Exact hole-induced $SU(N)$ flavor singlets in certain $U = \infty$ $SU(N)$ Hubbard models

Kyung-Su Kim (김경수)[1] and Hosho Katsura (桂法称)[2,3,4]

[1]*Department of Physics, Stanford University, Stanford, California 93405, USA*

[2]*Department of Physics, Graduate School of Science, The University of Tokyo, 7-3-1 Hongo, Tokyo 113-0033, Japan*

[3]*Institute for Physics of Intelligence, The University of Tokyo, 7-3-1 Hongo, Tokyo 113-0033, Japan*

[4]*Trans-scale Quantum Science Institute, The University of Tokyo, 7-3-1, Hongo, Tokyo 113-0033, Japan*

(Received 5 August 2023; revised 15 February 2024; accepted 23 February 2024; published 20 March 2024)

We prove that the motion of a single hole induces $SU(N)$ flavor singlets in the $U = \infty$ $SU(N)$ (Fermi) Hubbard model on a Husimi-like tree graph. The result is generalized to certain t-J models with singlet hopping terms typically neglected in the literature. This is an $SU(N)$ generalization of the "counter-Nagaoka theorem" introduced in [Phys. Rev. B **107**, L140401 (2023)]. Our results suggest the existence of resonating flavor singlet (RFS)-like polarons in the t-J models on a more realistic nonbipartite lattice. Such RFS polarons may be relevant for a novel strong-coupling mechanism of superconductivity or other exotic fractionalized phases of matter.

DOI: 10.1103/PhysRevResearch.6.013307

I. INTRODUCTION

The $SU(2)$ Hubbard model in the presence of a hole doping has been extensively studied as it is expected to capture essential features of the high-temperature superconductivity in cuprate superconductors [1–4]. Despite its deceptively simple form, the model presents significant challenges and complexity due to competing tendencies to develop various types of distinct ordered phases [5]. Even in the strong coupling ($U = \infty$) limit, an analytical solution on a bipartite lattice (e.g., square lattice) exists only for single-hole doping on a finite-sized system—the celebrated "Nagaoka theorem" states that such a system leads to a fully polarized ferromagnet [6–11]. In a physical context, the Nagaoka theorem implies the formation of the ferromagnetic Nagaoka polaron, which has been observed in numerics [12,13] and in cold-atom experiments [14].

On the other hand, it is known that the hole motion in the $U = \infty$ $SU(2)$ Hubbard model on a nonbipartite lattice (e.g., triangular lattice) induces antiferromagnetic correlations around it [15–18]. However, for such a nonbipartite lattice, even the single-hole problem is poorly understood due to the frustration inherent in antiferromagnetism. The problem has been recently solved in a frustration-free version of a nonbipartite lattice, which unambiguously demonstrated that a hole is surrounded by resonating valence bond (RVB)-like correlations [19]. Such a result suggests the formation of an RVB polaron on a more realistic nonbipartite lattice.

For systems with an emergent (or exact) $SU(N)$ symmetry with $N > 2$ [20–25], e.g., systems with degenerate multiple valleys or flavors [26–30], their physics may be characterized by the $SU(N)$ Hubbard model or its generalizations under suitable circumstances. If so, the magnetism at the $\frac{1}{N}$th filling (one fermion per site) in the strong coupling regime, $U \gg t$, is captured by the $SU(N)$ Heisenberg model with exchange interactions $J = 4t^2/U$. However, when $t \gg J$ ($U \to \infty$ limit), it is the motion of a hole that is responsible for the magnetism upon hole doping of such a Mott insulator. Therefore, $SU(N)$ generalizations of the Nagaoka and counter-Nagaoka theorems are needed. In Refs. [31,32], it is shown that, with the "unusual" sign of the hopping matrix element, $t < 0$, a single hole motion in such a $U = \infty$ $SU(N)$ Hubbard model leads to a fully flavor-polarized ground state. However, less is understood for the same problem with the "usual" sign of hopping $t > 0$, again due to the frustration inherent in antiferromagnetism.

In this paper, we study the dynamics of a single hole doped at the $\frac{1}{N}$th filling of the $U = \infty$ $SU(N)$ Hubbard and t-J models on certain solvable graphs. We first consider such a problem on an $(N+1)$-site graph that satisfies the connectivity condition (as defined later), and show that the ground state is in the $SU(N)$ flavor-singlet sector (Sec. II). Any other flavor configurations frustrate the hole motion. From such an $(N+1)$-site subgraph, we construct a subgraph tree, on which the single hole problem in the $SU(N)$ t-J model is exactly solvable (Secs. III and IV). The ground state is a positive superposition of $SU(N)$ flavor-singlet covering states. In Sec. V, we speculate on the possibility of exotic phases of matter in the presence of a dilute but finite hole concentration.

We note that the exact solvability of the single hole problem in a subgraph tree is due to the existence of an extensive number of local $SU(N)$ symmetries—in some sense, this is Hilbert space fragmentation [33–35] from restricted hole motion.

II. $SU(N)$ SINGLET IN AN $(N+1)$-SITE GRAPH

We start by solving a single hole problem in the $U = \infty$ $SU(N)$ Hubbard model ($N \geqslant 2$) on an $(N+1)$-site graph that satisfies the connectivity condition (to be defined below).

We assume that the hopping matrix elements are positive but otherwise arbitrary $t_{ij} > 0$:

$$\hat{H} = -\sum_{\langle i,j\rangle}\sum_{a=1}^{N} t_{ij}(c_{i,a}^{\dagger}c_{j,a} + \text{H.c.}) + \hat{V}(\{n_i\}) + [U = \infty]. \tag{1}$$

Here, $a = 1, 2, ..., N$ is a flavor index of a fermion in the fundamental representation, $i = 0, 1, 2, ..., N$ is a site index, and $\langle i, j\rangle$ is an edge of the graph. $\hat{V}(\{n_i\})$ describes arbitrary on-site terms and density-density interactions ($n_i \equiv \sum_{a=1}^{N} c_{i,a}^{\dagger}c_{i,a}$):

$$V(\{n_i\}) = \sum_i \epsilon_i n_i + \sum_{i,j} V_{ij} n_i n_j + \cdots. \tag{2}$$

The last $U = \infty$ term forbids any double occupancy.

Lemma: The ground state of the Hamiltonian (1) on an $(N + 1)$-site graph that satisfies the connectivity condition in the single hole sector is a unique $SU(N)$ flavor-singlet state.

In order to prove the Lemma, it is convenient to work in a particular many-body basis in a single hole sector. In doing so, we restrict ourselves to a flavor-balanced subspace, where each flavor $a = 1, 2, ..., N$ appears exactly once [36]. For example,

$$\begin{aligned}|\cdot, 1, 2, ..., N\rangle &\equiv c_{1,1}^{\dagger}c_{2,2}^{\dagger}\cdots c_{N,N}^{\dagger}|\emptyset\rangle \equiv |0, 1, ..., N\rangle \\ &\equiv c_{0,0}c_{0,0}^{\dagger}c_{1,1}^{\dagger}c_{2,2}^{\dagger}\cdots c_{N,N}^{\dagger}|\emptyset\rangle \end{aligned} \tag{3}$$

is a flavor-balanced state, where $|\emptyset\rangle$ is the vacuum state with no fermions, and 0 in the third expression denotes that the site $i = 0$ is unoccupied. This can be reexpressed as the final expression by creating a ghost fermion with flavor $a = 0$ at the hole site and annihilating it. This is a useful notation that will be used throughout the paper. From this state, we form a complete orthonormal basis in a flavor-balanced subspace by applying a permutation of $(N + 1)$ objects (a hole and N fermions), $\sigma \in S_{N+1}$, where S_{N+1} is the symmetric group of $(N + 1)$ objects:

$$\begin{aligned}|\sigma\rangle &\equiv |\sigma(0), \sigma(1), ..., \sigma(N)\rangle \equiv (-1)^{i}\text{sgn}(\sigma)c_{0,\sigma(0)}^{\dagger}c_{1,\sigma(1)}^{\dagger} \\ &\quad\times\cdots\times c_{i-1,\sigma(i-1)}^{\dagger}c_{i+1,\sigma(i+1)}^{\dagger}\cdots c_{N,\sigma(N)}^{\dagger}|\emptyset\rangle \\ &\equiv \text{sgn}(\sigma)c_{i,0}c_{0,\sigma(0)}^{\dagger}c_{1,\sigma(1)}^{\dagger}\cdots c_{N,\sigma(N)}^{\dagger}|\emptyset\rangle, \end{aligned} \tag{4}$$

where we assumed that the ith site is occupied by a hole, i.e., $\sigma(i) = 0$, and again we introduced a ghost fermion with flavor $a = 0$ in the last expression for convenience.

Among the states in the flavor-balanced subspace are the completely flavor-antisymmetric, $SU(N)$ flavor-singlet (FS) states with the hole at site i,

$$|i, \text{FS}\rangle \equiv \frac{1}{\sqrt{N!}}\sum_{\sigma\in S_{N+1}, \sigma^{-1}(0)=i} |\sigma(0), \sigma(1), ..., \sigma(N)\rangle. \tag{5}$$

Connectivity condition: An $(N + 1)$-site graph is said to satisfy the connectivity condition if all the basis states in Eq. (4) can be reached from one another by repeated applications of hopping operators in Eq. (1), $\hat{T}_{ij} \equiv -t_{ij}\sum_{a=1}^{N}(c_{i,a}^{\dagger}c_{j,a} + \text{H.c.})$. For example, Figs. 1(a)–1(c) are examples of graphs that satisfy the connectivity condition. In particular, in Fig. 1(c), starting from the state $|0, 1, 2, ..., N\rangle$,

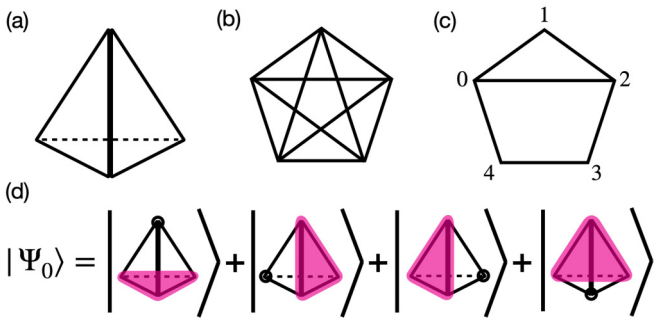

FIG. 1. (a), (b) Examples of a complete graph with fully connected edges. (c) An example of a noncomplete graph which nevertheless satisfies the connectivity condition. (d) The ground state of the $U = \infty$ $SU(3)$ Hubbard model in the presence of a single hole on a tetrahedron with uniform $t_{ij} = t$ and $\hat{V} = 0$ in Eq. (1). Magenta trimers denote $SU(3)$ flavor singlets, i.e., three fermions with complete flavor antisymmetry, and circles denote the location of the hole. The signs associated with the many-body states appearing in $|\Psi_0\rangle$ are defined implicitly in Eq. (5).

moving a hole around the triangular loop induces a transposition (1 2) and moving it around the largest, length $(N + 1)$, loop induces the N cycle $(1, 2, \ldots, N)$. These two permutations, together with hopping operations, generate S_{N+1}. More generally, Theorem 2 of Ref. [32] provides the sufficient condition for the connectivity condition.

Proof of the Lemma: Any two basis states in the flavor-balanced subspace, $|\sigma\rangle$ and $|\tau\rangle$, have a nonzero hopping matrix element only when they differ by one transposition involving a hole: $\sigma^{-1}(0) = \tau^{-1}(a)$ and $\tau^{-1}(0) = \sigma^{-1}(a)$ for some flavor a, and $\sigma^{-1}(k) = \tau^{-1}(k)$ for $k \neq 0, a$. Let $\sigma^{-1}(0) = i$ and $\tau^{-1}(0) = j$. Any such nonzero off-diagonal matrix element is negative:

$$\langle\sigma|\hat{T}_{ij}|\tau\rangle = -t_{ij} < 0. \tag{6}$$

Also, the interaction term $V(\{n_i\})$ only contributes to diagonal matrix elements. Therefore, the Perron-Frobenius theorem ensures that there exists a unique ground state $|\Psi_0\rangle$ which is a positive superposition of all the basis states ($A_\sigma > 0$):

$$|\Psi_0\rangle = \sum_{\sigma\in S_{N+1}} A_\sigma|\sigma\rangle. \tag{7}$$

Since this state has a nonzero overlap with a flavor-singlet state $|i, \text{FS}\rangle$, it must be a flavor-singlet state [if it were instead a superposition of multiple irreps of $SU(N)$, then it is possible to construct degenerate ground states, in contradiction to the uniqueness of the ground state]. Therefore, it is possible to rewrite Eq. (7) as a positive superposition ($A(i) > 0$) of $|i, \text{FS}\rangle$:

$$|\Psi_0\rangle = \sum_i A(i)|i, \text{FS}\rangle. \tag{8}$$

See Fig. 1(d) for the illustration of such a state. ■

III. $SU(N)$ FLAVOR-SINGLETS IN A SUBGRAPH TREE

It is now straightforward to generalize the previous result to a "subgraph tree" constructed as follows. Starting from an

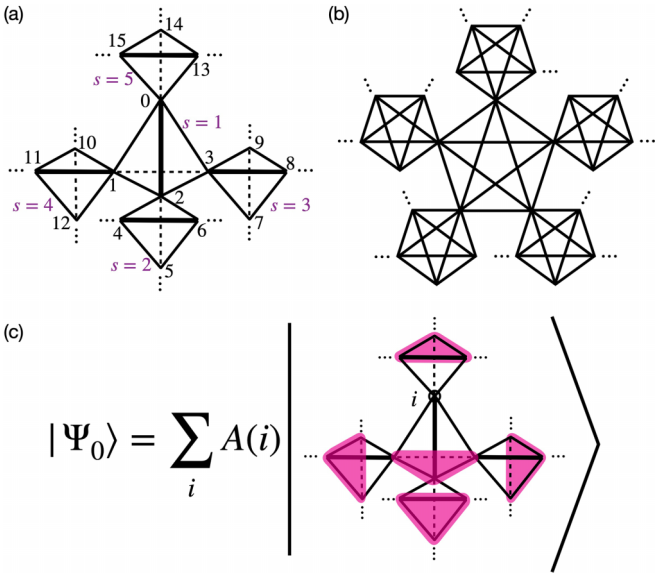

FIG. 2. (a), (b) Examples of subgraph tree. In (a), sites are numbered in the way specified in the main text above Eq. (9). (c) The ground state in the single hole sector of the $U=\infty$ $SU(3)$ Hubbard [Theorem] and certain t-J models [Corollary 2] is a positive ($A(i)>0$) superposition of the $SU(3)$ flavor-singlet covering states.

$(N+1)$-site subgraph that satisfies the connectivity condition, we attach other $(N+1)$-site subgraphs to some (or all) of the vertices of the initial subgraph, in such a way that it does not create any other cycles (loops of length $l \geqslant 3$ in which only the first and the last vertices are equal) than those contained within each subgraph. This generates depth 1 tree of $(N+1)$-site subgraph. Continuing this n times will generate a depth n subgraph tree, which has the property that all the cycles of the graph are contained within each subgraph. Let $N_{\rm SG}$ be the number of subgraphs constituting such a subgraph tree. The number of sites in such a graph is $NN_{\rm SG}+1$. Figures 2(a) and 2(b) are examples of such graphs. We will consider the Hamiltonian (1) on such a graph in the presence of a single hole.

The advantage of such a subgraph tree is that there is an $SU(N)$ symmetry associated with each subgraph, as can be seen as follows [37]. First, a many-body basis can be constructed by locating the site of the hole i, and then specifying the flavor configuration on the rest of the sites. Once the hole location is specified, it is easy to see that there is a unique N-mer covering of the lattice [see Fig. 2(c) for the illustration of such a covering]. In any step in which the hole hops to a neighboring site, one N-mer is moved, but in such a way that it remains inside the initial $(N+1)$-site subgraph in which it was contained. Thus, we can label the N-mers uniquely by a subgraph index $s=1,...,N_{\rm SG}$, and the total flavor $SU(N)$ symmetry is preserved for N fermions contained in each s N-mer. That is, there exists $SU(N)^{N_{\rm SG}} = SU(N)\otimes SU(N)\otimes\cdots\otimes SU(N)$ symmetry.

Thanks to such $SU(N)^{N_{\rm SG}}$ symmetry, it is enough to consider a subspace that is flavor balanced in each s N-mer. Any other states in the Hilbert space can be reached by repeated applications of raising and lowering operators on each s N-mer. (see Appendix B for the expression of those raising/lowering operators). We now construct a many-body basis restricted in such a flavor-balanced subspace analogously to Eqs. (3) and (4). We first occupy a hole at a particular location (call it $i=0$), which will define a unique N-mer covering as discussed above. For each s N-mer, we label the sites contained in it by $i=(s-1)N+1,\ (s-1)N+2,\cdots,\ sN$ [see Fig. 2(a) for the illustration of such a site numbering scheme along with subgraph indices s] and occupy it with fermions with flavors $a=1,\cdots,N$, respectively. This defines one basis state

$$\begin{aligned}&|0,(1,...,N),(1,...,N),...,(1,...,N)\rangle\\ &\equiv c_{0,0}c^\dagger_{0,0}(c^\dagger_{1,1}c^\dagger_{2,2}\cdots c^\dagger_{N,N})(c^\dagger_{N+1,1}\cdots c^\dagger_{2N,N})\\ &\quad\times\cdots\times\left(c^\dagger_{N\cdot(N_{\rm SG}-1)+1,1}\cdots c^\dagger_{N\cdot N_{\rm SG},N}\right)|\emptyset\rangle,\end{aligned}\tag{9}$$

where again, the ghost flavor index $a=0$ is introduced for convenience in $c_{0,0}$. Using the fact that fermions in different N-mers do not exchange one another due to the restricted dynamics of a hole, we might as well treat them as distinguishable and rename a flavor index a in s N-mer to be $(s-1)N+a$. Hence, the basis state (9) can be denoted by

$$\begin{aligned}&|0,1,...,N,N+1...,...,N\cdot N_{\rm SG}\rangle\\ &\equiv c_{0,0}c^\dagger_{0,0}(c^\dagger_{1,1}c^\dagger_{2,2}\cdots c^\dagger_{N,N})(c^\dagger_{N+1,N+1}\cdots c^\dagger_{2N,2N})\\ &\quad\times\cdots\times\left(c^\dagger_{N(N_{\rm SG}-1)+1,N(N_{\rm SG}-1)+1}\cdots c^\dagger_{NN_{\rm SG},NN_{\rm SG}}\right)|\emptyset\rangle.\end{aligned}\tag{10}$$

From this state, any other basis state that is flavor balanced for each s N-mer can be reached by repeated applications of hopping operators $\hat{T}_{ij}$. There are $(NN_{\rm SG}+1)(N!)^{N_{\rm SG}}$ different such (orthonormal) basis states. Each such basis state has a permutation operator $\sigma\in S_{NN_{\rm SG}+1}$ associated with it defined as a relative flavor configuration from the initial one in Eq. (10): if site i is occupied by the flavor a, then $\sigma(i)\equiv a$. (We emphasize that flavor indices are renamed to have values $a=0,1,...,NN_{\rm SG}$). Let P be the collection of all such permutations σ. We define the basis states $\{|\sigma\rangle:\ \sigma\in P\}$ with a particular sign structure analogous to Eq. (4):

$$\begin{aligned}|\sigma\rangle &\equiv |\sigma(0),...,\sigma(NN_{\rm SG})\rangle \equiv (-1)^i{\rm sgn}(\sigma)c^\dagger_{0,\sigma(0)}c^\dagger_{1,\sigma(1)}\\ &\quad\times\cdots\times c^\dagger_{i-1,\sigma(i-1)}c^\dagger_{i+1,\sigma(i+1)}\cdots c^\dagger_{NN_{\rm SG},\sigma(NN_{\rm SG})}|\emptyset\rangle\\ &={\rm sgn}(\sigma)c_{i,0}c^\dagger_{0,\sigma(0)}c^\dagger_{1,\sigma(1)}\cdots c^\dagger_{NN_{\rm SG},\sigma(NN_{\rm SG})}|\emptyset\rangle,\end{aligned}\tag{11}$$

where we again assumed that the ith site is occupied by a hole, i.e., $\sigma(i)=0$. The sign structure again allows us to write the $SU(N)$ flavor-singlet covering (FSC) state, the state with an $SU(N)$ flavor-singlet on every N-mer, as a uniform superposition of the basis states that have their hole at site i:

$$\begin{aligned}|i,{\rm FSC}\rangle &\equiv |i,{\rm FS}_1,\cdots,{\rm FS}_{N_{\rm SG}}\rangle\\ &=\frac{1}{\sqrt{(N!)^{N_{\rm SG}}}}\sum_{\substack{\sigma\in P\\ \sigma(i)=0}}|\sigma(0),\sigma(1),...,\sigma(NN_{\rm SG})\rangle.\end{aligned}\tag{12}$$

The following theorem is the main result of our paper.

Theorem: The ground state of the Hamiltonian (1) on a "subgraph tree" in the single hole sector is unique and is a

positive [$A(i) > 0$] superposition of the $SU(N)$ flavor-singlet covering (FSC) states [38]:

$$|\Psi_0\rangle = \sum_i A(i)|i, \mathrm{FSC}\rangle \tag{13}$$

[See Fig. 2(c) for an illustration of this state].

Proof of the Theorem: It is straightforward to show that any nonzero off-diagonal element of the Hamiltonian matrix is negative, $\langle\sigma|\hat{T}_{ij}|\tau\rangle = -t_{ij} < 0$, as in Eq. (6). Also, since any basis state $|\sigma\rangle$ can be reached from one another by repeated applications of $\hat{T}_{ij}$, one concludes from the Perron-Frobenius theorem that the ground state is unique and is a positive ($A_\sigma > 0$) superposition of all the basis states

$$|\Psi_0\rangle = \sum_{\sigma\in P} A_\sigma|\sigma\rangle. \tag{14}$$

This has a positive overlap with a flavor-singlet covering state $|i, \mathrm{FSC}\rangle$, and hence N fermions in every N-mer must be a flavor singlet. Hence, $|\Psi_0\rangle$ can be rewritten as a superposition of flavor-singlet covering states as in Eq. (13). ■

In Fig. 3 of Appendix A, we show the result of the finite size exact diagonalization study on the $SU(3)$ $U = \infty$ Hubbard model on the four-tetrahedron geometry. The result agrees with the Theorem.

IV. $SU(N)$ t-J MODEL

Now we generalize the previous results to the $SU(N)$ t-J model. In the presence of a finite but large U ($\gg t$) term, $\frac{U}{2}\sum_i \hat{n}_i(\hat{n}_i - 1)$, one can obtain the $SU(N)$ t-J model from the $SU(N)$ Hubbard model by projecting out the states with multiply occupied sites [39–41]:

$$\begin{aligned}\hat{H}_{t\text{-}J} &= \hat{H} + \sum_{\langle i,j\rangle} J_{ij}\left(\hat{\boldsymbol{\lambda}}_i\cdot\hat{\boldsymbol{\lambda}}_j - \frac{N-1}{2N}\hat{n}_i\hat{n}_j\right) \\ &\quad - \sum_{\langle i,j,k\rangle}\sum_{1\leqslant a<b\leqslant N} K_{ijk}\hat{\Delta}^{ab\dagger}_{jk}\hat{\Delta}^{ab}_{ij} + O\left(\frac{t^3}{U^2}\right) \\ &\equiv \hat{H} + \sum_{\langle i,j\rangle}\hat{J}_{ij} + \sum_{\langle i,j,k\rangle}\hat{K}_{ijk} + O\left(\frac{t^3}{U^2}\right).\end{aligned} \tag{15}$$

Here $\hat{H}$ is the Hamiltonian for the $U = \infty$ Hubbard model (1), $J_{ij} = 4t_{ij}^2/U$ and $K_{ijk} = 2t_{ij}t_{jk}/U$, $\langle i, j, k\rangle$ denotes the triplet of sites such that j is a nearest neighbor to i and k, and $\hat{\Delta}^{ab}_{ij} \equiv \frac{1}{\sqrt{2}}(c_{i,a}c_{j,b} - c_{i,b}c_{j,a})$ is the annihilation operator of a flavor-antisymmetric state on a bond $\langle i, j\rangle$. $\hat{\boldsymbol{\lambda}}_i = (\hat{\lambda}_i^{(1)}, ..., \hat{\lambda}_i^{(N^2-1)})$ denotes $(N^2 - 1)$ generators of the $SU(N)$ group at site i with the normalization $\mathrm{Tr}(\lambda_i^{(r)}\lambda_j^{(r')}) = \frac{1}{2}\delta_{r,r'}\delta_{i,j}$ [42]. The Heisenberg operator can be rewritten in terms of a flavor-permutation operator $\hat{P}_{ij}$ as $J_{ij}(\hat{\boldsymbol{\lambda}}_i\cdot\hat{\boldsymbol{\lambda}}_j - \frac{N-1}{2N}\hat{n}_i\hat{n}_j) = \frac{1}{2}J_{ij}(\hat{P}_{ij} - \hat{\mathbb{1}})\hat{n}_i\hat{n}_j$. In the last line, we defined $\hat{J}_{ij} \equiv J_{ij}(\hat{\boldsymbol{\lambda}}_i\cdot\hat{\boldsymbol{\lambda}}_j - \frac{N-1}{2N}\hat{n}_i\hat{n}_j)$ and $\hat{K}_{ijk} \equiv K_{ijk}\sum_{1\leqslant a<b\leqslant N}\hat{\Delta}^{ab\dagger}_{jk}\hat{\Delta}^{ab}_{ij}$. The following two corollaries generalize the Lemma and the Theorem to certain t-J models.

Corollary 1: Let us define $\hat{H}_{t\text{-}J}$ on an $(N + 1)$-site graph that satisfies the connectivity condition. $J_{ij} \geqslant 0$ and $K_{ijk} \geqslant 0$ do not have to be related to one another and can be arbitrary independent parameters. Then, the ground state of $\hat{H}_{t\text{-}J}$ in the presence of a single hole is unique and is a positive superposition of flavor-singlet states (8) as in the Lemma.

Corollary 2: For $\hat{H}_{t\text{-}J}$ defined on a subgraph tree, let $J_{ij} = J_s \geqslant 0$ be uniform within each subgraph and connect any two sites within it. Also, let $K_{ijk} \geqslant 0$ terms act only on three sites $\langle i, j, k\rangle$ fully contained within a subgraph. Again, J_{ij} and K_{ijk} can be independent parameters, except for the above constraints. Then, the ground state of $\hat{H}_{t\text{-}J}$ in the presence of a single hole is unique and is a positive superposition of flavor-singlet covering states (13) as in the Theorem [43].

Proof of Corollary 1: For a single hole problem in an $(N + 1)$-site graph, the total $SU(N)$ symmetry is intact even in the presence of $\hat{J}$ and $\hat{K}$ terms, and one can work in the flavor-balanced basis (4). Again, it is then sufficient to show that all the nonzero off-diagonal matrix elements are negative. In particular, for $\sigma \neq \tau$, $\langle\sigma|\hat{J}_{ij}|\tau\rangle$ is nonzero only when σ and τ differ by one transposition between occupied sites: $\sigma(i) = \tau(j) \neq 0$, $\sigma(j) = \tau(i) \neq 0$, and $\sigma(k) = \tau(k)$ for $k \neq i, j$. In such a case, one obtains

$$\langle\sigma|\hat{J}_{ij}|\tau\rangle = -J_{ij}/2 < 0. \tag{16}$$

Similarly, any nonzero off-diagonal element of $\hat{K}_{ijk}$ is negative:

$$\langle\sigma|\hat{K}_{ijk}|\tau\rangle = -K_{ijk}/2 < 0. \tag{17}$$

This completes the proof. ■

Proof of Corollary 2: For a subgraph tree, consider first the case when $\hat{J} = 0$. When K_{ijk} are nonzero only for triplets of sites $\langle i, j, k\rangle$ fully contained in a subgraph, $SU(N)^{N_{\mathrm{SG}}}$ symmetry is intact. Thus, one can still work in the flavor-balanced basis (11) and the same proof as in the Theorem can be applied.

When $\hat{J} \neq 0$, the $SU(N)^{N_{\mathrm{SG}}}$ symmetry is lost. However, for the special case where $J_{ij} = J_s$ is uniform within each subgraph and connects any two sites within it, one can rewrite the Heisenberg term as [density-density interactions in $\hat{J}$ can be absorbed in $\hat{V}$ term in Eq. (1)]:

$$\sum_{\langle i,j\rangle} J_{ij}\hat{\boldsymbol{\lambda}}_i\cdot\hat{\boldsymbol{\lambda}}_j = \sum_{s=1}^{N_{\mathrm{SG}}}\frac{J_s}{2}\left[\left(\sum_{i=1}^{N+1}\hat{\boldsymbol{\lambda}}_{(s,i)}\right)^2 - \sum_{i=1}^{N+1}\hat{\boldsymbol{\lambda}}^2_{(s,i)}\right]. \tag{18}$$

Here (s, i) denotes the site $i = 1, 2, ..., N + 1$ in a subgraph s. This Heisenberg operator takes the lowest possible eigenvalue for the flavor-singlet covering states (12):

$$\sum_{\langle k,l\rangle} J_{kl}\hat{\boldsymbol{\lambda}}_k\cdot\hat{\boldsymbol{\lambda}}_l|i, \mathrm{FSC}\rangle = -\frac{N^2-1}{4}\sum_{s=1}^{N_{\mathrm{SG}}} J_s|i, \mathrm{FSC}\rangle. \tag{19}$$

This means that the ground state of $\hat{H}_{t\text{-}J}$ is still in the flavor-singlet covering subspace spanned by states (12) and is of the form Eq. (13) with positive $A(i) > 0$. ■

V. DISCUSSION

Our result demonstrates the fundamental importance of the sign of the hopping matrix elements t_{ij} on a kinetic magnetism of the Hubbard model, which in turn manifests as a particle-hole asymmetry in the magnetic phase diagram. More precisely, in the usual $SU(2)$ Hubbard model, the particle-hole transformation $c_{i,\sigma} \to c^\dagger_{i,\sigma}$, with $\sigma = \uparrow, \downarrow$, maps the single doublon problem to the single hole problem with the opposite

sign of t_{ij} [4]. This implies that for a bipartite lattice—where the sign of t_{ij} can be changed by a gauge transformation—the phase diagram is particle-hole symmetric around half-filling. On the other hand, for a nonbipartite lattice the phase diagram exhibits a particle-hole asymmetry. For example, the single hole dynamics in the triangular lattice $U = \infty$ Hubbard model leads to a 120° antiferromagnetic ordering [16,17], whereas the single doublon problem satisfies the Nagaoka theorem and leads to a fully polarized ferromagnet (except for one singlet for a doublon). Performing such a particle-hole transformation to the $SU(N)$ Hubbard model, one maps a single hole problem at $1/N$ filling to a single N-on (N fermions at a site) problem at $(N-1)/N$ filling with the opposite sign of t_{ij}. Since $(N-1)$ fermions at the same site must be completely flavor antisymmetric, such $N-1$ electrons form a complex conjugate representation $\bar{N}$ of the fundamental representation. Hence, we see that with the usual sign of the hopping $t_{ij} > 0$, while the Nagaoka ferromagnetic state appears for a single fermion doping of the $(N-1)/N$ filled Mott insulator, a single hole doping at $1/N$ filling generically induces antiferromagnetism.

We note that in a more realistic nonbipartite lattice (e.g., a triangular or pyrochlore lattice), it is likely that the hopping operators $\hat{T}$ and exchange interactions $\hat{J}$ (or singlet hopping terms $\hat{K}$) favor different local magnetic correlations. In such a case, the hole can only delocalize in a finite number of sites, leading to the formation of an RVB polaron.

Going from such a single RVB/RFS polaron problem to a multipolaron (or multihole) problem requires yet another technical development, but we can speculate on possible outcomes (apart from a trivial phase separation scenario). First, it is possible to have a broken-$SU(N)$-symmetry phase with a long-range flavor-antiferromagnetic order when flavor singlets are supported over a sufficiently long distance [16–18,44]. When $SU(N)$ flavorsinglets are supported on sufficiently short distances, one can have a flavor-disordered phase with topological order [45–49]. The flavor-disordered state with a broken translation symmetry corresponds to various topologically ordered crystalline phases [50,51]. Finally, it is possible to have various exotic liquid phases with a topological character such as a $\mathbb{Z}_N$ topologically ordered Fermi liquid (FL* phase) [52] or high-temperature superconductivity.

ACKNOWLEDGMENTS

K.S.K. would like to acknowledge the hospitality of the Massachusetts Institute of Technology, where the majority of this work was done. K.S.K. appreciates Samuel Alipourfard, Zhaoyu Han, and Pavel Nosov for helpful discussions. K.S.K. also thanks Aidan Reddy for valuable discussions on the exact diagonalization method. H.K. would like to thank Tadahiro Miyao for useful comments on the manuscript. K.S.K. was supported by the Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering, under contract DE-AC02-76SF00515. H.K. was supported by JSPS KAKENHI Grants No. JP18K03445, No. JP23H01093, No. 23H01086, and MEXT KAKENHI Grant-in-Aid for Transformative Research Areas A "Extreme Universe" (KAKENHI Grant No. JP21H05191).

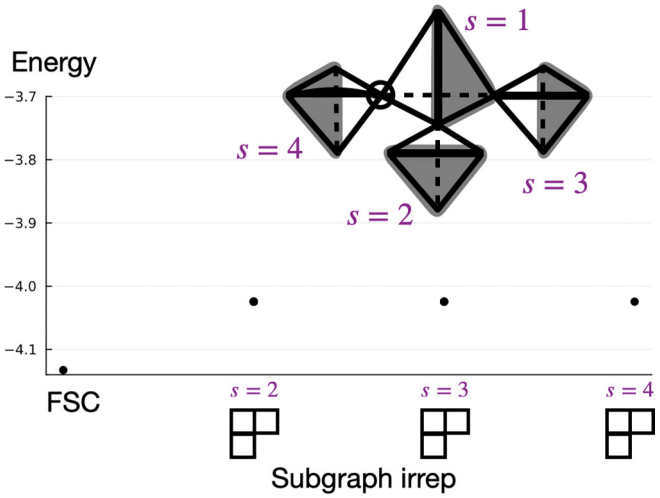

FIG. 3. Ground state and several first excited states of $SU(3)$ $U = \infty$ Hubbard model on the four-tetrahedron geometry. The horizontal axis denotes the Young diagram corresponding to the irrep of the $SU(3)$ group of the trimer (shown in gray) in the specified subgraph s. The three first excited states shown are the ones that have adjoint representation in $s = 2, 3, 4$ trimer, respectively; trimers in the subgraphs that are not specified are $SU(3)$ singlets. FSC is the sector which has $SU(3)$ singlet on every trimer. The ground state is of the form Eq. (13) and has the same energy as the noninteracting problem with the same hopping matrix elements, $E_{\mathrm{GS}} = -4.1326383$.

APPENDIX A: EXACT DIAGONALIZATION RESULT

In order to demonstrate the result of our main Theorem, we performed exact diagonalization calculation on the $SU(3)$ $U = \infty$ Hubbard model in the single-hole sector on a four-tetrahedron geometry as shown in Fig. 3 (13 sites; shown in the inset). Hopping matrix elements are set to $t_{ij} = 1$ for all bonds. The ground state is the positive superposition of $SU(3)$ flavor-singlet covering states, consistent with the result of the Theorem.

APPENDIX B: RAISING AND LOWERING OPERATORS

The local $SU(N)$ symmetry on each subgraph of the $U = \infty$ $SU(N)$ Hubbard model in the single-hole sector allows one to define raising and lowering operators on each s N-mer. Such operators for the $SU(2)$ case in terms of fermionic operators can be written as follows:

$$\hat{\mathbb{S}}_s^{\pm} = \sum_{i\in\mathcal{V}_1} \hat{h}_i \left(\prod_{j\notin\{i,2,3\}} \hat{n}_j \right) \hat{S}^{\pm}_{(23)} + \sum_{i\in\mathcal{V}_2} \hat{h}_i \left(\prod_{j\notin\{i,1,3\}} \hat{n}_j \right) \hat{S}^{\pm}_{(31)} + \sum_{i\in\mathcal{V}_3} \hat{h}_i \left(\prod_{j\notin\{i,1,2\}} \hat{n}_j \right) \hat{S}^{\pm}_{(12)}. \tag{B1}$$

Here $\hat{h}_i = 1 - \hat{n}_i$ is the hole number operator at site i and $\hat{S}^{\pm}_{(ij)}$ is the raising/lowering operator of the total spin of two fermions at sites i and j.$\mathcal{V}_{1,2,3}$ are the set of sites defined in Fig. 4. The operator $\hat{\mathbb{S}}_s^{\pm}$ is defined for every $s = 1, \ldots, N_{\mathrm{SG}}$. In the single hole sector, it is straightforward to show that they

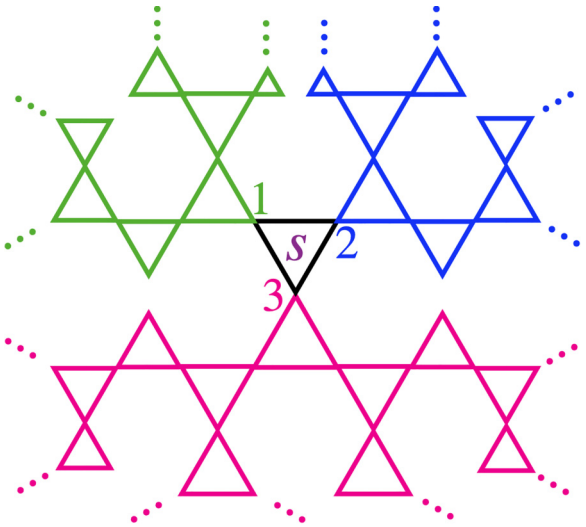

FIG. 4. One can classify sites according to the index of a branch stemming from sth subgraph. Green, blue, and magenta sites are in the first, second, and third branches of the s subgraph. The set of all sites contained in each branch can be denoted by $\mathcal{V}_1$, $\mathcal{V}_2$, and $\mathcal{V}_3$. $\mathcal{V}_1 \cup \mathcal{V}_2 \cup \mathcal{V}_3$ is the set of all sites in the graph.

commute with the hopping operators and number operators, and hence, with the Hamiltonian $\hat{H}$ (1) of the main text

$$\begin{aligned}\hat{P}_{\hat{N}_h=1}[\hat{\mathbb{S}}_s^{\pm}, \hat{T}_{ij}]\hat{P}_{\hat{N}_h=1} &= 0,\\ \hat{P}_{\hat{N}_h=1}[\hat{\mathbb{S}}_s^{\pm}, \hat{n}_i]\hat{P}_{\hat{N}_h=1} &= 0,\\ \hat{P}_{\hat{N}_h=1}[\hat{\mathbb{S}}_s^{\pm}, \hat{H}]\hat{P}_{\hat{N}_h=1} &= 0 \quad \forall s.\end{aligned} \tag{B2}$$

Here, $\hat{P}_{\hat{N}_h=1}$ is the projection to the single hole sector and $\hat{T}_{ij}$ is the electron hopping operator defined in the main text: $\hat{T}_{ij} \equiv -t_{ij}\sum_{a=1}^{N}(c_{i,a}^{\dagger}c_{j,a} + \text{H.c.})$. Note that "local" raising/lowering operators $\hat{\mathbb{S}}_s^{\pm}$ become nonlocal in terms of fermion operators.

APPENDIX C: DERIVATION OF EQ. (19)

Here, we show that the smallest eigenvalue of the following operator defined for each subgraph is $-\frac{N^2-1}{2}$ when the number of electrons is N or $N+1$:

$$\left(\sum_{i=1}^{N+1}\hat{\boldsymbol{\lambda}}_i\right)^2 - \sum_{i=1}^{N+1}(\hat{\boldsymbol{\lambda}}_i)^2. \tag{C1}$$

$\hat{\boldsymbol{\lambda}}_i \equiv \sum_{a,b=1}^{N} c_{i,a}^{\dagger}[\boldsymbol{\lambda}_i]_{a,b}c_{i,b}$ are $SU(N)$ generators in the fundamental representation in terms of fermion operators with normalization $\mathrm{Tr}(\lambda_i^{(r)}\lambda_j^{(r')}) = \frac{1}{2}\delta_{r,r'}\delta_{i,j}$. First, when the number of fermions is $N+1$, every site of the subgraph is occupied, so $(\hat{\boldsymbol{\lambda}}_i)^2 = \frac{N^2-1}{2N}\cdot\hat{\mathbb{1}}$. Also, the Casimir operator has the smallest eigenvalue when N of the fermions form a singlet [i.e., when $N+1$ fermions form a fundamental representation of $\sum_{i=1}^{N+1}\hat{\boldsymbol{\lambda}}_i$], so that $(\sum_{i=1}^{N+1}\hat{\boldsymbol{\lambda}}_i)^2 = \frac{N^2-1}{2N}\cdot\hat{\mathbb{1}}$. In such a case, $(\sum_{i=1}^{N+1}\hat{\boldsymbol{\lambda}}_i)^2 - \sum_{i=1}^{N+1}(\hat{\boldsymbol{\lambda}}_i)^2 = -\frac{N^2-1}{2}\cdot\hat{\mathbb{1}}$.

On the other hand, when the number of fermions is N, $(\sum_{i=1}^{N+1}\hat{\boldsymbol{\lambda}}_i)^2$ has the smallest eigenvalue, zero, when they form an $SU(N)$ singlet. Again, this implies $(\sum_{i=1}^{N+1}\hat{\boldsymbol{\lambda}}_i)^2 - \sum_{i=1}^{N+1}(\hat{\boldsymbol{\lambda}}_i)^2 = -\frac{N^2-1}{2}\cdot\hat{\mathbb{1}}$.

[1] P. W. Anderson, The resonating valence bond state in La_2CuO_4 and superconductivity, Science **235**, 1196 (1987).

[2] P. A. Lee, N. Nagaosa, and X.-G. Wen, Doping a Mott insulator: Physics of high-temperature superconductivity, Rev. Mod. Phys. **78**, 17 (2006).

[3] B. Keimer, S. A. Kivelson, M. R. Norman, S. Uchida, and J. Zaanen, From quantum matter to high-temperature superconductivity in copper oxides, Nature (London) **518**, 179 (2015).

[4] D. P. Arovas, E. Berg, S. A. Kivelson, and S. Raghu, The Hubbard model, Annu. Rev. Condens. Matter Phys. **13**, 239 (2022).

[5] E. Fradkin, S. A. Kivelson, and J. M. Tranquada, *Colloquium*: Theory of intertwined orders in high temperature superconductors, Rev. Mod. Phys. **87**, 457 (2015).

[6] Y. Nagaoka, Ferromagnetism in a narrow, almost half-filled s band, Phys. Rev. **147**, 392 (1966).

[7] H. Tasaki, Extension of Nagaoka's theorem on the large-U Hubbard model, Phys. Rev. B **40**, 9192 (1989).

[8] P. Fazekas, Lecture notes on electron correlation and magnetism, (World scientific, Budapest, 1999).

[9] H. Tasaki, Physics and mathematics of quantum many-body systems, (Springer, Tokyo, 2020).

[10] J. von Stecher, E. Demler, M. D. Lukin, and A. M. Rey, Probing interaction-induced ferromagnetism in optical superlattices, New J. Phys. **12**, 055009 (2010).

[11] J. P. Dehollain, U. Mukhopadhyay, V. P. Michal, Y. Wang, B. Wunsch, C. Reichl, W. Wegscheider, M. S. Rudner, E. Demler, and L. M. Vandersypen, Nagaoka ferromagnetism observed in a quantum dot plaquette, Nature (London) **579**, 528 (2020).

[12] L. Liu, H. Yao, E. Berg, S. R. White, and S. A. Kivelson, Phases of the infinite U Hubbard model on square lattices, Phys. Rev. Lett. **108**, 126406 (2012).

[13] S. R. White and I. Affleck, Density matrix renormalization group analysis of the Nagaoka polaron in the two-dimensional t-J model, Phys. Rev. B **64**, 024411 (2001).

[14] J. Koepsell, J. Vijayan, P. Sompet, F. Grusdt, T. A. Hilker, E. Demler, G. Salomon, I. Bloch, and C. Gross, Imaging magnetic polarons in the doped Fermi–Hubbard model, Nature (London) **572**, 358 (2019).

[15] K. Takano and K. Sano, Origin of resonating-valence-bond states for a Hubbard-type model, Phys. Rev. B **39**, 7367 (1989).

[16] J. O. Haerter and B. S. Shastry, Kinetic antiferromagnetism in the triangular lattice, Phys. Rev. Lett. **95**, 087202 (2005).

[17] C. N. Sposetti, B. Bravo, A. E. Trumper, C. J. Gazza, and L. O. Manuel, Classical antiferromagnetism in kinetically frustrated electronic models, Phys. Rev. Lett. **112**, 187204 (2014).

[18] Z. Zhu, D. N. Sheng, and A. Vishwanath, Doped Mott insulators in the triangular-lattice Hubbard model, Phys. Rev. B **105**, 205110 (2022).

[19] K.-S. Kim, Exact hole-induced resonating-valence-bond ground state in certain $U = \infty$ Hubbard models, Phys. Rev. B **107**, L140401 (2023).

[20] A. V. Gorshkov, M. Hermele, V. Gurarie, C. Xu, P. S. Julienne, J. Ye, P. Zoller, E. Demler, M. D. Lukin, and A. Rey, Two-orbital $SU(N)$ magnetism with ultracold alkaline-earth atoms, Nat. Phys. **6**, 289 (2010).

[21] S. Taie, R. Yamazaki, S. Sugawa, and Y. Takahashi, An $SU(6)$ Mott insulator of an atomic Fermi gas realized by large-spin Pomeranchuk cooling, Nat. Phys. **8**, 825 (2012).

[22] F. Scazza, C. Hofrichter, M. Höfer, P. De Groot, I. Bloch, and S. Fölling, Observation of two-orbital spin-exchange interactions with ultracold $SU(N)$-symmetric fermions, Nat. Phys. **10**, 779 (2014).

[23] X. Zhang, M. Bishof, S. L. Bromley, C. V. Kraus, M. S. Safronova, P. Zoller, A. M. Rey, and J. Ye, Spectroscopic observation of $SU(N)$-symmetric interactions in Sr orbital magnetism, Science **345**, 1467 (2014).

[24] C. Hofrichter, L. Riegger, F. Scazza, M. Höfer, D. R. Fernandes, I. Bloch, and S. Fölling, Direct probing of the Mott crossover in the $SU(N)$ Fermi-Hubbard model, Phys. Rev. X **6**, 021030 (2016).

[25] H. Ozawa, S. Taie, Y. Takasu, and Y. Takahashi, Antiferromagnetic spin correlation of $SU(N)$ Fermi gas in an optical superlattice, Phys. Rev. Lett. **121**, 225303 (2018).

[26] V. Calvera, S. A. Kivelson, and E. Berg, Pseudo-spin order of Wigner crystals in multi-valley electron gases, Fiz. Nyzk. Temp. **49**, 679 (2022).

[27] J. Kang and O. Vafek, Strong coupling phases of partially filled twisted bilayer graphene narrow bands, Phys. Rev. Lett. **122**, 246401 (2019).

[28] O. Vafek and J. Kang, Renormalization group study of hidden symmetry in twisted bilayer graphene with Coulomb interactions, Phys. Rev. Lett. **125**, 257602 (2020).

[29] N. Bultinck, E. Khalaf, S. Liu, S. Chatterjee, A. Vishwanath, and M. P. Zaletel, Ground state and hidden symmetry of magic-angle graphene at even integer filling, Phys. Rev. X **10**, 031034 (2020).

[30] B. A. Bernevig, Z.-D. Song, N. Regnault, and B. Lian, Twisted bilayer graphene. III. Interacting Hamiltonian and exact symmetries, Phys. Rev. B **103**, 205413 (2021).

[31] H. Katsura and A. Tanaka, Nagaoka states in the $SU(n)$ Hubbard model, Phys. Rev. A **87**, 013617 (2013).

[32] E. Bobrow, K. Stubis, and Y. Li, Exact results on itinerant ferromagnetism and the 15-puzzle problem, Phys. Rev. B **98**, 180101(R) (2018).

[33] T. Rakovszky, P. Sala, R. Verresen, M. Knap, and F. Pollmann, Statistical localization: From strong fragmentation to strong edge modes, Phys. Rev. B **101**, 125126 (2020).

[34] V. Khemani, M. Hermele, and R. Nandkishore, Localization from Hilbert space shattering: From theory to physical realizations, Phys. Rev. B **101**, 174204 (2020).

[35] S. Moudgalya, B. A. Bernevig, and N. Regnault, Quantum many-body scars and Hilbert space fragmentation: A review of exact results, Rep. Prog. Phys. **85**, 086501 (2022).

[36] It can be shown straightforwardly that such a flavor-balanced subspace contains a state in every irreducible representation (irrep) that appears in N-direct products of the fundamental representation $\boldsymbol{N}$, $\boldsymbol{N}^N \equiv \boldsymbol{N} \times \boldsymbol{N} \times \cdots \times \boldsymbol{N}$. Since any other states within each irrep can be reached by repeated applications of raising/lowering operators, it suffices to restrict ourselves to the flavor-balanced subspace.

[37] Ref. [19] deals with a special case $N = 2$.

[38] We note that when hopping matrix elements t_{ij} and on-site potentials ϵ_i satisfy certain relations, the Theorem reproduces the result of the Brandt-Giesekus model [53–56].

[39] A. H. MacDonald, S. M. Girvin, and D. Yoshioka, t/U expansion for the Hubbard model, Phys. Rev. B **37**, 9753 (1988).

[40] J. E. Hirsch, Attractive interaction and pairing in fermion systems with strong on-site repulsion, Phys. Rev. Lett. **54**, 1317 (1985).

[41] J. Oitmaa, C. Hamer, and W. Zheng, *Series Expansion Methods for Strongly Interacting Lattice Models* (Cambridge University Press, 2006).

[42] H. Georgi, *Lie Algebras in Particle Physics: From Isospin to Unified Theories* (Taylor & Francis, 2000).

[43] The results of Ref. [19] on the $SU(2)$ t-J model on a triangular cactus is the $N = 2$ case of Corollary 2.

[44] S. Liang, B. Doucot, and P. W. Anderson, Some new variational resonating-valence-bond-type wave functions for the spin-1/2 antiferromagnetic Heisenberg model on a square lattice, Phys. Rev. Lett. **61**, 365 (1988).

[45] D. S. Rokhsar and S. A. Kivelson, Superconductivity and the quantum hard-core dimer gas, Phys. Rev. Lett. **61**, 2376 (1988).

[46] R. Moessner and S. L. Sondhi, Resonating valence bond phase in the triangular lattice quantum dimer model, Phys. Rev. Lett. **86**, 1881 (2001).

[47] H. Lee, Y.-T. Oh, J. H. Han, and H. Katsura, Resonating valence bond states with trimer motifs, Phys. Rev. B **95**, 060413(R) (2017).

[48] G. Giudice, F. M. Surace, H. Pichler, and G. Giudici, Trimer states with Z_3 topological order in Rydberg atom arrays, Phys. Rev. B **106**, 195155 (2022).

[49] I. Kurečić, L. Vanderstraeten, and N. Schuch, Gapped $SU(3)$ spin liquid with Z_3 topological order, Phys. Rev. B **99**, 045116 (2019).

[50] H.-C. Jiang, T. Devereaux, and S. A. Kivelson, Holon Wigner crystal in a lightly doped kagome quantum spin liquid, Phys. Rev. Lett. **119**, 067002 (2017).

[51] K.-S. Kim and S. A. Kivelson, The quantum Hall effect in the absence of disorder, npj Quantum Mater. **6**, 22 (2021).

[52] T. Senthil, S. Sachdev, and M. Vojta, Fractionalized Fermi liquids, Phys. Rev. Lett. **90**, 216403 (2003).

[53] U. Brandt and A. Giesekus, Hubbard and Anderson models on perovskite-like lattices: Exactly solvable cases, Phys. Rev. Lett. **68**, 2648 (1992).

[54] A. Mielke, Exact results for the $U = \infty$ Hubbard model, J. Phys. A: Math. Gen. **25**, 6507 (1992).

[55] R. Strack, Exact ground-state energy of the periodic Anderson model in $d = 1$ and extended Emery models in $d = 1, 2$ for special parameter values, Phys. Rev. Lett. **70**, 833 (1993).

[56] H. Tasaki, Exact resonating-valence-bond ground state and possibility of superconductivity in repulsive Hubbard models, Phys. Rev. Lett. **70**, 3303 (1993).