PHYSICAL REVIEW E **90**, 022116 (2014)

Analysis and resolution of the ground-state degeneracy of the two-component Bose-Hubbard model

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(Received 13 June 2014; published 15 August 2014)

We study the degeneracy of the ground-state energy E of the two-component Bose-Hubbard model and of the perturbative correction E_1. We show that the degeneracy properties of E and E_1 are closely related to the connectivity properties of the lattice. We determine general conditions under which E is nondegenerate. This analysis is then extended to investigate the degeneracy of E_1. In this case, in addition to the lattice structure, the degeneracy also depends on the number of particles present in the system. After identifying the cases in which E_1 is degenerate and observing that the standard (degenerate) perturbation theory is not applicable, we develop a method to determine the zeroth-order correction to the ground state by exploiting the symmetry properties of the lattice. This method is used to implement the perturbative approach to the two-component Bose-Hubbard model in the case of degenerate E_1 and is expected to be a valid tool to perturbatively study the asymmetric character of the Mott insulator to superfluid transition between the particle and hole side.

DOI: 10.1103/PhysRevE.90.022116 PACS number(s): 05.30.Rt, 67.85.−d, 03.75.Mn

I. INTRODUCTION

Bosonic binary mixtures trapped in optical lattices have attracted considerable attention [1–13] in the past decade due to theoretic prediction of several new quantum phases originated by the interaction between the two components [6–11]. The mixture can consist of either two atomic species or the same species in two different internal states, with each component being described within the Bose-Hubbard (BH) picture [14,15]. The recent experimental realization of bosonic mixtures [2–4], in addition to their rich phenomenology, has reinforced the interest for this class of systems. The mixture is described by the two-component BH model as follows [6]:

$$H = H_a + H_b + U_{ab} \sum_{i=1}^{M} n_i^a n_i^b, \tag{1}$$

where U_{ab} represents the interspecies interaction, that is, the coupling between the two components $\mathcal{A}$ and $\mathcal{B}$. The local number operators $n_i^a = a_i^\dagger a_i$ and $n_i^b = b_i^\dagger b_i$ are defined in terms of space-mode bosonic operators a_i and b_i, relevant to species $\mathcal{A}$ and $\mathcal{B}$, respectively, satisfying the standard commutators $[a_r, a_i^\dagger] = [b_r, b_i^\dagger] = \delta_{ri}$, where $i,r \in [1,M]$ and M is the number of lattice sites. H_a and H_b are defined by the following:

$$H_c = \frac{U_c}{2} \sum_{i=1}^{M} n_i^c \left(n_i^c - 1\right) - T_c \sum_{(i,j)} I_{(i,j)}\, c_j^\dagger c_i\,, \quad c = a, b, \tag{2}$$

where U_c is the onsite intraspecies interaction, T_c is the hopping amplitude describing boson tunneling, and $I_{(i,j)}$ are the off-diagonal elements of the symmetric adjacency matrix in which bond $\{i,j\}$ runs through all pairs of sites with $i \neq j$. For the common case of nearest-neighbor hopping only, one has $I_{(i,j)} = 1$ on bonds $\{i,j\}$ connecting nearest-neighboring sites and zero otherwise. The study of mixtures by means of Monte Carlo simulations [12,13] has greatly contributed to disclose many fundamental properties of the system and provided an accurate, unbiased study of several aspects of the global phase diagram. On the other hand, the perturbation approach still represents a considerably effective tool to obtain a deep insight on the structure of the ground state and the microscopic processes governing the formation of quantum phases. By construction, the analytic character of this method clearly shows how microscopic processes incorporated in the perturbation term of the Hamiltonian along with nontrivial entanglement often characterizing mixtures influence the structure of ground states. In particular, entanglement between the two components is already present in the zeroth-order correction of the ground state for certain choices of boson numbers N_a and N_b, noncommensurate to M. In higher dimensions, other analytic techniques such as the Gutzwiller mean-field approach [10,15] are able to provide significant information for macroscopic states characterized by no or weak entanglement. In some simpler cases, mean-field techniques can be improved by introducing "local" entanglement between the two components [9,12].

We are interested in applying the perturbation method to the two-component BH model with the ultimate goal of gaining some insight on the structure of the ground state and the role of entanglement resulting from the interspecies interaction [16]. The application of the perturbation method, though, can be challenging, certainly analytically but also numerically, due to the remarkably high degree of degeneracy that often characterizes the ground state of the unperturbed Hamiltonian. In the sequel, we will assume the hopping amplitudes T_a and T_b of the two species as the perturbation parameters for the two-component BH model.

To understand the nature of the degeneracy and the challenges of the perturbative calculation we can consider the following simple example. Let us consider the transition of bosonic component $\mathcal{A}$ from the Mott insulator (MI) to the superfluid (SF) phase when component $\mathcal{B}$ is SF. This case,

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studied in Ref. [12,13] when component $\mathcal{B}$ is dilute, has revealed an evident asymmetric shift of the MI lobe of the (majority) component $\mathcal{A}$ between the particle and hole side of Mott lobe. This effect, in turn, appears to be related to a ground-state structure which features entanglement between $\mathcal{A}$ and $\mathcal{B}$ bosons which substantially differs in the particle and hole-excitation case [16]. The most elementary version of this transition is found in the limit $T_a,T_b \to 0$ by considering a SF component $\mathcal{B}$ with $N_b = k_b M + 1$ together with a Mott component $\mathcal{A}$ with $N_a = k_a M$ (where k_a,k_b are non-negative integers). The corresponding zeroth-order ground state is $|k_a\rangle \otimes \sum_s (b_s^\dagger/\sqrt{M})\,|k_b\rangle$, where $|k_c\rangle$, $c = a,b$ represents a Mott state with filling k_c, and $b_s^\dagger\,|k_b\rangle$ describes the creation of a solitary boson at site s causing the SF character of species $\mathcal{B}$. In the grand-canonical ensemble, when the energy cost for adding a boson to component $\mathcal{A}$ is zero, the transition to zeroth-order ground state of the form $\sum_{ik} F_{ik} a_i^\dagger b_k^\dagger\,|k_a\rangle \otimes |k_b\rangle$ corresponding to $\mathcal{A}$ and $\mathcal{B}$ both superfluid occurs. In order to minimize the contribution of the interspecies-interaction term to the ground-state energy E_0, the diagonal elements of the $M \times M$ matrix F must be zero. In general, the high degree of degeneracy (represented by the arbitrariness of F_{ik}) is removed by imposing the minimization of the first-order perturbative correction E_1 with respect to the undetermined parameters F_{ik}. This solution scheme, however, is viable only if E_1 is not degenerate, a condition whose validity can be shown to depend on the number of particles, the lattice properties, and possibly on model parameters.

While this simple case can be solved analytically [16], for situations with $N_a = k_a M + A$ and $N_b = k_b M + B$, where A and B are arbitrary integers $A,B \in [1,M-1]$, the determination of the zeroth-order ground-state amplitudes (e.g., matrix elements F_{ik} in the example illustrated above) cannot be done analytically and can easily become numerically costly. For this reason, determining general conditions for which the ground-state energy E of model H and the first-order correction E_1 are nondegenerate (without resorting to complicated either analytical or numerical calculations) represents a precious, essential information for implementing the perturbation method.

In this paper we show that both the ground-state energy E of H and the lowest eigenvalue of the perturbation term formed by the T_a and T_b-dependent terms in H are nondegenerate if the simple condition to have a *connected lattice* **G** is satisfied. Then, after observing that if the unperturbed ground-state energy E_0 is degenerate, then this degeneracy can be eliminated if the first-order correction E_1 is nondegenerate, we explore the conditions for which first-order correction E_1 is nondegenerate for different choices of A and B.

This paper is organized as follows. Section II is devoted to give some useful definitions and to recast the model interaction and hopping parameters into a form more advantageous for our perturbation approach. In Sec. III, we define the connectedness between states of the Fock basis and give the sufficient and necessary condition that links the lattice connectivity to the state connectedness. This allows us to apply the Perron-Frobenius theorem [17] to study the degeneracy properties of the ground-state energy. Concerning the definition of states' connectedness assumed in this paper, it should be noted that similar definitions, followed by the application of Perron-Frobenius theorem, are used in Katsura and Tasaki's recent work [18] in the proof of the degeneracy of the spin-1 Bose-Hubbard model and previously in Refs. [19–21] devoted to the study of ferromagnetism of the Hubbard model. Our method differs from previous studies in the fact that we define the connectedness in a different way in order to give an equivalence relation. This allows us to conveniently study the degeneracy of the ground-state energy and its first-order correction.

In Sec. IV we discuss the degeneracy of E_1 in two cases: (1) one of the two species is a MI while the other is SF; (2) there are $k_a M + 1$ (or $k_a M - 1$) species-$\mathcal{A}$ bosons while species $\mathcal{B}$ is SF with a generic number of bosons. In Sec. V, we extend our discussion to generic cases with the only requirement, $A + B < M - 1$ or $A + B > M + 1$. Our analysis shows that E_1 is nondegenerate if one assumes certain sufficient conditions on the connectivity of the lattice. These conditions are satisfied by most lattices.

Finally, in Sec. VI we show that when $A + B = M$, E_1 is degenerate independently on the connectivity of the lattice. We therefore discuss the determination of the unperturbed ground state in terms of symmetry properties of the lattice for N_a and N_b such that $A = 1$, $B = M - 1$ or $A = M - 1$, $B = 1$.

II. THE TWO-COMPONENT MODEL IN THE STRONGLY INTERACTING REGIME

We intend to study the two-component Bose-Hubbard model in the strongly interacting regime where $T_a,T_b \ll U_a,U_b,U_{ab}$. We assume that $T_a \approx T_b$, stating that the mobility of the bosons of the two components is essentially the same, and $0 \leqslant I_{(i,j)} \leqslant 1$. To avoid phase separation we also assume (repulsive) onsite interactions such that $U_{ab} < U_a,U_b$. Although in the following we will explicitly consider the case of soft-core bosons, i.e., $U_a,U_b < \infty$, the results presented are also valid for the case of hard-core bosons [22]. The application of the perturbation method suggests the definition of new interaction and hopping parameters,

$$T_a = T\,t_a, \quad T_b = T\,t_b, \quad U_a = U\,u_a, \quad U_b = U\,u_b,$$

entailing that model Hamiltonian H takes the form

$$H = U\left[\frac{u_a}{2}\sum_{i=1}^{M} n_i^a\big(n_i^a - 1\big) + \frac{u_b}{2}\sum_{i=1}^{M} n_i^b\big(n_i^b - 1\big) + \frac{U_{ab}}{U}\sum_{i=1}^{M} n_i^a n_i^b\right] + T\left[-t_a\sum_{(i,j)} I_{(i,j)}\,a_i^\dagger a_j - t_b\sum_{(i,j)} I_{(i,j)}\,b_i^\dagger b_j\right], \quad (3)$$

in which we call H_0 the U-dependent diagonal part of the Hamiltonian and TW represents the kinetic energy part of H [fourth and fifth T-dependent terms in Eq. (3)]. Then TW/U represents the perturbation and $\epsilon = T/U$ naturally identifies with the perturbation parameter.

The sites of the optical lattice and the set of all bonds $\{i,j\}$ with weight $I_{(i,j)} \neq 0$ define an edge-weighted graph

$\mathbf{G} = (\mathcal{V}(\mathbf{G}),\mathcal{E}(\mathbf{G}))$, where $\mathcal{V}(\mathbf{G})$ is the set of vertices, i.e., sites, $\mathcal{E}(\mathbf{G})$ is the set of edges, i.e., bonds (not necessarily nearest neighbors), and $I_{(i,j)}$ is the weight on bond $\{i,j\}$

In the following we will work in a finite-dimensional Hilbert space $\mathscr{H}$ corresponding to fixed particle numbers $N_a = k_a M + A$ and $N_b = k_b M + B$ for the two components, respectively[1]. Here k_a, k_b, A, and B are non-negative integers with $0 \leqslant A < M$, $0 \leqslant B < M$. The space $\mathscr{H}$ is spanned by an orthonormal basis of Fock states $|\xi\rangle \otimes |\gamma\rangle$,

$$|\xi\rangle \otimes |\gamma\rangle = \frac{\prod_{l=1}^{M} a_l^{\dagger\,\xi_l} \prod_{m=1}^{M} b_m^{\dagger\,\gamma_m} |0\rangle}{\sqrt{\prod_{l=1}^{M} \xi_l! \prod_{m=1}^{M} \gamma_m!}}, \tag{4}$$

where $|0\rangle$ is the vacuum state, i.e., every site in the lattice is empty, and ξ, γ are integers such that $\sum_{l=1}^{M} \xi_l = k_a M + A$, $\sum_{m=1}^{M} \gamma_m = k_b M + B$.

To simplify our notation we use $|\xi,\gamma\rangle$ to denote $|\xi\rangle \otimes |\gamma\rangle$. The ground state(s) of H_0 are labeled by $|\sigma,\lambda\rangle$. We call O the set of states $|\xi,\gamma\rangle$s and O_g the set of the states $|\sigma,\lambda\rangle$s. The operator W confined in the subspace spanned by $|\sigma,\lambda\rangle$'s is denoted by W_g. The matrix representation of W in terms of the basis $|\xi,\gamma\rangle$'s is denoted by $\mathbf{W}$ and the matrix representation of W_g in terms of $|\sigma,\lambda\rangle$'s is denoted by $\mathbf{W_g}$.

The explicit expression of matrix elements of $\mathbf{W}$ is given by the following:

$$\langle \xi,\gamma|W|\xi',\gamma'\rangle = -t_a\, \delta_{\gamma,\gamma'} \sum_{(i,j)} \left[I_{(i,j)} \sqrt{\xi_j + 1}\sqrt{\xi_i' + 1}\, \delta_{\xi_j+1,\xi_j'} \delta_{\xi_i,\xi_i'+1} \prod_{l\neq i,j}^{M} \delta_{\xi_l \xi_l'} \right] - t_b\, \delta_{\xi,\xi'} \sum_{(i,j)} \left[I_{(i,j)} \sqrt{\gamma_j + 1}\sqrt{\gamma_i' + 1}\, \delta_{\gamma_j+1,\gamma_j'} \delta_{\gamma_i,\gamma_i'+1} \prod_{m\neq i,j}^{M} \delta_{\gamma_m,\gamma_m'} \right]. \tag{5}$$

It is obvious that the matrix elements are nonpositive. Moreover, a matrix element is nonzero if and only if $\xi_i' = \xi_i + 1$, $\xi_j' + 1 = \xi_j$ on bond $\{i,j\}$ while all other $\xi_l' = \xi_l$ and $\gamma = \gamma'$ or $\gamma_i' = \gamma_i + 1$, $\gamma_j' + 1 = \gamma_j$ on bond $\{i,j\}$ while all other $\gamma_l' = \gamma_l$, and $\xi = \xi'$. This property of the matrix elements will be used below.

After recalling that in the strongly interacting regime we treat the term ϵW as a perturbation with $\epsilon = T/U$, the ground-state energy E of $H = U(H_0 + \epsilon W)$ and its eigenvector(s) $|\Psi_l\rangle$ $(l = 1,\ldots,f_E$, where f_E is the degeneracy of $E)$ can be expanded via the perturbative series $E = E_0 + \sum_{n=1}^{\infty} \epsilon^n E_n$ and $|\Psi_l\rangle = |\psi_l^0\rangle + \sum_{n=1}^{\infty} \epsilon^n |\psi_l^n\rangle$. Note that if $A + B > 0$, then H_0 has a degenerate ground-state energy E_0 with degeneracy f_{E_0}. If $f_{E_0} = f_E$, one can apply perturbation theory starting from any ground state of H_0. If $f_{E_0} > f_E$ and W fully lifts the extra degeneracy of E_0, then E_1 and $|\psi_l^0\rangle$ can be uniquely determined by solving the matrix eigenvalue problem (degenerate perturbation theory) as follows:

$$\sum_{\sigma',\lambda'} \langle \sigma,\lambda|W|\sigma',\lambda'\rangle \left\langle \psi_l^0 \middle| \sigma',\lambda' \right\rangle = E_1 \left\langle \psi_l^0 \middle| \sigma,\lambda \right\rangle. \tag{6}$$

On the other hand, if neither of the previous scenarios are true, then $|\psi_l^0\rangle$'s are not uniquely determined by solving Eq. (6). From this discussion, it becomes apparent that one needs to study the degeneracy of both E and E_1 and, in the case where Eq. (6) is not applicable, find an alternative method to determine $|\psi^0\rangle$.

As we will show in the following, the issue of degeneracy is closely related to the connectivity of the lattice.

III. DEGENERACY OF THE GROUND-STATE ENERGY, CONNECTIVITY OF LATTICE, AND CONNECTEDNESS BETWEEN STATES

In this section, we discuss the degeneracy of the ground-state energy of H by utilizing the notion of "connectedness" on the states of the basis and the Perron-Frobenius theorem (PFT). This theorem states that if $\mathbf{X}$ is a real symmetric matrix such that (i) off-diagonal elements are all nonpositive, (ii) for any two different indices p and q there exists an N such that $(\mathbf{X}^N)_{p,q} \neq 0$, then its lowest eigenvalue is nondegenerate and the corresponding eigenvector is positive [17]. In the following we will apply PFT theorem for the case of matrix $\mathbf{W}$ and $\mathbf{H}$.

To begin with, we define the "connectedness" on states via a symmetric linear operator X[2] (its corresponding matrix is denoted by $\mathbf{X}$).

Hence, we say that $|\xi,\gamma\rangle$ and $|\xi',\gamma'\rangle$ are connected by a symmetric linear operator X if there exists a finite sequence $\{|\alpha_1,\beta_1\rangle, |\alpha_2,\beta_2\rangle, \ldots, |\alpha_N,\beta_N\rangle\}$ with $|\alpha_1,\beta_1\rangle = |\xi,\gamma\rangle$ and $|\alpha_N,\beta_N\rangle = |\xi',\gamma'\rangle$ in the set O such that for any $1 \leqslant i < N$, $\langle \alpha_i,\beta_i|X|\alpha_{i+1},\beta_{i+1}\rangle \neq 0$ or $|\alpha_i,\beta_i\rangle = |\alpha_{i+1},\beta_{i+1}\rangle$. This definition includes the trivial case $|\xi,\gamma\rangle = |\xi',\gamma'\rangle$. The kinetic energy operator W and the Hamiltonian H are indeed symmetric linear operators. The connectedness associated with X defines an equivalence relation[3] $\mathfrak{R}_X$ on O such that

[1]Particle number operators commute with both H_0 and H.

[2]A linear operator X is symmetric if, for arbitrary states $|\phi\rangle$ and $|\psi\rangle$, $\langle\phi|X|\psi\rangle = \langle\psi|X|\phi\rangle$.

[3]A relation $\mathfrak{R}_X$ on a set O is a collection of ordered pairs $(|\xi,\gamma\rangle, |\xi',\gamma'\rangle)$ in O. If $(|\xi,\gamma\rangle, |\xi',\gamma'\rangle) \in O$, we say $|\xi,\gamma\rangle\, \mathfrak{R}_X\, |\xi',\gamma'\rangle$. $\mathfrak{R}_X$ is an equivalence relation on a set O if it satisfies (i) reflexivity, i.e., $|\xi,\gamma\rangle\, \mathfrak{R}_X\, |\xi,\gamma\rangle$; (ii) symmetry, i.e., $|\xi,\gamma\rangle\, \mathfrak{R}_X\, |\xi',\gamma'\rangle \rightarrow |\xi',\gamma'\rangle\, \mathfrak{R}_X\, |\xi,\gamma\rangle$; (iii) transitivity, i.e., $|\xi,\gamma\rangle\, \mathfrak{R}_X\, |\xi',\gamma'\rangle$, $|\xi',\gamma'\rangle\, \mathfrak{R}_X\, |\xi'',\gamma''\rangle \rightarrow |\xi,\gamma\rangle\, \mathfrak{R}_X\, |\xi'',\gamma''\rangle$. For a given relation $\mathfrak{R}_X$, $|\xi,\gamma\rangle / \mathfrak{R}_X$ denotes the set of all $|\xi',\gamma'\rangle$ related to $|\xi,\gamma\rangle$, and $O/\mathfrak{R}_X$ denotes the collection of all $|\xi,\gamma\rangle / \mathfrak{R}_X$'s. An

$|\xi,\gamma\rangle\, \mathfrak{R}_X\, |\xi',\gamma'\rangle$ if and only if the two states are connected by X. Given this equivalence relation, we can prove that:

Proposition 1. The following three conditions are equivalent: (a) $\mathbf{X}$ is irreducible,[4] (b) any $|\xi,\gamma\rangle$ and $|\xi',\gamma'\rangle$ are connected by X, and (c) property (ii) in the PFT is satisfied.

The proof is given in Appendix A.

A. Connectivity of G and the nondegeneracy of E

We want to prove that the ground state of H is nondegenerate by making use of PFT. Hence, we need to show that $\mathbf{H}$ satisfies the hypothesis of the theorem. We first notice that both H and W are symmetric linear operators. Moreover, $\langle\xi,\gamma|(H_0+\epsilon W)|\xi',\gamma'\rangle = \langle\xi,\gamma|H_0|\xi',\gamma'\rangle + \epsilon\,\langle\xi,\gamma|W|\xi',\gamma'\rangle = \epsilon\,\langle\xi,\gamma|W|\xi',\gamma'\rangle \leqslant 0$ for any $|\xi,\gamma\rangle \neq |\xi',\gamma'\rangle$, and hence $\mathbf{H}$ and $\mathbf{W}$ are both real matrices with nonpositive off-diagonal elements, as requested by condition (i) of the PFT. Moreover, $|\xi,\gamma\rangle$ and $|\xi',\gamma'\rangle$ are connected by H if and only if they are connected by W. The next step is to show that condition (ii) is also satisfied. In view of Proposition 1, it is sufficient to show that any $|\xi,\gamma\rangle$ and $|\xi',\gamma'\rangle$ are connected by W. From here on, we will assume that $\mathbf{G}$ is connected[5] (note that the connectivity of $\mathbf{G}$ differs from the connectedness on the basis). We can show that:

Proposition 2. Any $|\xi,\gamma\rangle$ and $|\xi',\gamma'\rangle$ are connected by W if and only if $\mathbf{G}$ is connected.

We first prove the sufficient condition. The general idea of the proof is to connect both states $|\xi,\gamma\rangle$ and $|\xi',\gamma'\rangle$ to a state such that all particles are sitting on the same lattice site k and then apply the transitivity property. Let us fix a site k. Then any other site is linked to k by a path. Since $|\xi'',\gamma''\rangle = c_i c_j^\dagger\,|\xi,\gamma\rangle\,/\|c_i c_j^\dagger\,|\xi,\gamma\rangle\,\|$, $c=a,b$, is connected to $|\xi,\gamma\rangle$ if $\{i,j\}$ is a bond [see Eq. (5)], we can apply $a_i a_j^\dagger$ or $b_i b_j^\dagger$ subsequently on the appropriate bonds $\{i,j\}$ in order to construct the special state $|\xi''',\gamma'''\rangle$ connected to $|\xi,\gamma\rangle$. $|\xi''',\gamma'''\rangle$ is such that all bosons are sitting on site k. Next, we perform a similar operation on $|\xi',\gamma'\rangle$ to connect it to $|\xi''',\gamma'''\rangle$. By transitivity of connectedness we have that $|\xi,\gamma\rangle$ and $|\xi',\gamma'\rangle$ are connected to each other. A similar construction of intermediate states is also used in Ref. [18].

Here we prove the necessary condition by contradiction. Let us assume that the lattice is not connected. Then there exists at least two sites k and l not linked by any path. Let K be the set of sites linked to k. Then the complement of K in $\mathcal{V}(\mathbf{G})$ is nonempty and is not linked to K[6]. Since there always exists states $|\xi,\gamma\rangle$ and $|\xi',\gamma'\rangle$ with different total number of particles on the sites belonging to K, then these two states are obviously not connected. We get contradiction.

We are now ready to apply PFT to conclude:

Theorem 1. If $\mathbf{G}$ is connected, then the ground-state energy of H is nondegenerate and it has a positive[7] ground state.

Corollary 1. If $\mathbf{G}$ is connected, then $\epsilon\, W$ has a negative nondegenerate ground-state energy with a positive ground state.

Another interesting result can be derived by setting the hopping amplitude of one of the components to zero, e.g., $T_b = 0$. Then, from Eq. (5), it is obvious that for any $|\xi,\gamma\rangle$, $|\xi',\gamma'\rangle$ with $|\gamma\rangle \neq |\gamma'\rangle$, the two states are not connected by W. One can show the following result (the proof is given in Appendix B):

Corollary 2. If $\mathbf{G}$ is connected and $T_a = 0, T_b \neq 0$ (or $T_b = 0, T_a \neq 0$), the degeneracy of the ground-state energy of W is M^{N_b} (M^{N_a}).

It is worth noting that the results presented in this section are quite general. They hold for the case of nearest-neighbor or longer-ranged hopping. Moreover, they are valid in both the weakly and strongly correlated regime and for both repulsive or attractive interspecies interaction. The only requirement is for the lattice to be connected and $T_{a,b}$, $I_{(i,j)}$ to be non-negative. Finally, we would like to mention that the results presented in this Sec. are also valid for the case of hard-core bosons, although the specifics of the proofs and the degeneracy in Corollary 2 differ [22]. Likewise, the results presented in the following hold for hard-core bosons as well since they are based on the results of Sec. III.

IV. DEGENERATE PERTURBATION THEORY

Theorem 1 states that the ground-state energy E of model 3 is nondegenerate. In the general case where at least one of the two component is doped away from integer filling, the ground state corresponding to E_0 is degenerate. Then the first-order correction E_1 can either be nondegenerate (i.e., W completely lifts the degeneracy of E_0), in which case $|\psi^0\rangle$ is uniquely determined, or degenerate, in which case $|\psi^0\rangle$ is not uniquely determined. In this section, we discuss degeneracy properties of E_1 in terms of graph theoretical properties of $\mathbf{G}$. In the case when E_1 is degenerate, we provide a method to determine $|\psi^0\rangle$ according to symmetry properties of $\mathbf{G}$, hence providing a rigorous solution to the degenerate perturbation theory Eq. (6). This case is discussed in Sec. VI.

A. Representing $|\sigma,\lambda\rangle$'s pictorially

At commensurate filling, i.e., $N_a = k_a M$ and $N_b = k_b M$, the potential energy is minimized when, on each site, there are k_a $\mathcal{A}$ bosons and k_b $\mathcal{B}$ bosons (recall we are considering $U_{ab} < U_a, U_b$). When one or both components are doped away from integer filling factor, the extra particles arrange themselves in order to minimize the interspecies-interaction term in H. In particular, a given site will accommodate at most $k_a + 1$ species-$\mathcal{A}$ bosons and $k_b + 1$ species-$\mathcal{B}$ bosons. Hence, we can specify an arbitrary ground state $|\sigma,\lambda\rangle$ of H_0 in terms of the sites which accommodate extra particles.

important property of equivalence relations is that $O/\mathfrak{R}_X$ is a partition of O [23]. It is easy to check that $\mathfrak{R}_X$ is well-defined here.

[4]A symmetric matrix is irreducible if and only if it cannot be block-diagonalized by permuting the indices.

[5]$\mathbf{G}$ is connected if any two sites can be linked by a path. Two sites i and j are linked if there exists a path $\{i,\ldots,k_l,\ldots,j\}$ in which every neighboring pair in the sequence forms a bond.

[6]Every site in K is not linked to any site in its complement.

[7]A vector is positive (in terms of the basis) if its expansion coefficients are all positive.

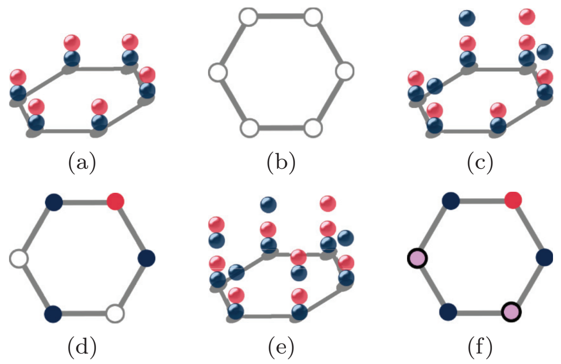

FIG. 1. (Color online) Panels (a), (c), and (e) are examples of states in $|\sigma,\lambda\rangle$s for the case of a one-dimensional lattice with periodic boundary condition and $M = 6$. These states correspond to ($k_a = 1, k_b = 1, A = 0, B = 0$), ($k_a = 1, k_b = 1, A = 3, B = 1$), and ($k_a = 1, k_b = 1, A = 5, B = 3$), respectively. The color (dark) blue refers to $\mathcal{A}$ bosons and (light) red to $\mathcal{B}$ bosons. They are represented pictorially by panels (b), (d), and (f), where blue (dark) sites form the set σ, red (light) sites form the set λ, purple (circled in black) sites form the intersection of σ and λ, and white (circled in gray) sites form the set of sites with neither extra $\mathcal{A}$ nor extra $\mathcal{B}$ bosons.

More specifically, when $A + B \leqslant M$, there are no sites with both an extra $\mathcal{A}$ and an extra $\mathcal{B}$ boson. Thus, the set of sites with an extra $\mathcal{A}$ boson has A elements, and the set of sites with an extra $\mathcal{B}$ boson has B elements. Such sets have an empty intersection. On the other hand, when $A + B > M$, there are $A + B - M$ sites with both an extra $\mathcal{A}$ and an extra $\mathcal{B}$ boson. In this case, the relevant sets have a nonempty intersection containing $A + B - M$ sites.

We can therefore identify an arbitrary ground state $|\sigma,\lambda\rangle$ in terms of the sets σ and λ corresponding to A sites with an extra $\mathcal{A}$ boson and B sites with an extra $\mathcal{B}$ boson, respectively. The set of ground states O_g is therefore represented by a collection of pairs of sets (σ,λ)s. In the following, for the sake of simplicity but without loss of rigor, we represent states $|\sigma,\lambda\rangle$ pictorially by coloring sites belonging to σ in blue (dark), sites belonging to λ in red (light), and sites belonging to the intersection between σ and λ in purple (circled in black). Site with neither extra $\mathcal{A}$ nor extra $\mathcal{B}$ bosons are colored in white (circled in gray). Examples of the mapping from $|\sigma,\lambda\rangle$ to (σ,λ) are shown in Fig. 1, where the states shown in Figs. 1(a), 1(c) and 1(e) are represented by Figs. 1(b), 1(d), and 1(f), respectively.

W_g is a symmetric linear operator in the subspace spanned by $|\sigma,\lambda\rangle$s, therefore we can define the connectedness between states $|\sigma,\lambda\rangle$s by W_g. From here on, we will describe connectedness by using the representation in terms of color of sites. For example, according to Eq. (5), when $A + B < M$, $\langle\sigma,\lambda|W_g|\sigma',\lambda'\rangle$ is nonzero if and only if one white site exchanges color with a blue or red site on a bond while all other colors remain unchanged. When $A = M - 1, B > 1$, $\langle\sigma,\lambda|W_g|\sigma',\lambda'\rangle$ is nonzero if and only if one purple site exchanges color with a blue or red site on a bond while all other colors remain unchanged[8].

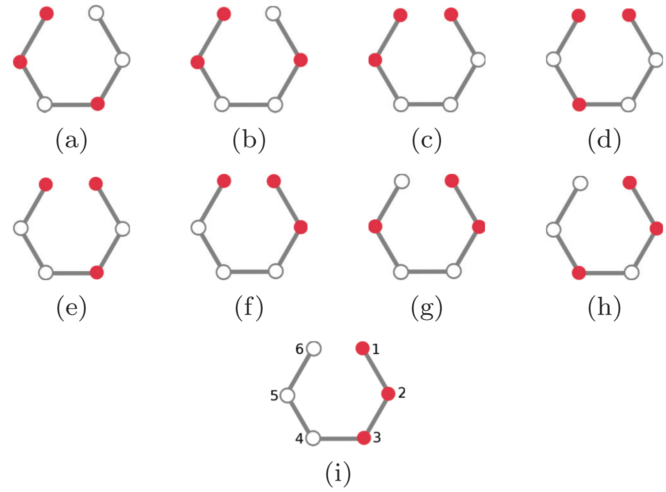

FIG. 2. (Color online) Panels (a)–(i) represent a sequence of states in O_g with $k_a = k_b = A = 0$ and $B = 3$ for the case of a connected one-dimensional lattice. The sequence connects states (a) and (i).

It should now be apparent that purple sites behave in the same way as white sites. Using this language, the rules to generate a connected state are as follows: (i) change the color of a white (or purple) site with a red or blue site on a bond and (ii) "exchange" the color of two sites with the same color on a bond (this operation is trivial and results from the definition of connectedness where two neighboring states in the connecting sequence can be identical). This second rule is introduced just for the sake of convenience in the remainder of our discussion.

In terms of the pictorial representation that we have described above, a sequence $\{|\sigma,\lambda\rangle, \ldots, |\chi_l,\theta_l\rangle, \ldots, |\sigma',\lambda'\rangle\}$ in O_g connecting $|\sigma,\lambda\rangle$ to $|\sigma',\lambda'\rangle$ can be represented by a sequence of pictures[9]. For example, Figs. 2(a) through 2(i) show a sequence connecting states in Figs. 2(a) and 2(i), with matrix elements of $\mathbf{W_g}$ between any two adjacent pictures being nonzero.

The next step is the study of the degeneracy of E_1. Since Proposition 1 and the PFT theorem also apply to W_g, it is sufficient to check for the existence of a sequence $\{|\sigma,\lambda\rangle, \ldots, |\chi_l,\theta_l\rangle, \ldots, |\sigma',\lambda'\rangle\}$ for any arbitrary $|\sigma,\lambda\rangle$ and $|\sigma',\lambda'\rangle$. In the following, we will study under which conditions arbitrary $|\sigma,\lambda\rangle$ and $|\sigma',\lambda'\rangle$ are connected. These conditions will differ depending on the values of A and B.

B. One of the species has commensurate filling factor, i.e., $A = 0$ or $B = 0$

It is obvious that when both species have commensurate filling factor, i.e., $A = 0$ and $B = 0$, E_0 is nondegenerate. In the strongly interacting regime one can apply the nondegenerate perturbation method. Let us therefore consider the case when only one of the species is at commensurate filling, e.g.,

[8]These rules can also be stated formally: $\langle\sigma,\lambda|W_g|\sigma',\lambda'\rangle$ is nonzero if and only if either set $\lambda = \lambda'$ while sets σ, σ' only differ by sites i and j belonging to the bond $\{i,j\}$, or set $\sigma = \sigma'$ while sets λ, λ' only differ by sites k and l belonging to the bond $\{k,l\}$.

[9]Formally, it is a sequence of pairs of sets $\{(\sigma,\lambda), \ldots, (\chi_l,\theta_l), \ldots, (\sigma',\lambda')\}$.

$A = 0, B \neq 0$. In this case, besides white sites, there are B red sites. The only assumption we are making on the lattice **G** is that it is connected (periodic boundary conditions do not necessarily need to be satisfied). Consider arbitrary $|\sigma,\lambda\rangle$ and $|\sigma',\lambda'\rangle$, e.g., states in Figs. 2(a) and 2(i). By using induction, one can show:

Proposition 3. When $A = 0, B \neq 0$ (or $A \neq 0, B = 0$), any $|\sigma,\lambda\rangle$ and $|\sigma',\lambda'\rangle$ are connected if and only if **G** is connected.

Let us prove the sufficient condition by induction. Let us assume that **G** is connected. Then it is always possible to label sites by $(i_1,i_2,\ldots,i_M)$ such that if we remove the first m sites in this sequence, the remaining $(i_{m+1},\ldots,i_M)$ sites still form a connected lattice for all $1 \leqslant m < M$ [24]. Figure 2(i) shows an example of labeling which satisfies this property. Constructing a state such that the color of i_1 (site 1 in our example) is the same as in $|\sigma',\lambda'\rangle$ can be done by first locating a site i_k (site 3 in our example) in $|\sigma,\lambda\rangle$ with the same color as i_1 in $|\sigma',\lambda'\rangle$. Next, we successively exchange the colors along a path linking i_1 to i_k [see, e.g., Figs. 2(a)–2(c)]. Let us assume that this can be done for an arbitrary i_m, with $1 \leqslant m < M$, and let us denote the constructed state by $|\chi_n,\theta_n\rangle$. Then, since $(i_{m+1},\ldots,i_M)$ forms a connected lattice, by applying the same procedure as for i_1 we can fix the color on i_{m+1} [see, e.g., Figs. 2(c)–2(f)]. Therefore, by induction, we have shown that $|\sigma,\lambda\rangle$ and $|\sigma',\lambda'\rangle$ are connected.

The necessary condition is proved by a similar argument as in Proposition 2, which implies that, if **G** is not connected, then there exist $|\sigma,\lambda\rangle$ and $|\sigma',\lambda'\rangle$ which are not connected.

A direct consequence of Proposition 1 and Proposition 3 is the following:

Theorem 2. When $A = 0, B \neq 0$ or $A \neq 0, B = 0$, E_1 is nondegenerate if **G** is connected.

C. Useful properties of a 2-connected lattice

Let us first introduce the notion of 2-connectivity. A lattice **G** is said to be 2-connected if the removal of any site leaves the remaining sites connected. In the one-dimensional example of Fig. 3(a), this is equivalent to introducing periodic boundary conditions to get Fig. 3(c). In higher dimensions, the 2-connectivity conditions is satisfied by square, triangular, honeycomb, cubic, fcc lattices, etc., with any boundary conditions. Some useful properties of 2-connectivity are as follows:

(a) if **G** is 2-connected then it is also connected;

(b) **G** is 2-connected if and only if, for any two distinct sites, there exist two disjoint paths linking them (two paths are disjoint if they only share the two ends). This is the global version of Menger's theorem [24];

(c) for any distinct sites i_1, i_2 and i_3, there exists a path linking i_1 and i_2 which avoids i_3 (this is a direct consequence of property (b));

(d) in any state with at least one white site, one can always move the blue or red color from an arbitrary site to another arbitrary site according to the rules given in Sec. IV A (we prove this property in Appendix C).

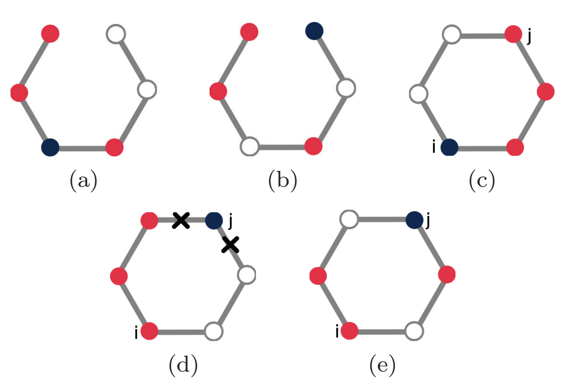

FIG. 3. (Color online) Panels (a) and (b) are two unconnected states in O_g for the case of a connected one-dimensional lattice with $A = 1, B = 3$. Panels (c) and (e) are two connected states in O_g for the case of a 2-connected lattice with $A = 1, B = 3$. Panel (d) is an intermediate state in the sequence connecting (c) to (e). The two crosses in (d) indicate that the removal of site j leaves the remaining lattice still connected.

D. $A = 1, 0 < B < M - 1$ and $A = M - 1, 1 < B \leqslant M - 1$

Although we will discuss our results explicitly for $A = 1, 0 < B < M - 1$, the case of $A = M - 1, 1 < B \leqslant M - 1$ can be mapped onto $A = 1, 0 < B < M - 1$ by replacing blue with red and vice versa and replacing purple with white. Since purple sites can be moved in the same manner as white sites the two cases are completely equivalent.

In the case $A = 1$, $0 < B < M - 1$, i.e., one blue and B red sites are present, the requirement that **G** is connected is not sufficient for any two states to be connected. This is shown with an example in Figs. 3(a) and 3(b), where the two states represented are not connected because it is not possible to move the blue color in Fig. 3(a) to its position in Fig. 3(b) according to the rules given in Sec. IV A. We need to impose that the lattice **G** is 2-connected. If this is the case, the following property holds:

Proposition 4. Any two states $|\sigma,\lambda\rangle$, $|\sigma',\lambda'\rangle$ with $A = 1$ and arbitrary $0 < B < M - 1$ (or $A = M - 1$ and arbitrary $1 < B \leqslant M - 1$) are connected if and only if **G** is 2-connected.

Let us start by proving the sufficient condition. Consider arbitrary $|\sigma,\lambda\rangle$ and $|\sigma',\lambda'\rangle$. Without loss of generality, assume that the blue color is on site i in $|\sigma,\lambda\rangle$ and on site j in $|\sigma',\lambda'\rangle$. Due to property (d) of 2-connectivity, the blue color can be moved from i to j. In other words, we can construct a state $|\chi_n,\theta_n\rangle$ connected with $|\sigma,\lambda\rangle$ in which j is blue. An example of states $|\sigma,\lambda\rangle$, $|\chi_n,\theta_n\rangle$ and $|\sigma',\lambda'\rangle$ is displayed in Figs. 3(c), 3(d), and 3(e), respectively. Moreover, the 2-connectivity of **G** implies that removal of site j leaves the rest of the lattice still connected [see Fig. 3(d)]. Removing site j leaves state $|\sigma,\lambda\rangle$ with red and white sites only. Thus, following a similar argument as for the case $A = 0, B \neq 0$ in Proposition 3, we can show that $|\chi_n,\theta_n\rangle$ is connected to $|\sigma',\lambda'\rangle$. Therefore, by transitivity of connectedness, $|\sigma,\lambda\rangle$ is connected to $|\sigma',\lambda'\rangle$.

The necessary condition is proved by contradiction. For simplicity but without loss of generality we choose a counter example with a single white site. If **G** is not 2-connected [e.g., the lattice shown in Fig. 4(a)], then there exists at least one site i (site 3 in our example) whose removal leaves the remaining sites partially unconnected. Let J and K denote the two unlinked sets [in our example (1,2) and (4,5) in Fig. 4(a)]. Let us consider two states, e.g., Figs. 4(a) and 4(d), with

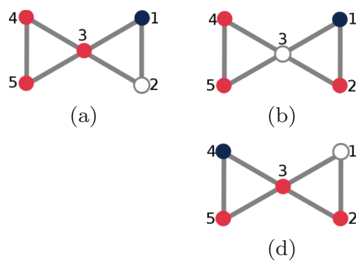

FIG. 4. (Color online) Panels (a)–(d) represent states in O_g with $A = 1, B = 3$ for the case of a lattice which is *not* 2-connected. The absence of 2-connectivity implies that the removal of the site 3 leaves the remaining lattice unconnected. Panels (a), (b), and (c) are connected with each other, but they are not connected with (d).

the blue color on J and K, respectively. In the attempt of transferring the blue color from J to K one can move the white color as shown in Figs. 4(b) and 4(c). At this point, though, the blue color cannot be moved to any site in K, because all sites in K are red. So it is not possible to connect state Fig. 4(c) to state Fig. 4(d).

Finally, we can conclude the following:

Theorem 3. In the case $A = 1$, $0 < B < M - 1$ (or $A = M - 1$, $1 < B \leqslant M - 1$), E_1 is nondegenerate if $\mathbf{G}$ is 2-connected.

V. NONDEGENERACY OF E_1 IN THE GENERAL CASES $A + B < M - 1$ AND $A + B > M + 1$

We extend the results of Sec. IV D to the general case $A + B < M - 1$. Replacing white with purple, the case $A + B > M + 1$ can be mapped onto $A + B < M - 1$.

In general, for $A + B < M - 1$, 2-connectivity is not a sufficient condition for any two states to be connected. This is shown by an example in Figs. 5(a) and 5(b) for a one-dimensional system with periodic boundary conditions. For later convenience we refer to this type of lattice as circle[10]. When there are at least two blue and two red sites, the order of the color on the circle becomes important. Note that the order of color only includes red and blue, since white sites can be freely moved as explained previously. It is obvious that one cannot change the order of the color in Fig. 5(a) to construct Fig. 5(b). However, it is easy to check that two states on a circle are connected if they have the same order of color. The sequence connecting them can be constructed by successively moving the white color on the circle. Using this property one can show that:

Proposition 5. For $A + B < M - 1$ (or $A + B > M + 1$), if $\mathbf{G}$ is a circle with one added path linking two unbonded sites on the circle, then any $|\sigma,\lambda\rangle$, $|\sigma',\lambda'\rangle$ are connected.

An example displaying the assumption of Proposition 5 on the lattice is shown in Fig. 10(i). The proof of this proposition is given in Appendix D. Note that $\mathbf{G}$ being 2-connected is equivalent to $\mathbf{G}$ being constructed as follows: (1) start from a circle; (2) add a path which starts and ends on two distinct sites on the circle; (3) successively add paths to the already constructed lattice in the same manner as in (2) [24] [see, e.g., Fig. 6(a)][11].

By using this equivalence and Proposition 5, we give a necessary and sufficient condition in order for any two states to be connected for generic cases (including all cases we discussed above) with $A + B < M - 1$(or $A + B > M + 1$):

Proposition 6. Any two states $|\sigma,\lambda\rangle$, $|\sigma',\lambda'\rangle$ with arbitrary $A + B < M - 1$ (or arbitrary $A + B > M + 1$) are connected

[10]A circle is a path where the two ends are the same.

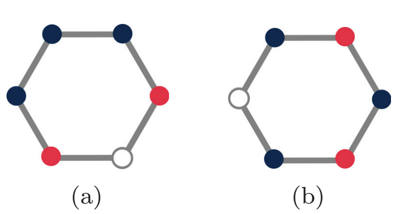

FIG. 5. (Color online) 5(a) and 5(b) are two unconnected states in O_g for the case of a one-dimensional lattice of $M = 6$ sites with periodic boundary condition and $A = 3, B = 2$.

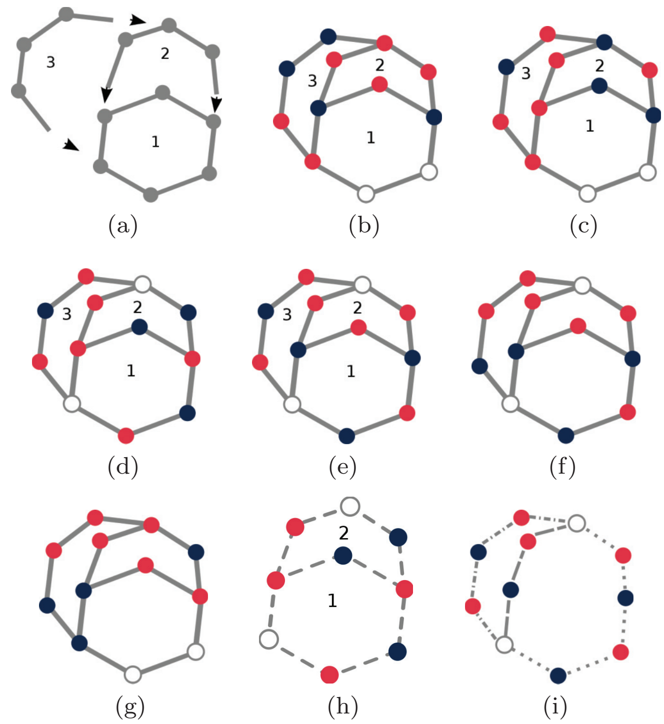

FIG. 6. (Color online) Panel (a) displays a 2-connected lattice constructed by adding path 2 and 3 to the original circle 1. Panels (b) and (g) represent two connected states in O_g for the case of the lattice represented in (a). Here $M = 12$ and $A = 4, B = 6$. Panels (c)–(f) are intermediate states in the sequence connecting (b) to (g). Panels (h) and (i) show states (d) and (e) on sublattices. Panel (i) also shows three different paths (dashed, dot-dashed, and dotted lines) linking the end points of path 3 (see text).

[11]Note that in the remainder of this subsection all added paths are nontrivial in the sense that they add new sites to the already constructed lattice. Adding trivial bonds does not change our conclusions as it keeps the 2-connectivity properties of the lattice.

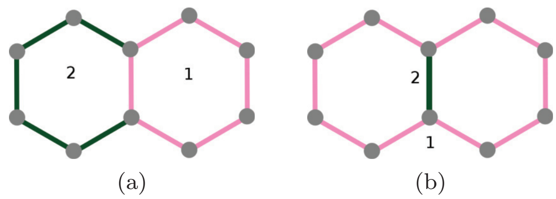

FIG. 7. (Color online) Panels (a) and (b) display two different ways of viewing the same lattice. They can both be viewed as an already constructed lattice plus an added path. In (a), two ends of the added path (dark green) form a bond on the already constructed lattice (light pink). In (b), two ends of the added path (dark green) does not form a bond on the already constructed lattice (light pink).

if and only if **G** is 2-connected and is not a circle of 5 or more sites[12].

We will show that this is true with a specific example. The argument, though, can be straightforwardly generalized to the general case. Let us start by proving the sufficient condition. Consider a 2-connected lattice (not a circle of 5 or more sites) as displayed in Fig. 6(a), and arbitrary $|\sigma,\lambda\rangle$, $|\sigma',\lambda'\rangle$ as displayed in Figs. 6(b) and 6(g). Note that, with $A+B<M-1$, there exists at least two white sites. In this example we only consider two white sites[13]. Because the white color can be moved to any site in the lattice, without loss of generality, we choose the white sites to be the same for $|\sigma,\lambda\rangle$ and $|\sigma',\lambda'\rangle$ as shown Figs. 6(d) and 6(g). Starting from $|\sigma,\lambda\rangle$, we first construct an intermediate state $|\chi_n,\theta_n\rangle$ [Fig. 6(c)] connected to $|\sigma,\lambda\rangle$ such that the number of blue and red sites on the inner circle labeled by 1, and on the paths (in the context of this proof when we count the number of colors in the added paths we exclude the end points from the paths) labeled by 2 and 3, is the same as in $|\sigma',\lambda'\rangle$. This can be done according to property (d) of Sec. IV C. Specifically, this is done by first fixing the colors on path 3 next, since the remaining lattice is still 2-connected, on path 2. Obviously, at this point, the colors on circle 1 are automatically fixed.

Next, we construct a sequence starting forward from $|\chi_n,\theta_n\rangle$ [Fig. 6(c)] and backward from $|\sigma',\lambda'\rangle$ [Fig. 6(g)], by first moving the white color from the original circle to the two ends of path 3, only through sites on circle 1 and path 2. This step generates the state in Fig. 6(d) from that in Fig. 6(c) and the state in Fig. 6(f) from that Fig. 6(g). In order to connect Fig. 6(d) to Fig. 6(f) we notice that path 2 combined with circle 1 [see Fig. 6(h)] satisfies the assumption of Proposition 5[14], therefore we can construct the state in Fig. 6(e) such that colors on circle 1 and path 2 are the same as in Fig. 6(f). Next, we notice that both lattices in Figs. 6(b) and 6(h) are 2-connected, therefore there exist three disjoint paths linking the two ends of path 3: path 3 itself and two paths belonging to circle 1 combined with path 2. This is shown in Fig. 6(i). Hence, we can apply Proposition 5 again to show that states in Figs. 6(e) and 6(f) are connected. In conclusion, due to transitivity of connectedness, we have shown that $|\sigma,\lambda\rangle$ and $|\sigma',\lambda'\rangle$ are connected.

To prove the necessary condition, we simply observe that if **G** is not 2-connected or is a circle with 5 or more sites, as shown in examples Fig. 4(a)–4(d) and Fig. 2, there exist some cases for which not every two states are connected.

In view of Proposition 1 and Proposition 6 we can formulate the following theorem:

Theorem 4. In case of arbitrary $A+B<M-1$ (or arbitrary $A+B>M+1$), E_1 is nondegenerate if **G** is 2-connected and not a circle with 5 or more sites.

In the case $A+B=M-1$ (or $A+B=M+1$), finding a necessary and sufficient condition on the connectivity of a lattice for any two states to be connected is still an open question. Sufficient conditions for a specific model are provided by Tasaki [21] and Katsura [25][15].

VI. DETERMINATION OF $|\psi^0\rangle$ WITH N_a, N_b SUCH THAT $A=1, B=M-1$

In the general case of $A+B=M$, there are neither white nor purple sites. Hence, according to the rules given in Sec. IV A, any two different states are *not* connected. This statement is valid independently on the connectivity properties of **G**. Therefore, all matrix elements in $\mathbf{W_g}$ are zero, which results in $E_1=0$ and degenerate. We are interested in the case $A=1,B=M-1$ $(A=M-1,B=1)$ which correspond to doping species $\mathcal{A}$ ($\mathcal{B}$) with one particle and species $\mathcal{B}$ ($\mathcal{A}$) with one hole. In this case, $|\psi^0\rangle$ is not uniquely determined by solving Eq. (6). In the following we will take advantage of the symmetry properties of the lattice to uniquely determine $|\psi^0\rangle$.

Let us start by defining a symmetry operation r on the lattice and its corresponding operator S_r. We say r is a (bond-weighted) lattice automorphism of **G** if r maps $\mathcal{V}(\mathbf{G})$ one to one onto itself and satisfies that (i) $\{i,j\}$ is a bond if and only if $\{r(i),r(j)\}$ is a bond and (ii) $I_{(i,j)}=I_{(r(i),r(j))}$. The inverse of r, r^{-1}, is also a lattice automorphism. Given a lattice automorphism r, one can define a linear operator S_r on $\mathscr{H}$ such that $S_r\,|\xi,\gamma\rangle=|\xi',\gamma'\rangle$, where $\xi'_i=\xi_{r(i)}$ and $\gamma'_i=\gamma_{r(i)}$.

[12]Two states on a circle with 4 or less sites are always connected, as shown in Lemma 4.6 of Tasaki's work [17]. In Ref. [17] the authors discuss the degeneracy problem of the ground-state energy of Fermi-Hubbard model with infinite U at fixed number of spin-up (-down) fermions and in the presence of a single hole. It is interesting noting that the basis $|\sigma,\lambda\rangle$ that we define here is equivalent to the corresponding basis defined in Ref. [17].

[13]Nothing would change if more than two white sites are present since the white color can be freely moved on the lattice.

[14]If the two ends of any added path form a bond on the already constructed lattice as shown in Fig. 7(a), where pink indicates the already constructed lattice and green indicates the added path, then, since the path adds at least one new site, the "new" lattice we consider includes all sites as shown in Fig. 7(b) by pink bonds with an added green trivial path. Now, in order to apply Proposition 5, we regard the green bond in Fig. 7(b) as the added path.

[15]In Ref. [25] the authors study the degeneracy of the ground-state energy of the SU(n) Fermi-Hubbard model with $U=\infty$ and with exactly one hole. Another sufficient condition for the SU(2) Fermi-Hubbard model requiring the lattice to be constructed by "exchange bond" was given in Ref. [21].

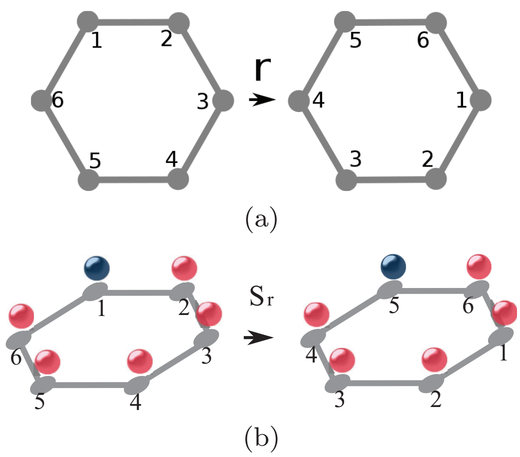

FIG. 8. (Color online) Panel (a) displays a lattice automorphism r on an hexagon. Panel (b) displays the action on Fock states of the corresponding operator S_r: The lattice is rotated while the physical position of particles is unchanged.

If we take the example of Fig. 8 with equal weight on all bonds ($I_{(i,j)} = 1$ for every $\{i,j\}$), the lattice automorphism r is a $2\pi/3$ clockwise rotation [see Fig. 8(a)]. The action of the corresponding S_r is shown in Fig. 8(b), where the lattice is rotated while the physical position of particles is unchanged.

Since r is invertible, S_r also has an inverse, ${S_r}^{-1}$. It is easy to show that $S_{r^{-1}} = S_r^{-1}$. Moreover, by definition $|\xi',\gamma'\rangle = S_r\,|\xi,\gamma\rangle$ is also a normalized Fock state. Therefore S_r preserves the norm $\sqrt{\langle\psi|\psi\rangle}$ for any arbitrary state $|\psi\rangle$ in a finite-dimensional $\mathscr{H}$. Hence, S_r is a unitary operator, i.e., ${S_r}^{\dagger} = {S_r}^{-1}$, and thus a bounded operator[16].

Note that, by definition, the state $S_r\,|\xi,\gamma\rangle$ has exactly the same spatial configuration of bosons as $|\xi,\gamma\rangle$. Then the interaction-dependent terms in H are unchanged. Hence, state $S_r\,|\xi,\gamma\rangle$ has the same eigenvalue of H_0 as $|\xi,\gamma\rangle$, and thus S_r commutes with H_0. Moreover, according to Eq. (5) and the definition of r,

$$\begin{aligned}\langle\xi,\gamma|S_r^{-1}WS_r|\xi',\gamma'\rangle = &-\delta_{\gamma,\gamma'}t_a\sum_{(r(i),r(j))}\left[I_{r(i),r(j)}\sqrt{\xi_{r(j)}+1}\sqrt{\xi'_{r(i)}+1}\;\delta_{\xi_{r(j)}+1,\xi'_{r(j)}}\delta_{\xi_{r(i)},\xi'_{r(i)}+1}\prod_{l\neq r(i),r(j)}^{M}\delta_{\xi_{r(l)}\xi'_{r(l)}}\right]\\ &-\delta_{\xi,\xi'}t_b\sum_{(r(i),r(j))}\left[I_{r(i),r(j)}\sqrt{\gamma_{r(j)}+1}\sqrt{\gamma'_{r(i)}+1}\;\delta_{\gamma_{r(j)}+1,\gamma'_{r(j)}}\delta_{\gamma_{r(i)},\gamma'_{r(i)}+1}\prod_{m\neq r(i),r(j)}^{M}\delta_{\gamma_m,\gamma'_m}\right]\\ &= \langle\xi,\gamma|W|\xi',\gamma'\rangle\,. \end{aligned} \tag{7}$$

Therefore S_r also commutes with H.

The boundedness of S_r implies the following:

$$S_r\,|\Psi\rangle = S_r\,|\psi^0\rangle + \sum_{n=1}^{\infty}\epsilon^n S_r\,|\psi^n\rangle\,. \tag{8}$$

Since E is nondegenerate and $HS_r\,|\Psi\rangle = ES_r\,|\Psi\rangle$, then $S_r\,|\Psi\rangle = e^{i\theta}\,|\Psi\rangle$. More specifically,

$$S_r\,|\psi^0\rangle + \sum_{n=1}^{\infty}\epsilon^n S_r\,|\psi^n\rangle = e^{i\theta}\,|\psi^0\rangle + \sum_{n=1}^{\infty}\epsilon^n e^{i\theta}\,|\psi^n\rangle\,. \tag{9}$$

Taking the limit $\epsilon\to 0$, we have $S_r\,|\psi^0\rangle = e^{i\theta}\,|\psi^0\rangle$. Furthermore, multiplying by $\langle\xi,\gamma|$ Eq. 9, we obtain two power series of ϵ as follows:

$$\begin{aligned}&\langle\xi,\gamma|S_r|\psi^0\rangle + \sum_{n=1}^{\infty}\epsilon^n\,\langle\xi,\gamma|S_r|\psi^n\rangle\\ &= e^{i\theta}\,\langle\xi,\gamma|\psi^0\rangle + \sum_{n=1}^{\infty}\epsilon^n e^{i\theta}\,\langle\xi,\gamma|\psi^n\rangle\,.\end{aligned} \tag{10}$$

Because the series are analytic in a small neighborhood of $\epsilon = 0$, we can equate the coefficients at each order n to get $\langle\xi,\gamma|S_r|\psi^n\rangle = e^{i\theta}\,\langle\xi,\gamma|\psi^n\rangle$. In other words, $|\psi^n\rangle$ is S_r invariant (apart from a phase factor) for any lattice automorphism r.

In the following we will use these properties to determine the expansion coefficients of the first-order correction to the ground state Eq. (6). Let us consider arbitrary states $|\sigma,\lambda\rangle$ and $|\sigma',\lambda'\rangle$. We denote the unique blue site (recall $A = 1$ so all sites but one are red) on these states by i and j, respectively. If there exists a lattice automorphism r such that $r(j) = i$, then $|\sigma',\lambda'\rangle = S_r\,|\sigma,\lambda\rangle$. Moreover, as shown above, $\langle\sigma',\lambda'|S_r|\psi^0\rangle = \langle S_r^{\dagger}\sigma',\lambda'|\psi^0\rangle = \langle S_r^{-1}\sigma',\lambda'|\psi^0\rangle = \langle S_{r^{-1}}\sigma',\lambda'|\psi^0\rangle = \langle\sigma,\lambda|\psi^0\rangle = e^{i\theta}\,\langle\sigma',\lambda'|\psi^0\rangle$. If we choose $|\Psi\rangle$ to be positive (see Theorem 1), in the limit of ϵ arbitrarily small, all $\langle\sigma,\lambda|\psi^0\rangle$ are also positive. This implies $\langle\sigma,\lambda|\psi^0\rangle = \langle\sigma',\lambda'|\psi^0\rangle$. Therefore we can conclude the following:

Theorem 5. If $\mathbf{G}$ is connected and for any two sites i and j there exists a lattice automorphism mapping j to i, then $\langle\sigma,\lambda|\psi^0\rangle = 1/\sqrt{M}$.

The assumption made on the lattice is very easily satisfied by any regular lattice with periodic boundary conditions (e.g., hypercubic, triangular, and honeycomb) as long as $I_{(i,j)} = I_{\mathbf{i}-\mathbf{j}}$, where $\mathbf{i},\mathbf{j}$ refer to the position of sites i,j. We also note that this assumption seems to be independent from the size of the lattice.

VII. CONCLUSION

We have studied the degeneracy of the ground-state energy E of the two-component Bose-Hubbard model and of the

[16] A unitary operator is always bounded. Then, if an operator S_r is bounded, $(|\psi^0\rangle + \sum_{n=1}^{\infty}\epsilon^n\,|\psi^n\rangle) \to |\Psi\rangle$ implies $(S_r\,|\psi^0\rangle + \sum_{n=1}^{\infty}\epsilon^n S_r\,|\psi^n\rangle) \to S_r\,|\Psi\rangle$.

perturbative correction E_1 in terms of connectivity properties of the optical lattice. We have shown that the degeneracy properties of E and E_1 are closely related to the connectivity properties of the lattice. We can summarize our main results as follows:

(i) The ground-state energy E is nondegenerate if the lattice is connected.

(ii) When $A = 0, B \neq 0$ ($B = 0, A \neq 0$), E_1 is nondegenerate if the lattice is connected.

(ii) When $A = 1, 0 < B < M - 1$ or $A = M - 1, 1 < B \leqslant M - 1$, E_1 is nondegenerate if the lattice is 2-connected.

(iv) In generic cases with $A + B < M - 1$ or $A + B > M + 1$, E_1 is nondegenerate if the lattice is 2-connected and not a circle with 5 or more sites.

(v) When $A + B = M$, E_1 is degenerate independently on the connectivity of the optical lattice. In the case of $A = M - 1, B = 1$ ($A = 1, B = M - 1$), we have determined the 0th-order correction of state ψ^0. We have shown that ψ^0 possesses equal expansion coefficient provided that there exists a lattice automorphism mapping a generic site of the lattice into another one.

These results are used to ensure a valid perturbative approach of the two-component Bose-Hubbard model also in the case of degenerate E_1. We expect that the analysis developed in this paper and the results about the ground-state degeneracy provide an effective tool to study the asymmetric character of the Mott insulator to superfluid transition between the particle and hole side and, more generally, the entanglement properties that appear to characterize this process.

ACKNOWLEDGMENTS

The work of one of the authors (V.P.) was partially supported by the M.I.U.R. project Collective quantum phenomena: From strongly correlated systems to quantum simulators (Project No. PRIN 2010LLKJBX).

APPENDIX A: PROOF OF PROPOSITION 1

We only prove the equivalence between (a) and (b). A proof based on the connectivity of the underlying graph of matrices is given in Ref. [26]. The equivalence between (b) and (c) is a direct consequence of Theorem 4.3 in Ref. [17].

Let us first prove the necessary condition by contradiction. Let us assume that $|\xi,\gamma\rangle$ and $|\xi',\gamma'\rangle$ are not connected by X. Then $|\xi,\gamma\rangle/\Re_X \neq |\xi',\gamma'\rangle/\Re_X$ and they both belong to $O/\Re_X$. So $O/\Re_X$ is a nontrivial partition of O, i.e., it includes more than one subset of O, and thus $\mathbf{X}$ is reducible. We get contradiction. Therefore we proved the necessary condition.

Let us now prove the sufficient condition also by contradiction. Let us assume $\mathbf{X}$ is reducible. Then there exists a nontrivial partition of O containing at least two disjoint nonempty subsets O_1 and O_2 of O, and the blocks $\mathbf{X}_{O_1\times O_1{}^c}$ (${O_1}^c$ is the complement of O_1 in O), $\mathbf{X}_{O_1{}^c\times O_1}$, $\mathbf{X}_{O_2\times O_2{}^c}$, and $\mathbf{X}_{O_2{}^c\times O_2}$ are zero. On the other hand, by hypothesis, for any $|\xi,\gamma\rangle$ and $|\xi',\gamma'\rangle$ which belong respectively to O_1 and O_2, there exists a finite sequence in the basis $\{|\alpha_1,\beta_1\rangle, |\alpha_2,\beta_2\rangle, \ldots, |\alpha_N,\beta_N\rangle\}$ such that $|\alpha_1,\beta_1\rangle = |\xi,\gamma\rangle$, $|\alpha_N,\beta_N\rangle\} = |\xi',\gamma'\rangle$ and for any $1 \leqslant i < N$, $\langle\alpha_i,\beta_i|X|\alpha_{i+1},\beta_{i+1}\rangle \neq 0$. Hence, for some $1 \leqslant i < N$, $|\alpha_i,\beta_i\rangle \in {O_2}^c$ and $|\alpha_{i+1},\beta_{i+1}\rangle \in O_2$ with $\langle\alpha_i,\beta_i|X|\alpha_{i+1},\beta_{i+1}\rangle \neq 0$, which implies $\mathbf{X}_{O_2\times O_2{}^c} \neq 0$. We get contradiction, hence $\mathbf{X}$ is irreducible.

APPENDIX B: PROOF OF COROLLARY 2

Let us consider $t_b = 0$, $t_a \neq 0$ ($\leftrightarrow T_b = 0$, $T_a \neq 0$). The basic idea is to show that $\mathbf{W}$ can be block diagonalized in terms of M^{N_b} identical blocks. Let us start by noticing that matrix elements of W,

$$\langle\xi,\gamma|W|\xi',\gamma'\rangle = -t_a\delta_{\gamma,\gamma'}\sum_{\{i,j\}\in\mathcal{E}(\mathbf{G})}\Bigg[I_{(i,j)}\sqrt{\xi_j+1}\sqrt{\xi_i'+1} \times \delta_{\xi_j+1,\xi_j'}\delta_{\xi_i,\xi_i'+1}\prod_{l\neq i,j}^{M}\delta_{\xi_l\xi_l'}\Bigg] \tag{B1}$$

are nonzero only when $\gamma = \gamma'$. Moreover, if $\gamma = \gamma'$, the value of matrix elements is independent of γ.

Let us define a function f which provides a one-to-one mapping from the set P of all $|\gamma\rangle$s onto $O/\Re_W$, such that for any $|\gamma\rangle$, $f(|\gamma\rangle) = |\xi,\gamma\rangle/\Re_W$. The mapping f can be easily defined and one just needs to show that f is one-to-one and onto.

Let $|\gamma\rangle$ and $|\gamma'\rangle$ differ. It is obvious that any member in $f(|\gamma\rangle)$ is not connected with any member in $f(|\gamma'\rangle)$ by W, hence $f(|\gamma\rangle) \neq f(|\gamma'\rangle)$, i.e., f is one-to-one. Next, let $x \in O/\Re_W$, i.e., $x = |\xi'',\gamma''\rangle/\Re_W$ for some $|\xi'',\gamma''\rangle$. Let us now consider $f(|\gamma''\rangle) = |\xi''',\gamma''\rangle/\Re_W$ for some $|\xi'''\rangle \neq |\xi''\rangle$. By using connection properties of W, one can show that $|\xi'',\gamma''\rangle\,\Re_W\,|\xi''',\gamma''\rangle$. So $|\xi'',\gamma''\rangle/\Re_W = |\xi''',\gamma''\rangle/\Re_W$ and thus $x = f(|\gamma''\rangle)$, i.e., f is onto. In conclusion, f is a one-to-one mapping from P onto $O/\Re_W$.

The total number of elements in P is M^{N_b}, hence $O/\Re_W$ is a nontrivial partition of O. Then, it is obvious that for any $O_i \in O/\Re_W$, $\mathbf{W}_{O_i\times O_i{}^c}$ and $\mathbf{W}_{O_i{}^c\times O_i}$ are zero matrices. In other words, $O/\Re_W$ block-diagonalizes $\mathbf{W}$.

Next, we show that each block is an irreducible nonnegative matrix and all blocks have the same set of eigenvalues. Let $|\gamma\rangle \in P$, then $f(|\gamma\rangle) \in O/\Re_W$. We can express $f(|\gamma\rangle)$ as $f(|\gamma\rangle) = Q \otimes \{|\gamma\rangle\}$, where Q is the set of all $|\xi\rangle$'s. From Frobenius theorem, one can conclude that $\mathbf{W}_{f(|\gamma\rangle)\times f(|\gamma\rangle)}$ has a nondegenerate ground-state energy. Since $f(|\gamma\rangle) = Q \otimes \{|\gamma\rangle\}$, one can use the identity map on Q, so for any $|\gamma\rangle \neq |\gamma'\rangle$, a one-to-one mapping from $\mathbf{W}_{f(|\gamma\rangle)\times f(|\gamma\rangle)}$ onto $\mathbf{W}_{f(|\gamma'\rangle)\times f(|\gamma'\rangle)}$ can be constructed. By construction, this mapping keeps matrix element identical, i.e., the two matrices have the same set of eigenvalues.

In conclusion, we have shown that the ground-state energy of W is M^{N_b} degenerate.

APPENDIX C: PROOF OF PROPERTY (D) IN SEC. IV C

We only consider the case of blue color. The proof for the red color is trivially equal.

Consider an arbitrary state and arbitrary sites i and j, where i is blue. We want to move the blue color from i to j according to the rules given in Sec. IV A. Because $\mathbf{G}$ is connected, there exists a path $\{i, i_2, \ldots, j\}$ linking i to j. The idea of following proof is to move the blue color along this path.

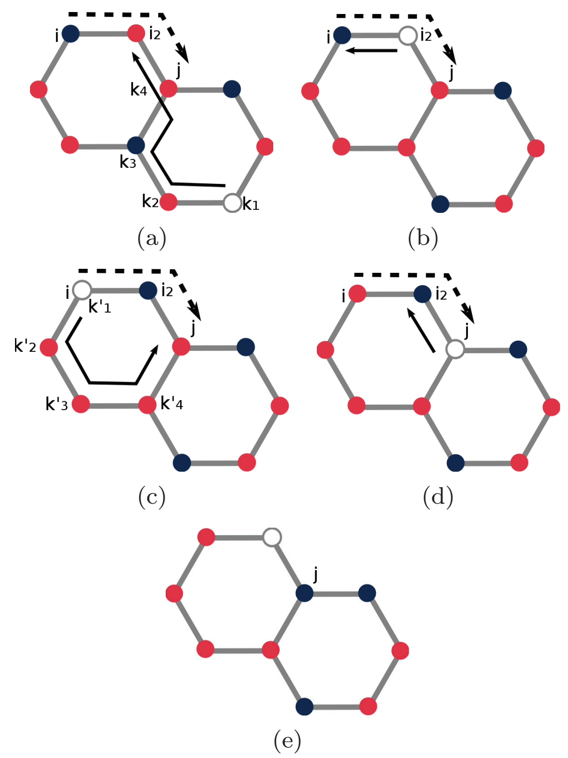

FIG. 9. (Color online) Panels (a)–(e) are examples of states in O_g on a 2-connected lattice with $A = 3, B = 6$. The steps for moving the (dark) blue color from site i to j are explained in the text and displayed pictorially in the sequence (a)–(e). The dashed arrow indicates a path connecting i and j. Black arrows indicate the path along which the white (circled in gray) color is moved at each step.

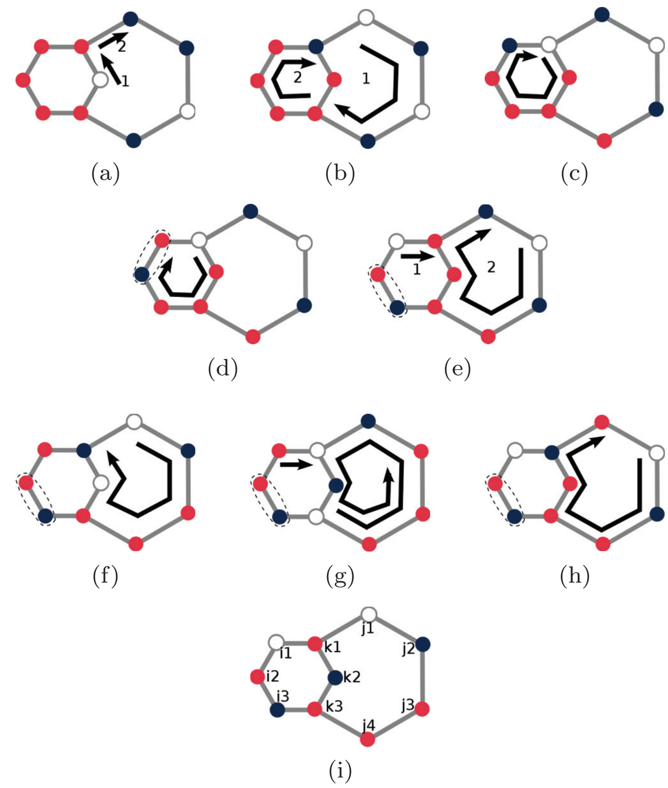

FIG. 10. (Color online) Panels (a)–(i) represent states in O_g for the case of a lattice consisting of a circle with one added path linking to unbonded sites. In this example $A = 3, B = 5$. States (a) and (i) are connected through the sequence (b)–(h). Black arrows indicate how the white (circled in gray) color is moved at each step. The dashed circle shows the order of the color which needs to be keep fixed (see text).

To illustrate the proof, we give an example in Fig. 9, where Figs. 9(a) is the starting state, and the path $\{i,i_2, \ldots ,j\}$ is indicated by a dashed arrow. To move the blue color along the path, e.g., from i_n to i_{n+1}, we need to, first, move a white color to i_{n+1} and then exchange the color on the bond $\{i_n,i_{n+1}\}$. In order to do so we observe that, due to the 2-connectivity of **G**, there also exists a path $\{k_1,k_2, \ldots ,i_2\}$ which avoids i but links a white site k_1 to i_2. The white color can be moved successively on $\{k_1,k_2, \ldots ,i_2\}$ so i_2 becomes white. Note that the fact that the path $\{k_1,k_2, \ldots ,i_2\}$ avoids i is important, because it allows us to keep the blue color on i while moving the white color to i_2. The next step consists of exchanging the color on the bond $\{i,i_2\}$ so i_2 becomes blue. The last two steps can be repeated successively (i.e., finding a path $\{k'_1,k'_2, \ldots ,i_3\}$ linking a white site k'_1 to i_3 and avoiding i_2, moving the white color along this path until i_3 becomes white, exchanging the color on bond $\{i_2,i_3\}$ so i_3 becomes blue and so on) until j acquires the blue color. This process is illustrated in Figs. 9(a) through 9(e) where solid black arrows indicate the path along which the white color is moved at each step.

APPENDIX D: PROOF OF PROPOSITION 5

For simplicity, but without loss of generality, we prove the proposition for the specific example shown in Fig. 10. The general case only differs in the number of sites on the circle and the extra path connecting the two sites which are unbounded in the original circle and in the color of sites.

Let us consider the lattice shown in Fig. 10(i). We denote by i_l, j_l, k_1, and k_3 the sites belonging to the original circle. Sites on the extra path connecting the initially unbounded sites k_1 and k_3 are denoted by k_l (in this case we only have k_2). This path separates the original circle into the left and right circles. Let us now consider arbitrary $|\sigma,\lambda\rangle$ and $|\sigma',\lambda'\rangle$ displayed by, e.g., Figs. 10(a) and 10(i), respectively. Because the white color can be moved to any site of the lattice according to the rules given in Sec. IV A, we choose $|\sigma',\lambda'\rangle$ such that both the left and right circles have one white site. Note that the proof below does not depend on the number of white sites.

The proof is based on the fact that we can first construct a generic state connected with $|\sigma,\lambda\rangle$ and such that the order of color on the i sites is the same as in $|\sigma',\lambda'\rangle$. In our particular example, because one of the i sites is white, this reduces to fixing the color on the bond specified by the dashed line in Figs. 10(d)–10(h). In order to do so, we first construct a state connected to $|\sigma,\lambda\rangle$ where k_1 is blue, as shown in Fig. 10(b). This process is depicted in Fig. 10(a) by black arrows indicating how the white color moves. This process is always possible due to the fact that **G** is 2-connected (see a similar argument given to prove Proposition 4). We keep moving the white color as depicted by black arrows in Figs. 10(b)–10(d) in order to construct the sequence Figs. 10(c)–10(e). We have finally constructed a state such that the order of the color on i sites is the same as $|\sigma',\lambda'\rangle$. Similar procedures can be followed if the color of more than two i sites need to be fixed.

Next we need to fix the order of color on the right circle. In a general case, this is equivalent to switching the order of color on a certain number of bonds. In our case, we only need to do so for the color on bond $\{j_1,k_1\}$ of state Fig. 10(e). The procedure is depicted by black arrows in Figs. 10(e)–10(g), so we end up with state Fig. 10(h). The idea of the procedure is to transfer the pair of colors on bond $\{j_1,k_1\}$ to bond $\{k_1,i_1\}$ [see Fig. 10(f)] and then move white sites in order to transfer the pair of colors back to the original bond $\{j_1,k_1\}$ [see Fig. 10(h)] but with the order of the color inverted. In general, this procedure will ensure that the order of the color on $\{j_1,k_1\}$ is inverted. Now the order of color on the right circle is the same as in $|\sigma',\lambda'\rangle$. The last step consists of moving the white color (which does not change the order of color) on the right circle in order to reach the state $|\sigma',\lambda'\rangle$. This is depicted by the black arrow in Fig. 10(h).

In a more general case that the one described here, one simply needs to repeat similar procedures to switch the color on bonds on the right circle as needed.

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