Rapid Communications

Exact results on itinerant ferromagnetism and the 15-puzzle problem

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We apply a result from graph theory to prove exact results about itinerant ferromagnetism. Nagaoka's theorem is extended to all nonseparable graphs except single polygons with more than four vertices by applying the solution to the generalized 15-puzzle problem, which studies whether the hole's motion can connect all possible tile configurations. This proves that the ground state of a $U \to \infty$ Hubbard model with one hole away from the half filling on a two-dimensional honeycomb lattice or a three-dimensional diamond lattice is fully spin polarized. Furthermore, the condition of connectivity for N-component fermions is presented, and Nagaoka's theorem is also generalized to SU(N)-symmetric fermion systems on nonseparable graphs.

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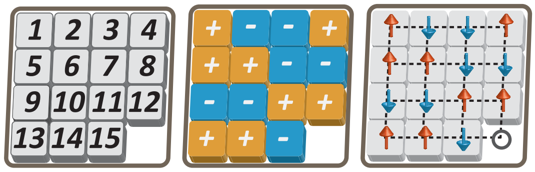
Introduction. The origin of itinerant ferromagnetism based on Fermi-surface splitting rather than the ordering of local spin moments is a difficult question in condensed matter physics [1–24]. As illustrated by Stoner's criterion, itinerant ferromagnetism arises from Fermi statistics—parallel spin alignment leads to the antisymmetrization of electron spatial wave functions, which reduces the repulsive interaction energy [3]. However, spin polarization suffers from a kinetic energy cost, which often dominates the gain of the exchange energy. As a result, electrons typically remain unpolarized even in the presence of strong interactions, developing highly correlated wave functions to reduce interaction energy. Hence, nonperturbative results and exact theorems in particular are desired for the study of itinerant ferromagnetism to set up reliable benchmarks. Known theorems include Nagaoka's theorem [9] and its various generalizations [11,12,25] and flat-band ferromagnetism [13,15]. Inspired by the orbital activity characterized by Hund's coupling in most ferromagnetic metals, a set of theorems of itinerant ferromagnetism in orbital band systems driven by Hund's coupling have been recently proven [22,25], identifying phases of ferromagnetism with a large range of electron fillings and finite bandwidth [26].

Nagaoka's theorem, the first exact result showing itinerant ferromagnetism [9], proves the existence and uniqueness, up to spin degeneracy, of the fully polarized ground state for the single-band Hubbard model. It applies for the case with a single hole away from half filling in the limit of $U \to \infty$, in which the only energy is the hole's kinetic energy. Intuitively, the hole's motion is fully coherent in the background of a fully polarized spin configuration, while it becomes incoherent if spins are unpolarized. Hence, the kinetic energy is optimized with a configuration of the maximum total spin. The proof of Nagaoka's theorem was simplified by Tasaki [11] through use of the Perron-Frobenius theorem, which has two key conditions—nonpositivity and connectivity. Nonpositivity means that all the off-diagonal matrix elements of the many-body Hamiltonian are negative or zero, which is feasible for a single hole under a suitably defined basis but generally not for more than one hole due to fermionic statistics. Connectivity means that the hole's motion can connect all configurations of spins and holes.

The connectivity condition is typically difficult to verify on a general lattice. It has been shown to hold on lattices composed of loops of size three or four [11,12]. In this case, the hole's hopping around each loop generates arbitrary permutations of spins. The two-dimensional (2D) square and triangular lattices and the three-dimensional (3D) cubic lattices satisfy this condition, and Nagaoka's theorem applies to them. However, for lattices consisting of loops of more than four sites, such as the 2D honeycomb lattice and 3D diamond lattice, it remains unclear from previous work whether Nagaoka's theorem holds. It is thus interesting to ask whether necessary and sufficient conditions can be determined under which connectivity is satisfied.

Graph theory has been a useful tool in solving physical problems. A celebrated example is the diagrammatic expansion of field theory, in which graph theory is used to guide the loop expansion and the one-particle irreducible vertex expansion [27]. In the $1/N$ expansion of the large N method, Feynman diagrams are sorted based on their degree of planarity, and the leading-order contribution comes from the planar diagrams [28]. Graph theory also plays an important role in the study of polymer configuration [29], phase transitions in Ising and Potts models [30], and electric network designs [31]. Physical problems defined on graphs have also attracted considerable attention, including random walks [32], field theory [33], phase transitions [34], and dynamic processes [35].

In this Rapid Communication, we find an interesting connection between the study of itinerant ferromagnetism and the celebrated 15-puzzle problem of graph theory. In its original form, the 15-puzzle consists of a 4×4 grid of tiles numbered from 1 to 15, with the 16th cell on the grid being the hole. The hole can be transposed with neighboring tiles, and the goal is to permute a scrambled configuration to put the tiles in order, as shown in Fig. 1. The generalized version of the 15-puzzle problem was examined on arbitrary graphs in Ref. [36]. By relating the connectivity condition of lattices to the



(a) (b) (c)

FIG. 1. (a) The solved configuration of the original 15-puzzle. The goal of the puzzle is to return to this configuration from any scrambled starting one. (b) For the 15-puzzle analogous to spin-1/2 particles, there are only two labels. A sample configuration on a 4×4 grid is shown here with $+$ for spin up and $-$ for spin down. It is mapped to a spin configuration with a single hole in a square lattice in (c).

15-puzzle problem, we find that connectivity holds for spin-$\frac{1}{2}$ electrons *if and only if* the lattice (graph) is nonseparable and not a single polygon larger than a quadrilateral. This generalizes Nagaoka's theorem to a large class of lattices including the honeycomb lattice and the diamond lattice for which Nagaoka's theorem has not been previously proven. We also provide criteria for the connectivity condition for SU(N) fermions in the fundamental representation, leading to a generalized SU(N) Nagaoka's theorem.

In what follows, we refer to a"graph" instead of a "lattice" since the results require a finite number of sites and do not depend on a regular lattice structure. Consider a spin-$\frac{1}{2}$ Hubbard model on a general graph,

$$H = \sum_{i,j,\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}, \tag{1}$$

where σ is the spin index, $n_{i,\sigma} = c^\dagger_{i\sigma} c_{i\sigma}$, and t_{ij} is a symmetric matrix of hopping amplitudes that encodes the graph structure. If sites i and j are connected, then $t_{ij} > 0$, otherwise $t_{ij} = 0$. In the limit of $U \to \infty$, states with doubly occupied sites are projected out, and every site has exactly one electron apart from the site with a hole. On a bipartite graph, the overall sign of t_{ij} does not influence physical properties, since the sign can by changed by a gauge transformation $c_{i\sigma} \to -c_{i\sigma}$ on all sites i in one of the two subgraphs.

In order to consider a general graph structure, we now summarize Tasaki's proof of Nagaoka's theorem [11]. Since the Hamiltonian of Eq. (1) is SU(2) symmetric, the Hilbert space decomposes into sectors labeled by the z component of total spin $S_{z,\mathrm{tot}}$. Without loss of generality, consider the sector where $S_{z,\mathrm{tot}} = 0$ or 1/2 for cases with an even or odd number of spins, respectively, since any SU(2) multiplet has a component in this sector. The basis is defined as

$$|h, \{\sigma\}\rangle = (-1)^h {\prod_i}' c^\dagger_{i,\sigma_i}(\mathbf{r}_i)|0\rangle, \tag{2}$$

where $c^\dagger_{i,\sigma_i}$ is ordered following an arbitrary but fixed sequence of the vertex indices, h is the index of hole's location, and the primed product excludes the creation operator at the hole's vertex. In this basis, the Hamiltonian matrix satisfies a nonpositivity condition in that its elements are all 0 or $-t_{ij}$. Suppose that the Hamiltonian additionally satisfies a connectivity condition, which requires that there exists a positive integer power N for any two basis elements $|h, \{\sigma\}\rangle$ and $|h', \{\sigma'\}\rangle$ such that

$$\langle h', \{\sigma'\}|H^N|h, \{\sigma\}\rangle \neq 0. \tag{3}$$

This connectivity condition intuitively means that any configuration of the spins and hole in the S_z sector can be converted into any other configuration through a sequence of hole hopping.

According to the Perron-Frobenius theorem, if both nonpositivity and connectivity are satisfied, Eq. (1) has a unique ground state,

$$|\psi_g\rangle = \sum_{h,\{\sigma\}} \alpha_{h,\{\sigma\}} |h, \{\sigma\}\rangle, \tag{4}$$

with a positive-definite wave function, meaning $\alpha_{h,\{\sigma\}} > 0$ for all states in the selected S_z sector. To determine the total spin of $|\psi_g\rangle$, a trial state $|\psi_t\rangle$ is constructed by summing over all states in the S_z sector with equal weight, $|\psi_t\rangle = \sum_{h,\{\sigma\}} |h, \{\sigma\}\rangle$. Such a state is fully symmetric under permutation of spin configurations and is thus fully spin polarized. Since $\langle\psi_g|\psi_t\rangle > 0$, $|\psi_g\rangle$ shares the same quantum numbers as $|\psi_t\rangle$, meaning the ground state must also be fully spin polarized.

In order to determine conditions under which the connectivity condition holds, it is useful to consider the generalized 15-puzzle problem, which was examined on arbitrary graphs in Ref. [36]. Through induction on the number of loops in the graph, it is proven that, apart from two classes of exceptions, any permutation can be performed on a nonseparable, nonbipartite graph, and any even permutation can be performed on a nonseparable, bipartite graph. Here "nonseparable" means that the graph remains path connected if any single vertex is removed. The first class of exceptions consists of single polygons larger than a triangle, and the second class consists of the so-called θ_0 graph which is a single hexagon with an extra vertex in the middle that connects two opposite hexagon vertices, as shown in Fig. 3 in the Supplemental Material (SM) I [37].

We can now relate the connectivity condition to the generalized 15-puzzle problem. Each electron is labeled by "+" or "−" according to its eigenvalue $S_z = \pm\frac{1}{2}$ and electrons of the same label are indistinguishable. For example, Fig. 1(b) illustrates a 4×4 lattice, in which each square plaquette represents a vertex of the corresponding graph. The basis elements Eq. (2) correspond to an assignment of $+$, $-$, or the hole to each location. The connectivity condition is satisfied if any configuration of labels can be converted to any other with the same total numbers of $+$ and $-$ by a sequence of transposing the hole with neighboring labels. On a general graph, this takes the form of the generalized 15-puzzle with only two distinct tile labels. Based on the solution to the general 15-puzzle problem [36], we have the following theorem.

Theorem 1. The Hamiltonian in Eq. (1) on a graph G satisfies the connectivity condition of Eq. (3) if and only if G is nonseparable and G is not a polygon with $V \geqslant 5$ vertices. The ground state of the model in Eq. (1) is then fully spin polarized and unique up to spin degeneracy when $U \to \infty$ and there is exactly one hole.

Proof. We first prove sufficiency. The connectivity condition can be verified if G is a single triangle or quadrilateral simply by cycling the hole around the loop and noting that at least two spins are identical in the quadrilateral case since there are only two distinct spin labels. Connectivity also holds on the θ_0 diagram, as shown in SM I [37]. For the remaining nonseparable, nonpolygonal graphs, we note that since spin only has two labels, the permutations of the spins and hole are a subset of the possible permutations in the corresponding 15-puzzle problem where every vertex has a distinct label. Hence, for the nonbipartite graphs, where all permutations can be performed in the 15-puzzle problem with all labels distinct, the connectivity condition is immediately satisfied. For the bipartite graphs, the vertex number is larger than 4, and there are thus at least two vertices occupied by the same spin label. Since exchanging these two identical spin labels is an identity operation, any odd permutation can be composed with an exchange of two identical spin labels to produce an even permutation with the same effect on the labels. Hence generating all the even permutations on the bipartite graph is equivalent to generating all permutations when there is a repeated label. Since the 15-puzzle problem on the bipartite graphs allows for any even permutation, connectivity is satisfied.

Next, we prove necessity by demonstrating that the connectivity condition is satisfied for neither polygons with vertex number $V \geqslant 5$ nor for separable graphs. For the polygons with $V \geqslant 5$, permutations leaving the hole fixed are cyclic permutations, all generated by a single $V-1$ cycle, on the spin labels and thus cannot connect all configurations in the S_z sector in general since these cyclic permutations cannot exchange neighboring spins unless every spin but one has the same label. This can also be seen by counting the number of configurations in the $S_{z,\text{tot}} = 0$ or $1/2$ sector, where the total configuration number is $N_c = V!/[m!(V-m-1)!]$, where $m = \frac{V-1}{2}$ or $\frac{V-2}{2}$ for odd or even V, respectively. Cycling the hole around the polygon can at most generate $V(V-1)$ configurations, which is less than N_c for $V \geqslant 5$. For the separable graphs, we only need to consider a general connected but separable graph, which can be divided into two subgraphs A and B with a single vertex O connecting them. A and B are thus disconnected, and the overall graph is disconnected, if O is removed. If the hole is initially at O, then if the hole moves to A, it cannot enter B without passing O, and vice versa. As a result, the hole's motion cannot be used to move spins between A and B, and permutations can only be performed within A and O, or B and O, but not between A and B.

Theorem 1 ensures Nagaoka ferromagnetism for all regular lattices, which goes beyond the previous results in literature applying for graphs composed of triangles and quadrilaterals [11,12]. For example, this demonstrates Nagaoka ferromagnetism on lattices where the minimal loops are hexagons. To our knowledge, this was previously an open problem. We thus have the following corollary.

Corollary. Nagaoka ferromagnetism applies to both the 2D honeycomb lattice and the 3D diamond lattice.

We can explicitly demonstrate connectivity in the honeycomb lattice using 3-cycles, and the same method applies to the diamond lattice as well. Figure 2(a) presents that a 3-cycle for any three adjacent vertices in a hexagon loop can be performed for the 15-puzzle problem without affecting other vertices, and a construction of such a 3-cycle is given in SM II [37]. For the case of spins, two opposite labels on any edge can be exchanged without affecting other vertices as shown in Fig. 2(b). Without loss of generality, assume vertices 1 and 2 are occupied with spin labels ↑ and ↓, respectively. If site 3 has spin-↓, then simply applying the cycle (123) will be exchange the spins at sites 1 and 2. Otherwise, if site 3 has spin-↑, performing the cycle twice, or (321), will exchange the spins. Next, consider any two vertices $1'$ and $2'$ with opposite spin labels. We can choose a path connecting them. If the hole is not on the path, it is straightforward to show that by successively applying exchanges between adjacent vertices along the path can exchange $1'$ and $2'$ without affecting other vertices. If the hole is on the path, move it away, and after the exchange is performed, reverse the hole's motion. Since all the permutations of spins can be generated by exchanges, they can also be performed. In other words, the 3-cycles of adjacent vertices generate all 3-cycles on the lattice. This establishes connectivity on the honeycomb lattice.

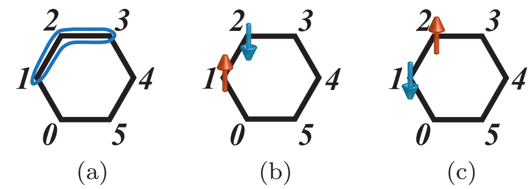


FIG. 2. (a) A three-cycle for any adjacent three vertices 1, 2, and 3 can be performed in a hexagon loop with concrete steps given in SM II [37]. (b) Vertices 1 and 2 are occupied by spin-↑ and spin-↓. Apply (123) or (132) when 3 is ↑ and ↓, respectively, then spins on 1 and 2 are exchanged without affecting other vertices as shown in (c).

The above demonstration of Nagaoka ferromagnetism on the honeycomb and diamond lattices can serve as a starting point for further studies. An interesting question is the stability of the fully polarized Nagaoka state in the presence of multiple holes. Following the method in Refs. [38,39], we have shown in SM III [37] that the ground-state energy E_g satisfies the bounds of

$$E_N \leqslant E_g \leqslant E_N + t\,O\big(N_h^{1/\alpha}/M\big), \tag{5}$$

where $E_N = -zN_h t$ with N_h the number of holes, z the coordination number, M the total number of sites, and $\alpha = 1/2$ and $2/5$ for the honeycomb and diamond lattices, respectively. When N_h scales with M more slowly than M^α, the upper and lower bounds meet in the thermodynamic limit and the Nagaoka state is degenerate with the ground state. The stability of the Nagaoka state against finite hole densities has been studied by analytic estimations [40] and a recent numeric density-matrix-renormalization-group simulation [17]. It would be interesting to further explore exact results at finite hole density in the thermodynamic limit.

Extensions. Recently, SU(N) symmetric fermionic systems have attracted considerable attention in the context of cold atom physics, where they can be realized by alkalineearth fermions [41–43]. Consider the SU(N) Hubbard model,

$$H = \sum_{ij,\alpha=1}^{N} t_{ij} c_{i,\alpha}^{\dagger} c_{j,\alpha} + \frac{U}{2} \sum_{i} n_i (n_i - 1), \qquad (6)$$

where $1 \leqslant \alpha \leqslant N$ labels the fermion component, n_i is the number operator $n_i = \sum_\alpha c_{i,\alpha}^{\dagger} c_{i,\alpha}$, and $t_{ij} > 0$ for connected sites i and j with $t_{ij} = 0$ otherwise. In the $U \to \infty$ limit with one hole away from $1/N$ filling, where every site but one has exactly one fermion, Nagaoka's theorem was previously generalized to this SU(N) system on triangular, kagome, and hypercubic lattices [44]. Without loss of generality, below we only consider the case where N is less or equal to the particle number, i.e., $N \leqslant V - 1$. The fermions considered here are in the fundamental representation of SU(N), yielding N-component fermions.

It is natural to generalize Nagaoka's theorem to the SU(N) case on general graphs with the help of the 15-puzzle problem. The nonpositivity of the Hamiltonian matrix of Eq. (6) can be established under a many-body basis constructed similarly to Eq. (2). For the connectivity condition, consider the nonseparable graphs other than the θ_0 graph and polygons. For nonbipartite graphs, the connectivity condition holds even when all the occupied vertices have different fermion components, which places no further requirements on N. For bipartite graphs, since only even permutations can be performed, at least two vertices must be occupied by fermions in the same component to allow a 3-cycle involving two identical fermions to behave as an odd permutation. Satisfying connectivity thus requires $V \geqslant N + 2$ for bipartite graphs. For polygons, connectivity only holds on the triangle and quadrilateral for the SU(2) case, and it does not holds on any polygons with $V \geqslant 4$ for $N \geqslant 3$. For the θ_0 graph, connectivity holds only for $N = 2$. Summarizing the reasoning above, we have the following theorem.

Theorem 2. Consider the SU(N) Hamiltonian Eq. (6) for $N > 2$ on a graph G with vertex number $V \geqslant N + 1$ in the limit of $U \to +\infty$ with a single hole. The connectivity condition is satisfied for G a nonseparable graph other than the θ_0 graph and polygons with $V \geqslant 4$, with an additional condition that $V \geqslant N + 2$ for G bipartite. Then the ground state is in the fully symmetric one-row SU(N) representation and is unique up to the SU(N) degeneracy.

We can also generalize the ferromagnetism to hard-core bosons with the same Hamiltonian Eq. (6). The Perron-Frobenius theorem together with the 15-puzzle problem can be used to prove a fully spin-polarized ground state. For bosons, the hopping amplitudes need to be $t_{ij} < 0$ for links to satisfy the nonpositivity of the Hamiltonian matrix elements. As opposed to the fermion case, extension to multiple holes is possible since bosons do not suffer from the minus sign when switching two holes, allowing nonpositivity to hold. Connectivity continues to hold for nonseparable graphs other than single polygons larger than a triangle and the θ_0 graph, since a single hole can still be used to solve the 15-puzzle and the remaining holes can be considered labels. When there are at least two holes, connectivity holds on θ_0 as well, as shown in SM IV [37]. This yields Theorem 3.

Theorem 3. Consider the Hubbard model of Eq. (6) for SU(N) hard-core bosons in the $U \to +\infty$ limit on a graph G. The connectivity condition for $N > 2$ is satisfied for any number of bosons $N_b \leqslant V - 1$ if and only if G is a nonseparable graph other than θ_0 and polygons with $V \geqslant 4$ with an additional condition that $V \geqslant N + 2$ in the case of only a single hole in a bipartite graph. If there are at least two holes or $N \leqslant 2$, connectivity holds if G is θ_0 as well. Then the ground state is in the fully symmetric, one-row representation of SU(N), which is unique up to SU(N) degeneracy.

Conclusions. The graph theorem of the generalized 15-puzzle problem has been applied to establish the Nagaoka ferromagnetic state of the infinite-U Hubbard model on general graphs with a single hole away from half filling. We have found that for the SU(2) case, the Nagaoka state is the unique ground state up to spin degeneracy for all nonseparable graphs other than single polygons with vertex number $V \geqslant 5$, as established by Theorem 1. This extends Nagaoka's theorem to the 2D honeycomb lattice and the 3D diamond lattice, whose minimal loops contain six vertices and are hence beyond previous results in the literature. Furthermore, Nagaoka's theorem can also be extended to the case of a single hole in an otherwise $1/N$-filled SU(N) Hubbard model. In the SU(N) case, the result is valid on nonseparable graphs other than the θ_0 graph and single polygons with an additional condition of $V \geqslant N + 2$ for bipartite graphs, as established by Theorem 2. Similar results can also be generalized to SU(N) hard-core boson systems. These results are helpful for further analytic and numeric studies of the mechanism for itinerant ferromagnetism and searches for novel ferromagnetic states in condensed matter and ultracold atom systems.

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[37] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevB.98.180101 for the θ_0 graph and connectivity on the θ_0 graph; connectivity for the honeycomb lattice; stability of the Nagaoka state with multiple holes; and connectivity on the θ_0 graph for bosons with multiple holes.
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