

Nagaoka states in the $SU(n)$ Hubbard model

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(Received 20 October 2012; published 17 January 2013)

We present an extension of Nagaoka's theorem in the $SU(n)$ generalization of the infinite- U Hubbard model. It is shown that, when there is exactly one hole, the fully polarized states analogous to the ferromagnetic states in the $SU(2)$ Hubbard model are ground states. For a restricted class of models satisfying the connectivity condition, these fully polarized states are the unique ground states up to the trivial degeneracy due to the $SU(n)$ symmetry. We also give examples of lattices in which the connectivity condition can be verified explicitly. The examples include the triangular, Kagomé, and hypercubic lattices in $d (\geq 2)$ dimensions, among which the cases of $d = 2$ and 3 are experimentally realizable in ultracold atomic gases loaded into optical lattices.

DOI: [10.1103/PhysRevA.87.013617](https://doi.org/10.1103/PhysRevA.87.013617)

PACS number(s): 03.75.Ss, 71.10.Fd, 67.85.-d, 37.10.Jk

I. INTRODUCTION

The (fermionic) Hubbard model has attracted considerable attention as a model for describing correlated electrons in solids. Despite its apparent simplicity, it is difficult to analyze the model in a consistent way, and exact and/or rigorous results are very limited [1–3]. A number of approximate treatments have been developed to understand the model. A systematic approach from the large- n limit of the $SU(n)$ Hubbard model was initiated by Affleck and Marston in the context of high-temperature superconductivity [4]. In this approach, the $SU(n)$ symmetry used is just a theoretical tool rather than a physical reality. Therefore, the model at finite n did not attract much attention and was much less studied. However, a realization of the $SU(n)$ Hubbard model [5] and its two-orbital generalization [6] have recently been proposed theoretically in the context of ultracold fermionic atoms. These systems were later realized experimentally using ultracold Yb atoms [7,8]. The enlarged symmetry of the system results from the hyperfine spin degrees of freedom. In the large- U limit, these models with $m (< n)$ atoms per site reduce to $SU(n)$ spin Hamiltonians in which a variety of exotic states including chiral spin liquids are found to be ground states [9,10].

In this paper, we present an extension of Nagaoka's theorem [11]. The original theorem is the first rigorous result about the ferromagnetism in the Hubbard model. Nagaoka proved that when there is exactly one hole, the ferromagnetic state is the ground state of the infinite- U Hubbard model if the lattice satisfies certain connectivity conditions. A generalized version of this theorem with a simplified proof was given by Tasaki [12]. A natural analog of the Nagaoka ferromagnetic state in a system with $SU(n)$ symmetry is a fully polarized state characterized by the Young tableau having one row with N_f boxes, where N_f is the total number of fermions. In this paper, we show that an analog of Nagaoka's theorem holds in the $SU(n)$ Hubbard model and those fully polarized states are indeed the ground states if certain conditions are satisfied. Note that the analog of the Nagaoka state in the $SU(4)$ Hubbard model on small clusters was studied in Ref. [13] and, very recently, the existence of a fully polarized phase in the $SU(3)$ case at certain fillings was indicated in Ref. [14].

The rest of the paper is organized as follows. In Sec. II, we give a precise definition of the model and describe the

symmetries of the Hamiltonian. Our main results are then presented as theorems. In Sec. III, we first construct a basis in which all of the off-diagonal elements of the Hamiltonian are nonpositive. Then we give the definition of the connectivity condition and give proofs of the theorems. In Sec. IV, we give several examples of lattices that satisfy the connectivity condition. We conclude with a summary and outlook in Sec. V.

II. THE MODEL AND THE RESULTS

A. The Hamiltonian

We begin with the definition of the $SU(n)$ Hubbard model. Let Λ be a finite lattice of N_s sites. The model is described by the following Hamiltonian:

$$H = \sum_{x,y \in \Lambda} \sum_{\alpha=1}^n t_{x,y} c_{x,\alpha}^\dagger c_{y,\alpha} + V(\{n_x\}) + \frac{U}{2} \sum_{x \in \Lambda} n_x(n_x - 1), \quad (1)$$

where $c_{x,\alpha}^\dagger$ ($c_{x,\alpha}$) creates (annihilates) a fermion with flavor α at site x , and the number of fermions at site x is defined by $n_x = \sum_{\alpha=1}^n n_{x,\alpha}$ with $n_{x,\alpha} = c_{x,\alpha}^\dagger c_{x,\alpha}$. The hopping matrix elements are arbitrary as long as they are real, $t_{x,x} = 0$, and $t_{x,y} = t_{y,x} \geq 0$. Although this requirement might look odd, $t_{x,y} \leq 0$ can be achieved, in the case of bipartite lattices, by local gauge transformations ($c_{x,\alpha}^\dagger \rightarrow -c_{x,\alpha}^\dagger$) for one sublattice. Furthermore, it has recently been proposed that a sign change of the hopping matrix elements can be achieved by shaking optical lattices [15,16]. The second term $V(\{n_x\})$ is an arbitrary real-valued function of the number operators n_x . Typical examples are on-site potentials and charge-charge interactions between any pair of sites. In cold-atom systems, an external harmonic trap is usually unavoidable. Such a confinement term can be taken into account by setting

$$V(\{n_x\}) = \sum_{x \in V} \frac{1}{2} m \omega^2 |\mathbf{R}_x|^2 n_x, \quad (2)$$

where m is the mass of atoms, ω is the trapping frequency, and \mathbf{R}_x is the position vector for the site x . Since we are concerned with the model on finite lattices, the expectation value of $V(\{n_x\})$ in Eq. (2) in any state is finite provided that

$m\omega^2 < \infty$. The third term in Eq. (1) represents the on-site Coulomb repulsion ($U > 0$).

B. Symmetries of the Hamiltonian

Let us first consider symmetries of the Hamiltonian H . In addition to the trivial conservation of the total number of fermions, the Hamiltonian exhibits $U(n) = U(1) \times SU(n)$ symmetry. To see this, we define a set of number operators and flavor-raising and -lowering operators as

$$F^{\alpha,\alpha} = \sum_{x \in \Lambda} n_{x,\alpha}, \quad F^{\alpha,\beta} = \sum_{x \in \Lambda} c_{x,\alpha}^\dagger c_{x,\beta}. \quad (3)$$

They satisfy the commutation relation $[F^{\alpha,\beta}, F^{\gamma,\delta}] = \delta_{\beta,\gamma} F^{\alpha,\delta} - \delta_{\delta,\alpha} F^{\gamma,\beta}$, which follows from the relation

$$[c_{x,\alpha}^\dagger c_{x,\beta}, c_{y,\gamma}^\dagger c_{y,\delta}] = \delta_{x,y} (\delta_{\beta,\gamma} c_{x,\alpha}^\dagger c_{x,\delta} - \delta_{\alpha,\delta} c_{x,\gamma}^\dagger c_{x,\beta}). \quad (4)$$

Using a similar relation, one can confirm that $[F^{\alpha,\beta}, n_x] = 0$ and $[F^{\alpha,\beta}, \sum_{\gamma=1}^n c_{x,\gamma}^\dagger c_{y,\gamma}] = 0$, and thus the Hamiltonian H commutes with $F^{\alpha,\beta}$, i.e., $[H, F^{\alpha,\beta}] = 0$. From the operators $F^{\alpha,\beta}$, one can construct new operators that also commute with the Hamiltonian:

$$N = \sum_{x \in \Lambda} n_x, \quad (5)$$

$$T^a = \sum_{x \in \Lambda} \sum_{\alpha, \beta} c_{x,\alpha}^\dagger \mathcal{T}_{\alpha,\beta}^a c_{x,\beta} \quad (a = 1, \dots, n^2 - 1), \quad (6)$$

where $\mathcal{T}_{\alpha,\beta}^a$ are the generators of $SU(n)$ Lie algebra. Therefore it is concluded that the Hamiltonian has a global $U(n) = U(1) \times SU(n)$ symmetry. As a side remark, we note that the restriction of the Hamiltonian to the subspace where each site is occupied by at most two fermions has an enhanced symmetry [17]. Moreover, this projected model in one dimension is exactly solvable by means of the Bethe ansatz [18–20].

C. Fully polarized states

In this section, we introduce the notion of fully polarized states in the $SU(n)$ Hubbard model. Since the numbers of α fermions, $F^{\alpha,\alpha}$, are conserved, the eigenstates of H are separated into disconnected sectors labeled by the eigenvalues of $F^{\alpha,\alpha}$ ($\alpha = 1, \dots, n$). In what follows, we shall denote eigenvalues of $F^{\alpha,\alpha}$ by N_α . The off-diagonal operators $F^{\alpha,\beta}$ ($\alpha \neq \beta$) play a role in connecting degenerate eigenstates in different subspaces. For instance, starting from a fully polarized state Φ_1 that is an eigenstate of H in the subspace $N_1 = N_f$, $N_2 = \dots = N_n = 0$, one can obtain degenerate states with the same energy by applying $F^{\alpha,\beta}$ repeatedly:

$$\Phi_1^{(N_1, \dots, N_n)} = (F^{n,1})^{N_n} \dots (F^{3,1})^{N_3} (F^{2,1})^{N_2} \Phi_1, \quad (7)$$

where $N_1 = N_f - \sum_{\alpha=2}^n N_\alpha$. Note that we have assumed that $\sum_{\alpha=2}^n N_\alpha \leq N_f$, where N_f is the total number of fermions.

To show that the above state is indeed the eigenstate, we shall prove by induction that the squared norm of $\Phi_1^{(N_1, \dots, N_n)}$ is nonvanishing. We first set $N_2 = \dots = N_n = 0$. Then the statement is trivial because $|\Phi_1|^2 > 0$. Next, we suppose that the squared norm of the state

$$\Phi_1^{(N_1, \dots, N_k)} = (F^{k,1})^{N_k} \dots (F^{3,1})^{N_3} (F^{2,1})^{N_2} \Phi_1 \quad (8)$$

is nonvanishing. Then from the commutation relation $[F^{1,k+1}, F^{k+1,1}] = F^{1,1} - F^{k+1,k+1}$ and the fact that $F^{1,k+1} \Phi_1^{(N_1, \dots, N_k)} = 0$, we have

$$\begin{aligned} F^{1,k+1} (F^{k+1,1})^m \Phi_1^{(N_1, \dots, N_k)} \\ = m(N_1 - m + 1) (F^{k+1,1})^{m-1} \Phi_1^{(N_1, \dots, N_k)} \end{aligned} \quad (9)$$

for $m = 1, 2, \dots, N_{k+1}$. Using the above chain of relations, we obtain

$$\begin{aligned} |\Phi_1^{(N_1, \dots, N_k, N_{k+1})}|^2 &= |(F^{k+1,1})^{N_{k+1}} \Phi_1^{(N_1, \dots, N_k)}|^2 \\ &= \frac{N_1! N_{k+1}!}{(N_1 - N_{k+1})!} |\Phi_1^{(N_1, \dots, N_k)}|^2, \end{aligned} \quad (10)$$

and find that the squared norm of $\Phi_1^{(N_1, \dots, N_{k+1})}$ is nonvanishing when $N_{k+1} \leq N_1$. The desired result $|\Phi_1^{(N_1, \dots, N_n)}|^2 > 0$ then follows by induction.

The above argument ensures that the number of the states with the same energy as Φ_1 is at least

$$d_{\text{deg}} = \binom{N_f + n - 1}{N_f} = \frac{(N_f + n - 1)!}{N_f! (n - 1)!}. \quad (11)$$

This number coincides with the number of standard Young tableaux having one row with N_f boxes. When $n = 2$, $d_{\text{deg}} = N_f + 1$, which is the number of ferromagnetic states in the $SU(2)$ Hubbard model with N_f fermions. In this paper, we will henceforth refer to states of the form Eq. (7) as *fully polarized states*.

D. Theorems

We prove two generalizations of Nagaoka's theorem in the $SU(n)$ Hubbard model. The first one is weaker and does not require the connectivity condition. However, this version of the theorem does not establish that the fully polarized states are the unique ground states. The second one is a strict extension of the original theorem in the $SU(2)$ Hubbard model, which ensures the uniqueness of the ground states.

Theorem 1. Consider the $SU(n)$ Hubbard Hamiltonian (1) with $t_{x,y} \geq 0$, V arbitrary, $U = \infty$, and $N_f = N_s - 1$. Then among the ground states, there are d_{deg} states [see Eq. (11)] that are the fully polarized states.

Theorem 2. Consider the $SU(n)$ Hubbard Hamiltonian (1) with $t_{x,y} \geq 0$, V arbitrary, $U = \infty$, and $N_f = N_s - 1$. We further assume that the model satisfies the connectivity condition. Then the ground states are fully polarized states and are nondegenerate apart from the trivial d_{deg} -fold degeneracy due to the $SU(n)$ symmetry.

III. PROOF

In this section we shall prove the theorems. We first define the basis we work with and clarify the connectivity condition under which Theorem 2 holds. Then we prove Theorem 1 by using the variational principle. Theorem 2 is proved as a consequence of the Perron-Frobenius theorem.

A. Basis states

In the limit $U \rightarrow \infty$, a state with a site occupied by two or more fermions has infinite energy. We are interested only in

the finite-energy states and hence consider the Hilbert space \mathcal{H} which is spanned by states of the form

$$\Psi_\Gamma = \text{sgn}[x] \left(\prod_{y \in \Lambda \setminus \{x\}} c_{y, \alpha_y}^\dagger \right) \Phi_{\text{vac}}, \quad (12)$$

where Φ_{vac} is the vacuum (no-particle) state, and the index $\Gamma = (x, \alpha)$ represents a position x of the hole (the site without a fermion) and a flavor configuration $\alpha = (\alpha_y)_{y \in \Lambda \setminus \{x\}}$ with $\alpha_y = 1, 2, \dots, n$. Here, we have assumed that the product is ordered according to an arbitrary order introduced in Λ , and $\text{sgn}[x]$ takes -1 if x is an odd-numbered position and 1 otherwise. More explicitly, the states (12) can be written as

$$\Psi_\Gamma = c_{x, \beta} \left(\prod_{y \in \Lambda} c_{y, \tilde{\alpha}_y}^\dagger \right) \Phi_{\text{vac}}, \quad (13)$$

where the flavor configuration $\tilde{\alpha} = (\alpha_y)_{y \in \Lambda}$ is defined by $\tilde{\alpha}_x = \beta$ for the site x and $\tilde{\alpha}_y = \alpha_y$ for all $y \in \Lambda \setminus \{x\}$. It is noted that the collection of the states (12) as well as (13) form an orthonormal basis.

Since each number N_α of fermions with flavor α is a conserved quantity, the Hilbert space \mathcal{H} can be further decomposed into subspaces labeled by $(N_\alpha)_{\alpha=1}^n$ with $\sum_{\alpha=1}^n N_\alpha = N_s - 1$. Note that N_s denotes the number of sites in Λ . In the following, we denote by $\mathcal{H}[(N_\alpha)]$ the subspace with fixed $(N_\alpha)_{\alpha=1}^n$.

B. Connectivity condition

Consider the matrix representation of H in the basis defined by Eq. (12). We say that two states labeled by Γ and Γ' are directly connected if $\langle \Psi_{\Gamma'}, H \Psi_\Gamma \rangle \neq 0$, and express this fact by writing $\Gamma \leftrightarrow \Gamma'$. Let $\alpha_{y \rightarrow x}$ be the flavor configuration on $\Lambda \setminus \{y\}$ obtained from α on $\Lambda \setminus \{x\}$ by moving α_y from y to x . One can easily see that $\Gamma = (x, \alpha)$ and $\Gamma' = (y, \alpha')$ are directly connected if $t_{x,y} \neq 0$ and $\alpha' = \alpha_{y \rightarrow x}$, since we have

$$\left\langle \Psi_{\Gamma'}, \left(\sum_{\alpha=1}^n t_{x,y} c_{x, \alpha}^\dagger c_{y, \alpha} \right) \Psi_\Gamma \right\rangle = -t_{x,y}. \quad (14)$$

Here, we note that the negative sign is attributed to the sign factor in the definition of basis states (12). We also note that an off-diagonal matrix element of H , i.e.,

$$\langle \Psi_{(y, \alpha')}, H \Psi_{(x, \alpha)} \rangle = -t_{x,y} (\leq 0), \quad (15)$$

comes solely from the hopping term and is nonvanishing only if $(y, \alpha') \leftrightarrow (x, \alpha)$.

For two indices Γ and Γ' , if there is a sequence of $\mathbf{\Gamma} = (\Gamma_1, \Gamma_2, \dots, \Gamma_l)$ such that $\Gamma = \Gamma_1 \leftrightarrow \Gamma_2 \leftrightarrow \dots \leftrightarrow \Gamma_l = \Gamma'$, we say Γ and Γ' are connected and write $\Gamma \leftarrow \mathbf{\Gamma} \rightarrow \Gamma'$. Then the model is said to satisfy the connectivity condition if all indices corresponding to the basis states with common $(N_\alpha)_{\alpha=1}^n$ are connected with each other.

Remarks. The direct connectivity $(x, \alpha) \leftrightarrow (y, \alpha_{y \rightarrow x})$ implies that the hopping term of the Hamiltonian H transfers the hole from site x to site y , and vice versa. Similarly, the connectivity (x, α) and (y, α') implies that there is a hopping process by which the hole is exchanged between x and y .

A simple sufficient condition for the connectivity condition in the SU(2) case was found in Ref. [12]. In the SU(n) case,

however, it is more difficult to examine the connectivity condition for given hopping matrix $t_{x,y}$ and the number of flavors n . This is because the connectivity condition of our model depends not only on $t_{x,y}$ but also on n . It may even happen that the model with n less than a certain integer n_0 satisfies the connectivity condition but the one with $n \geq n_0$ does not (e.g., see Ref. [13]). In Sec. IV, we will give several examples where we can verify the connectivity condition explicitly.

C. Proof of Theorem 1

Let Φ_G be a ground state of H , which is expanded as $\Phi_G = \sum_\Gamma \psi_\Gamma \Psi_\Gamma$ with certain coefficients ψ_Γ . Let us write $\Psi_{(x,1)}$ for the basis states of $\mathcal{H}[(N_\alpha)]$ with $N_1 = N_f$ and $N_2 = \dots = N_n = 0$, i.e.,

$$\Psi_{(x,1)} = c_{x,1} \left(\prod_{y \in \Lambda} c_{y,1}^\dagger \right) \Phi_{\text{vac}}. \quad (16)$$

Then, consider the trial state $\Phi_1 = \sum_{x \in \Lambda} \phi_x \Psi_{(x,1)}$ with $\phi_x = (\sum_\alpha |\psi_{(x,\alpha)}|^2)^{1/2}$ where the sum is taken over all flavor configurations.

Let us consider the expectation value of H in Φ_1 . We first find that $\langle \Phi_1, \Phi_1 \rangle = \sum_x |\phi_x|^2 = \sum_x \sum_\alpha |\psi_{(x,\alpha)}|^2 = \langle \Phi_G, \Phi_G \rangle$. Next, noting that $\langle \Psi_{(x,1)}, V(\{n_x\}) \Psi_{(x,1)} \rangle = \langle \Psi_{(x,\alpha)}, V(\{n_x\}) \Psi_{(x,\alpha)} \rangle$, which follows from

$$n_x \Psi_{(y,\alpha)} = \begin{cases} 0 & \text{if } x = y, \\ \Psi_{(y,\alpha)} & \text{otherwise,} \end{cases} \quad (17)$$

for any flavor configuration α , we get

$$\begin{aligned} \langle \Phi_1, V(\{n_x\}) \Phi_1 \rangle &= \sum_x |\phi_x|^2 \langle \Psi_{(x,1)}, V(\{n_x\}) \Psi_{(x,1)} \rangle \\ &= \sum_x \sum_\alpha |\psi_{(x,\alpha)}|^2 \langle \Psi_{(x,\alpha)}, V(\{n_x\}) \Psi_{(x,\alpha)} \rangle \\ &= \langle \Phi_G, V(\{n_x\}) \Phi_G \rangle. \end{aligned} \quad (18)$$

For the hopping term, we have

$$\begin{aligned} &\left\langle \Phi_1, \left(\sum_{\alpha=1}^n t_{x,y} c_{x, \alpha}^\dagger c_{y, \alpha} \right) \Phi_1 \right\rangle \\ &= -t_{x,y} \phi_y \phi_x \leq -t_{x,y} \sum_\alpha \psi_{(y, \alpha_{y \rightarrow x})}^* \psi_{(x, \alpha)} \\ &= \left\langle \Phi_G, \left(\sum_{\alpha=1}^n t_{x,y} c_{x, \alpha}^\dagger c_{y, \alpha} \right) \Phi_G \right\rangle. \end{aligned} \quad (19)$$

Here, we have used the Schwarz inequality

$$\begin{aligned} \sum_\alpha \psi_{(y, \alpha_{y \rightarrow x})}^* \psi_{(x, \alpha)} &\leq \left(\sum_\alpha |\psi_{(y, \alpha_{y \rightarrow x})}|^2 \right)^{1/2} \left(\sum_\alpha |\psi_{(x, \alpha)}|^2 \right)^{1/2} \\ &= \phi_y \phi_x. \end{aligned} \quad (20)$$

As a consequence of the relations obtained above, we find

$$\frac{\langle \Phi_1, H \Phi_1 \rangle}{\langle \Phi_1, \Phi_1 \rangle} \leq \frac{\langle \Phi_G, H \Phi_G \rangle}{\langle \Phi_G, \Phi_G \rangle}, \quad (21)$$

which shows that Φ_1 is also a ground state. Then the theorem follows by taking Φ_1 as one of the ground states and using the global SU(n) symmetry discussed in Sec. IIC.

D. Proof of Theorem 2

Let us fix $(N_\alpha)_{\alpha=1}^n$ and consider the matrix representation of H for the basis states Ψ_Γ in $\mathcal{H}[(N_\alpha)]$. Then, as we noted below (14), all the off-diagonal matrix elements are nonpositive. Furthermore, the connectivity condition ensures that the matrix is not decomposable. Therefore, the Perron-Frobenius theorem is applicable to the present matrix, implying that the lowest-energy state in the subspace $\mathcal{H}[(N_\alpha)]$ is unique.

This fact together with the statement of Theorem 1 will complete the proof of Theorem 2. However, we give here a simple proof which relies only on the Perron-Frobenius theorem. We use another consequence of the Perron-Frobenius theorem: the lowest-energy state in each subspace is given by a certain linear combination of all Ψ_Γ with positive coefficients.

Let $\Phi_{1,G}$ be the lowest-energy state with energy E in the subspace where all fermions have flavor 1. Using the operators $F^{\alpha,\beta}$ in Eq. (3), one can construct the state with the same energy E in the subspace $\mathcal{H}[(N_\alpha)]$ as

$$(F^{n,1})^{N_n} \dots (F^{3,1})^{N_3} (F^{2,1})^{N_2} \Phi_{1,G}. \quad (22)$$

Here note that the state (22) can be expanded in terms of Ψ_Γ with positive coefficients. Since the lowest-energy state in $\mathcal{H}[(N_\alpha)]$ also has positive coefficients, it is not orthogonal to the state (22). Therefore, the state (22) is exactly the lowest-energy state in the subspace $\mathcal{H}[(N_\alpha)]$. This implies that the ground state is unique apart from the degeneracy due to the $SU(n)$ symmetry.

IV. EXAMPLES

In this section we give three examples where the connectivity condition can be verified explicitly. Before proceeding, let us introduce some terminology. A pair $\{x,y\}$ of sites in Λ is called a *bond* if $t_{x,y} \neq 0$. By a *path* from x to y , we mean an ordered set $\{x_1, x_2, \dots, x_l\}$ of l sites such that $x_1 = x$, $x_l = y$, and $\{x_m, x_{m+1}\}$ is a bond for all $m = 1, \dots, l-1$. A path $\{x_1, x_2, \dots, x_l\}$ is called a *loop* if $\{x_1, x_l\}$ is a bond. A lattice Λ is said to be connected if one can find a path for any two sites x and y in Λ . A connected lattice Λ is said to be twofold connected, if one cannot make it disconnected by removing a single site.

The connectivity of Λ implies that one can bring the hole to any site in Λ by successive hops. It should be noted, however, that the connectivity of Λ itself does not necessarily mean the connectivity of the model. This is because the motion of the hole around the lattice may not generate all the configurations $\Gamma = (x, \alpha)$ with common $(N_\alpha)_{\alpha=1}^n$.

A. Closed chain with one next nearest neighbor bond

The first example is the $SU(n)$ Hubbard Hamiltonian on a closed chain, i.e., the one-dimensional lattice $\Lambda = \{0, 1, \dots, L\}$ with bonds $\{l, l+1\}$ ($l = 0, 1, \dots, L-1$) and $\{L, 0\}$. It is, furthermore, assumed that there is one next-nearest-neighbor bond, say $\{0, 2\}$. Let us take a fixed $(N_\alpha)_{\alpha=1}^n$ and examine the connectivity of indices $\Gamma = (x, \alpha)$ in this subspace. Since the lattice Λ is obviously twofold connected, one can bring the hole to any site. Thus, one can fix the location of the hole, say 0, and see whether the motion of the hole generates all the flavor configurations $(0, \alpha)$ in the subspace.

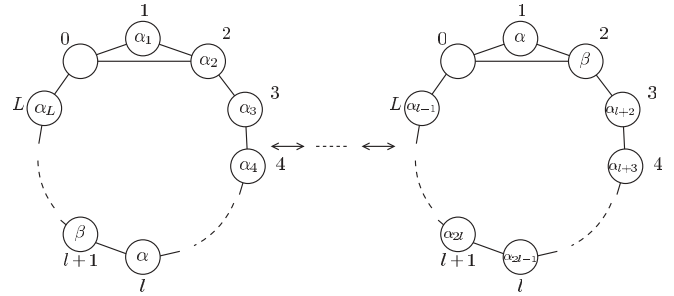


FIG. 1. By letting the hole move around the chain in the clockwise direction $l-1$ times, one can bring the fermions from sites l and $l+1$ to sites 1 and 2, respectively.

For this purpose, we show below that, for any bond $\{x,y\}$, $(0, \alpha)$ and $(0, \alpha_{x \leftrightarrow y})$ are connected, where $\alpha_{x \leftrightarrow y}$ is the flavor configuration obtained from α by switching α_x and α_y . This property implies that one can generate any flavor configuration α' from α by successively switching the flavors on a pair of neighboring sites in an appropriate way. Let us assume that $\alpha_l = \alpha$ and $\alpha_{l+1} = \beta$. By letting the hole move around the closed chain in the clockwise direction $l-1$ times, we first obtain the flavor configuration α' in which $\alpha'_1 = \alpha$ and $\alpha'_2 = \beta$ (see Fig. 1). Next we let the hole move around the triangle loop $\{0, 1, 2\}$ in the clockwise direction once, by which the flavor α'_1 is exchanged with α'_2 (see Fig. 2). Finally, by letting the hole move along the chain in the opposite (counterclockwise) direction $l-1$ times, we get the flavor configuration α'' with $\alpha''_1 = \beta, \alpha''_{l+1} = \alpha$ without changing the flavor configuration outside $\{l, l+1\}$. This proves that the model satisfies the connectivity condition.

A few comments are in order: The presence of the single next-nearest-neighbor bond changes drastically the nature of ground states. In fact, in the purely one-dimensional chain in which the connectivity condition is not satisfied, all the flavor configurations become degenerate at $U = \infty$ in the same way as in the standard $SU(2)$ case [21]. This degeneracy is removed if $U < \infty$ and the ground states form a unique antisymmetric multiplet, which can be proved using the Perron-Frobenius argument [22]. In particular, the ground state is a unique $SU(n)$ singlet if the number of fermions is a multiple of n .

B. Twofold connected lattice with triangle loops

The second example is a class of models defined on twofold connected lattices containing at least one triangle loop. Typical

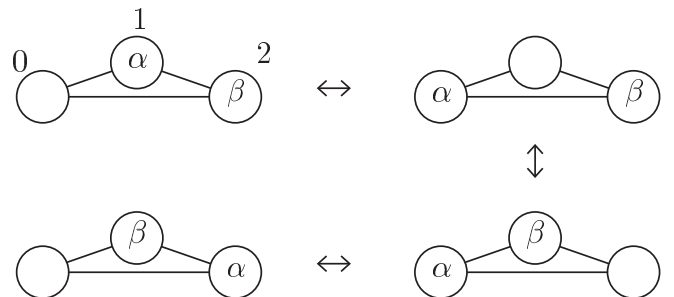


FIG. 2. The flavors at sites 1 and 2 are exchanged when the hole hops around the loop $\{0, 1, 2\}$ in the clockwise direction once.

examples are the triangular and Kagomé lattices. Let us show that the model of this class satisfies the connectivity condition. Let $\{u, v, w\}$ be a triangle loop, and let $\{x, y\}$ be an arbitrary bond in the lattice Λ . Since Λ is connected, we can find a path from x to u and another path from y to v . Suppose that these two paths share the same site z and one cannot find other paths that do not intersect. Then, the removal of the site z makes Λ disconnected. This contradicts the fact that Λ is twofold connected. Thus one can always find two nonintersecting paths, one from x to u and the other from y to v . It follows from this that there is a loop containing two bonds $\{u, v\}$ and $\{x, y\}$ in Λ . Noting that $\{u, v\}$ belongs to the triangle loop, we can repeat the same argument as in the previous example, which gives the conclusion that the connectivity condition is satisfied in the model.

C. Lattice consisting of loops of four sites

In the previous two examples, the existence of a loop of three sites plays an important role in establishing the connectivity condition. It is then natural to ask whether the connectivity condition is satisfied or not in a model on a lattice without any triangle. However, it seems difficult to answer this question in a general setting. Here, we instead give a concrete example: the model on a lattice consisting only of loops of length 4. Our lattice Λ can be constructed as follows. Let C_1 be a loop of four sites having four bonds. Let C_l with $l = 2, \dots, L$ be identical copies of C_1 . We construct Λ_2 by adding C_2 to $\Lambda_1 = C_1$ in such a way that Λ_1 and C_2 share one bond. Similarly, we construct Λ_l by adding C_l to Λ_{l-1} in such a way that C_l shares at least one bond with Λ_{l-1} and shares at most one bond with each $C_{l'}$ ($l' = 1, \dots, l - 1$) that forms Λ_{l-1} . Our lattice is then obtained as $\Lambda = \Lambda_L$. Typical examples are square and cubic lattices.

In the following, we shall prove that the model on Λ with $N_s \geq n + 2$ satisfies the connectivity condition, i.e., any pair of indices $\Gamma = (z, \alpha)$ and $\Gamma' = (z', \alpha')$ with common $(N_\alpha)_{\alpha=1}^n$ are connected. To see this, let us consider the subspace with fixed $(N_\alpha)_{\alpha=1}^n$. Since we have assumed that $N_s \geq n + 2$, the fermion number N_f satisfies $N_f = N_s - 1 \geq n + 1$. It is thus ensured that there is a flavor σ such that $N_\sigma \geq 2$. The presence of two fermions with flavor σ plays an important role in the

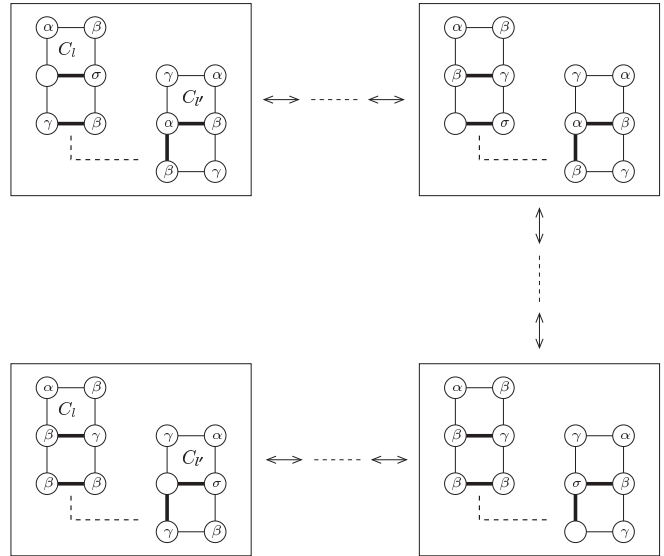


FIG. 4. A pair of the hole and a fermion with flavor σ in loop C_l can be moved to any other loop $C_{l'}$ through shared bonds emphasized by thick lines.

proof below. As in the previous examples, it suffices to show that (z, α) and $(z, \alpha_{x \leftrightarrow y})$ are connected for any bond $\{x, y\}$ since the lattice Λ is obviously twofold connected.

Before proceeding, we give two remarks on the connectivity and the motion of the hole: (i) In a loop C_l containing three fermions and the hole, the motion of the hole does not change the order of flavors in the clockwise (counterclockwise) direction (see Fig. 3). (ii) One can bring a pair of the hole and a fermion with a fixed flavor from a loop C_l to any other loop $C_{l'}$. This is confirmed by the first property (i) and the construction of Λ . In fact, there is a sequence of $C_l = C_{l_1}, C_{l_2}, \dots, C_{l_k} = C_{l'}$ such that C_{l_i} and $C_{l_{i+1}}$ share a bond, and, by occupying these shared bonds, a pair of the hole and a fermion can move from C_l to $C_{l'}$ (see Fig. 4).

Let us prove the connectivity of (z, α) and $(z, \alpha_{x \leftrightarrow y})$ for an arbitrary bond $\{x, y\}$ by explicitly constructing a sequence Γ such that $(z, \alpha) \leftarrow \Gamma \rightarrow (z, \alpha_{x \leftrightarrow y})$. Here we assume that $\alpha_x = \alpha$ and $\alpha_y = \beta$. From the construction of Λ , it is possible to find a loop $C_l = \{x, y, u, v\}$ and a path from z to v that contains neither x nor y . This means that we have $\Gamma^{(1)}$ such that $(z, \alpha) \leftarrow \Gamma^{(1)} \rightarrow (z^{(1)}, \alpha^{(1)})$ where $z^{(1)}$ ($\neq x, y$) is a site in C_l and $\alpha^{(1)}$ is a certain flavor configuration. We recall that there is a flavor σ with $N_\sigma \geq 2$. By using two fermions with flavor σ , we will construct a process in which α_x and α_y are switched.

Now suppose that one of the fermions with flavor σ is in $C_{l'}$. We can find a sequence of shared bonds from C_l to $C_{l'}$, as mentioned above. If x or $y \in C_l$ (or both of them) touches the shared bond we transfer the two fermions on $\{x, y\}$ to the sites on $\{u, v\}$. Then we can bring the hole in C_l to $C_{l'}$ through sites touching the shared bonds, and from (ii) we can bring back the pair of the hole and the fermion with flavor σ from $C_{l'}$ to C_l . Thus we can find $\Gamma^{(2)}$ which connects $(z^{(1)}, \alpha^{(1)})$ to $(z^{(2)}, \alpha^{(2)})$, where $z^{(2)}$ is a site in $C_l = \{x, y, u, v\}$, and $\alpha^{(2)}$ is a certain flavor configuration. We note that now there are three

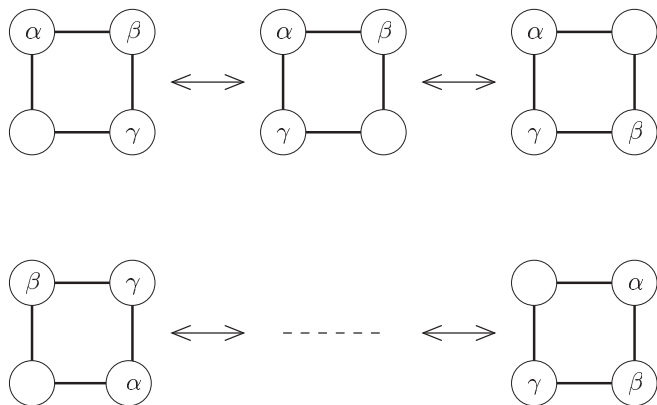


FIG. 3. Three fermions and the hole in a loop C_l . The motion of the hole does not change the order of flavors in the clockwise (counterclockwise) direction.

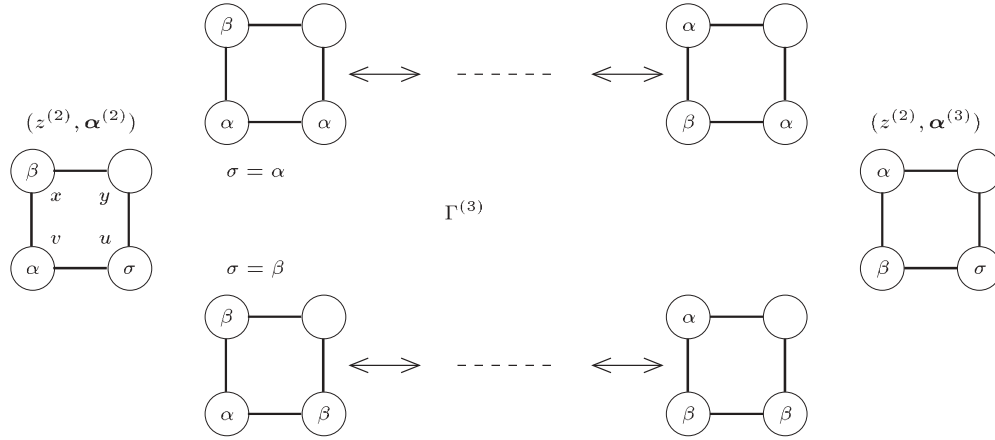


FIG. 5. $\Gamma^{(3)}$ connecting $(z^{(2)}, \alpha^{(2)})$ to $(z^{(2)}, \alpha^{(3)})$. It is assumed that $\{y, u\}$ is a shared bond, so that fermions with flavor α and β were transferred in the process $\Gamma^{(2)}$. In $(z^{(2)}, \alpha^{(2)})$, the position of the hole is $z^{(2)} = y$, and the local flavor configuration is $\alpha_x^{(2)} = \beta$, $\alpha_y^{(2)} = \alpha$, and $\alpha_u^{(2)} = \sigma$, while, in $(z^{(2)}, \alpha^{(3)})$, the local flavor configuration is changed to $\alpha_x^{(3)} = \alpha$, $\alpha_y^{(3)} = \beta$, and $\alpha_u^{(3)} = \sigma$. $\Gamma^{(3)}$ exchanges the flavors on the bond $\{v, x\}$ without changing the configuration outside $\{v, x\}$

fermions with flavors α , β , and σ in C_l . [See Fig. 5 for an example of a local flavor configuration $(\alpha_x^{(2)}, \alpha_y^{(2)}, \alpha_u^{(2)}, \alpha_v^{(2)})$.]

If α or β equals σ , as depicted in Fig. 5, we can find the sequence $\Gamma^{(3)}$ which connects $(z^{(2)}, \alpha^{(2)})$ to $(z^{(2)}, \alpha^{(3)})$, where $\alpha^{(3)}$ is obtained from $\alpha^{(2)}$ by switching two flavors α and β on a bond in C_l . Then, by tracing the motion of the pair of the hole and the fermion with flavor σ backwards, we find the sequence $\overline{\Gamma^{(2)}}$ such that $(z^{(2)}, \alpha^{(3)}) \leftarrow \overline{\Gamma^{(2)}} \rightarrow (z^{(1)}, \alpha_{x \leftrightarrow y}^{(1)})$. Similarly, we can find the sequence $(z^{(1)}, \alpha_{x \leftrightarrow y}^{(1)}) \leftarrow \overline{\Gamma^{(1)}} \rightarrow (z, \alpha_{x \leftrightarrow y})$ by tracing the hole motion backwards. A desired sequence Γ is then obtained by setting $\Gamma = (\Gamma^{(1)}, \Gamma^{(2)}, \Gamma^{(3)}, \overline{\Gamma^{(2)}}, \overline{\Gamma^{(1)}})$.

If neither α nor β equals σ , we have to find another fermion with flavor σ in a certain loop. Repeating the above argument, we can find $\Gamma^{(4)}$ which connects $(z^{(2)}, \alpha^{(2)})$ to $(z^{(2)}, \alpha^{(4)})$ where the local flavor configuration of $\alpha^{(4)}$ is indicated in Fig. 6. Then, as shown in Fig. 7, we have $(z^{(2)}, \alpha^{(4)}) \leftarrow \Gamma^{(5)} \rightarrow (z^{(2)}, \alpha^{(5)})$, where $\alpha^{(5)}$ is obtained from $\alpha^{(4)}$ by switching two flavors α and β on a bond in C_l . By introducing $\overline{\Gamma^{(4)}}$ in the same manner as above, we find

$$\begin{aligned} (z^{(2)}, \alpha^{(5)}) &\leftarrow (\overline{\Gamma^{(4)}}, \overline{\Gamma^{(2)}}) \rightarrow (z^{(1)}, \alpha_{x \leftrightarrow y}^{(1)}) \\ &\leftarrow \overline{\Gamma^{(1)}} \rightarrow (z, \alpha_{x \leftrightarrow y}), \end{aligned}$$

which gives the desired sequence

$$\Gamma = (\Gamma^{(1)}, \Gamma^{(2)}, \Gamma^{(4)}, \Gamma^{(5)}, \overline{\Gamma^{(4)}}, \overline{\Gamma^{(2)}}, \overline{\Gamma^{(1)}}).$$

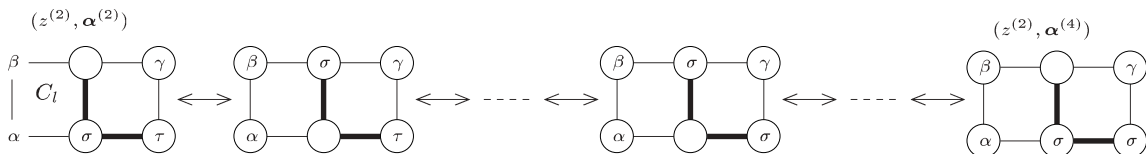


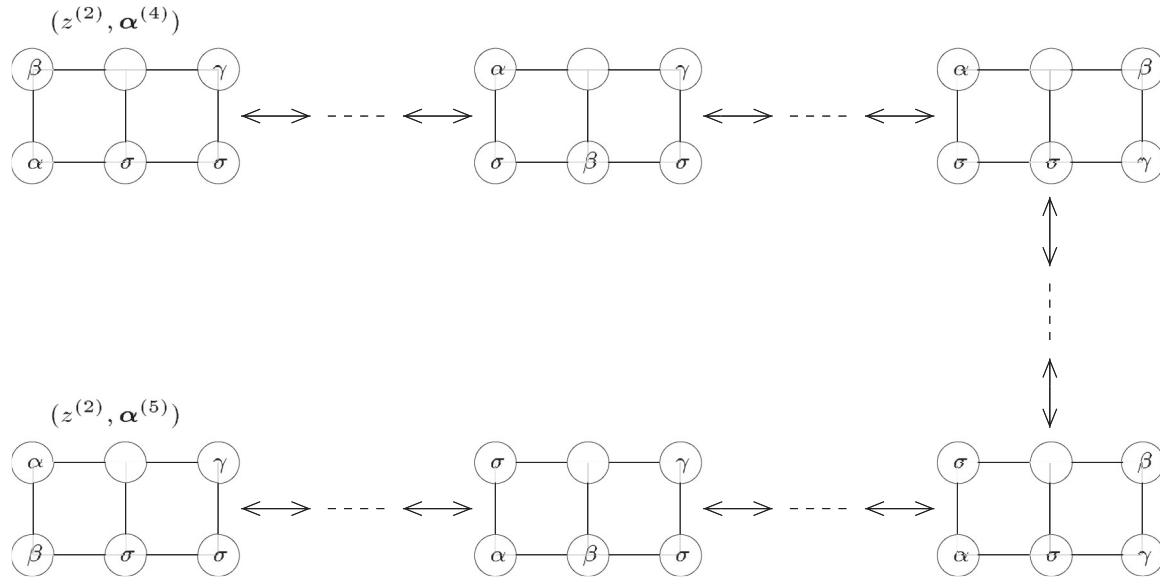
FIG. 6. $\Gamma^{(4)}$ connecting $(z^{(2)}, \alpha^{(2)})$ to $(z^{(2)}, \alpha^{(4)})$. The thick lines represent shared bonds.

V. CONCLUSION AND OUTLOOK

We have presented an extension of Nagaoka's theorem to the infinite- U Hubbard model with $SU(n)$ symmetry. As in the $SU(2)$ case, for the model with one hole, we found that (i) the fully polarized (Nagaoka) states analogous to the ferromagnetic states are ground states; (ii) these Nagaoka states are the only possible ground states if the connectivity condition is satisfied. However, unlike the $SU(2)$ case, here it is not easy to verify the connectivity condition for given n and lattice structure. A simple sufficient condition for the connectivity condition is that the lattice contains at least one triangle loop. We also found a class of lattices consisting of loops of length 4 that satisfy the connectivity condition when the total number of sites N_s is large enough ($N_s \geq n + 2$). Examples include hypercubic lattices in $d \geq 2$ dimensions.

An interesting question is whether the Nagaoka states discussed in the present paper can be detected experimentally. For the $SU(2)$ case, a controllable scheme to detect Nagaoka ferromagnetism in optical superlattices has been proposed [23]. In this scheme, we need to prepare an array of isolated plaquettes each of which consists of four lattice sites with three fermions. The Nagaoka transition and the variation of the total spin in the ground state can then be probed using a band mapping analysis [24] after switching off the superlattice potential.

We now extend the above scheme to the $SU(n)$ case with $n > 2$. Since positive hopping amplitudes are more difficult to achieve experimentally, we focus on the case where the lattice is bipartite and is formed by loops of length 4 (see Sec. IV C). In this case, one needs to prepare an array of clusters

FIG. 7. $\Gamma^{(5)}$ connecting $(z^{(2)}, \alpha^{(4)})$ to $(z^{(2)}, \alpha^{(5)})$.

each of which consists of more than $n + 2$ sites. A simple choice is to take each cluster as a cube with eight lattice sites, which implies that $n \leq 6$. Fortunately, preparation of the SU(6) Hubbard system is feasible in current experiments with ^{173}Yb atoms [7]. Furthermore, an array of cubes can be easily created by superimposing optical lattices with different periodicities. We thus expect that the onset of the Nagaoka states in the SU(n) Hubbard model can be studied experimentally with currently available techniques.

Finally, we remark on the instability of the Nagaoka states. In the standard SU(2) case, one can prove that the Nagaoka states are *not* the ground states for large enough densities of holes by constructing a variational state with one overturned spin which has a lower energy than the Nagaoka states [25–27]. For the model on a square lattice, for example, an extension

of the earlier work yields the best estimate of the critical hole density $\delta_{\text{cr}} = 0.251$, above which the Nagaoka state is unstable [28]. The same variational argument applies to the SU(n) case, because the model in the subspace with $N_1 + N_2 = N_f$ and $N_3 = \dots = N_n = 0$ is described by the SU(2) Hubbard Hamiltonian. Thus we see that the SU(n) Nagaoka states are also unstable with respect to the finite concentration of holes, implying the importance of the precise control of hole densities in a possible realization of the fully polarized states.

ACKNOWLEDGMENTS

We thank Leon Balents and Alexey Gorshkov for stimulating discussions. H.K. was supported in part by Grand-in-Aid for Young Scientists (B) (Grant No. 23740298).

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