mathcal{H}^{(\gamma)}) + \frac{1}{2} E_0(\mathcal{H}^{(\delta)}),$$
 (A14)

where $E_0(\mathcal{H}^{(\gamma)})$ and $E_0(\mathcal{H}^{(\delta)})$ are the ground-state energies of Hamiltonian \hat{H}_1 in the subspaces $\mathcal{H}^{(\gamma)}$ and $\mathcal{H}^{(\delta)}$, respectively. Therefore, one of them must be less than or equal to E_0 , which is the global ground-state energy of the system. Otherwise, inequality (A14) cannot hold. Now, if we can show that the corresponding subspace is also strictly less unhomogeneous than $\mathcal{H}^{(\beta)}$, then Lemma 1 is proven.

As mentioned above, by their construction, one of subspaces $\mathcal{H}^{(\gamma)}$ and $\mathcal{H}^{(\delta)}$ is already known to be strictly less unhomogeneous than $\mathcal{H}^{(\beta)}$. Therefore, if another one is also strictly less unhomogeneous than $\mathcal{H}^{(\beta)}$, then we reach Lemma 1 without further ado. Consequently, we need only to consider the other possibility, i.e., the second subspace, say $\mathcal{H}^{(\delta)}$, is more unhomogeneous than $\mathcal{H}^{(\beta)}$.

However, in this case, the ground-state energy of \hat{H}_1 in $\mathcal{H}^{(\delta)}$ must be larger than the global ground-state energy E_0 . In other words, we have

$$E_0(\mathcal{H}^{(\delta)}) \ge E_0(\mathcal{H}^{(\beta)}) = E_0. \tag{A15}$$

It is due to the very definition of $\mathcal{H}^{(\beta)}$, which is the least unhomogeneous member of set \mathcal{N} . By substituting this inequality into Eq. (A14), we find that $E_0(\mathcal{H}^{(\gamma)}) \leq E_0$. Therefore, $\Psi_0^{(\gamma)}$ is also a global ground state of \hat{H}_1 . In the meantime, subspace $\mathcal{H}^{(\gamma)}$ is strictly less unhomogeneous than $\mathcal{H}^{(\beta)}$. That ends our proof of Lemma 1. QED.

Before finishing this appendix, we would like to make a remark. From the above discussion, one can easily see that inequality (A12) plays a vital role in proving Lemma 1. An interesting question is whether this inequality can be made strict under some additional condition. Previously, this problem has been addressed by several authors. For instance, a concise discussion on this issue can be found in the appendix of Ref. 41. An important conclusion is that if

$$\langle \xi_l^L(\beta) | \hat{H}_L | \xi_l^L(\beta) \rangle \neq \langle \chi_l^R(\beta) | \hat{H}_R | \chi_l^R(\beta) \rangle$$
 (A16)

for some basis vector $\xi_l^L(\beta) \otimes \chi_l^R(\beta)$, then inequality (A12) is strict.

Applying this result to \hat{H}_1 , we see that if the unhomogeneous subspace $\mathcal{H}^{(\beta)}$ is created from one of the homogeneous subspaces $\mathcal{H}^{(1)}$ and $\mathcal{H}^{(2)}$ by an odd number of index replacements, then the subspace on the left sublattice cannot be isomorphic to the one on the right-hand side of plane *P*. Therefore, there exists, at least, a pair of configurations $\xi_l^L(\beta)$

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and $\chi_{I}^{R}(\beta)$, which makes Eq. (A16) satisfied. It implies that

inequality (A12) as well as inequality (A14) must be strict.

As a result, the ground state $\Psi_0^{(eta)}$ of \hat{H}_1 in subspace $\mathcal{H}^{(eta)}$

cannot be a global ground state. We should mention that the

above mentioned conclusion is also confirmed by our nu-

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