Characterization of solvable spin models via graph invariants

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Exactly solvable models play an essential role in many-body physics and in quantum Hamiltonian complexity. Such models—and their solutions—often yield deep insight into physical phenomena. In the context of quantum information, these insights can be leveraged for quantum computing using ground states of exactly solvable models such as *cluster states* [1–5], or related states [6–8], or to show that seemingly complex and highly entangled ground states are in fact easy to find on a classical computer [9, 10]. For the problem of Hamiltonian simulation, the complexity is similarly informed by a physical property of the system, such as its locality [11] or stoquasticity [12].

In the setting of many-body spin-1/2 (qubit) systems, an important class of exactly solvable models consists of those that can be mapped to free fermions hopping on a graph. The paradigmatic example of this method is the Jordan-Wigner transformation [13], which provides an exact solution to the XY model [9] through a description by free fermions in one spatial dimension. A generalization to the Jordan-Wigner transformation to two dimensions can be seen in the exact solution to the Kitaev honeycomb model [10]. The dynamics of free-fermion models is closely connected to the quantum computational model of *matchgate circuits* [14, 15], which have an extensive complexity-theoretic characterization [16–22]. These circuits were originally investigated in the context of counting perfect matchings in a graph [23–26], which is efficiently solved for planar graphs using the so-called Fisher-Kasteleyn-Temperley algorithm [27, 28], despite being #P-complete [29] in general.

A free-fermion solution maps the problem of simulating a system of n qubits, with Hilbert space dimension 2^n, to one of simulating a single particle hopping on a lattice of $O(n)$ sites. In this talk, we will describe the results of Ref. [30], where we give a complete characterization of quantum Hamiltonians that can be solved this way, via a generalization to the Jordan-Wigner transformation. We will show that the problem of recognizing free-fermion-solvable spin models is equivalent to the graph-theoretic problem of recognizing line graphs, which can be done efficiently, and has in-fact been solved optimally. Furthermore, our results lead to a complete classification of the "obstructions" to a Jordan-Wigner-like solution. Our result extends the numerous applications enjoyed by free-fermion models and matchgate circuits to the widest possible class of systems.

Background: Let us define the *Majorana modes* $\{\gamma_j\}$ as a set of Hermitian operators satisfying the canonical anticommutation relations

$$\{\gamma_j, \gamma_k\} = 2\delta_{jk} I \qquad \gamma_j^\dagger = \gamma_j \quad \forall\ j. \tag{1}$$

A *free-fermion model* has a Hamiltonian that can be described in terms of quadratics in the n Majorana modes

$$H = i\boldsymbol{\gamma} \cdot \boldsymbol{h} \cdot \boldsymbol{\gamma}^{\mathrm{T}} \equiv i \sum_{j,k} h_{jk} \gamma_j \gamma_k. \tag{2}$$

The eigenvalues and eigenstates of the model are completely described by the $n \times n$ antisymmetric *single-particle Hamiltonian* $\boldsymbol{h}$, and so such a model is exactly solvable classically.

Next consider an n-qubit many-body Hamiltonian, written in a given Pauli basis as

$$H = \sum_{\boldsymbol{j}} h_{\boldsymbol{j}} \sigma^{\boldsymbol{j}}, \tag{3}$$

where $\boldsymbol{j} \in \{0, x, y, z\}^{\times n}$ labels an n-qubit Pauli operator in the natural way, and $h_{\boldsymbol{j}}$ is a real coupling strength. Since the terms in this definition only either commute or anticommute, we can define a graph relating to H:

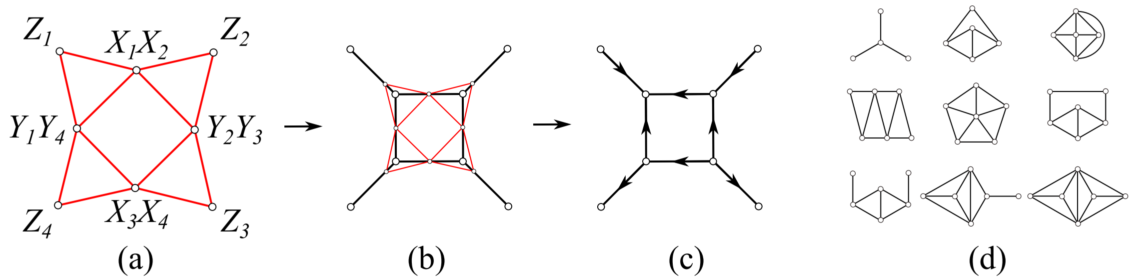

FIG. 1. A visual summary of our characterization. (a) Given a Hamiltonian expressed in a given basis of Paulis, construct its frustration graph. (b) If the frustration graph (red) can be realized as the line graph of another graph (the root graph, black), then the model can be faithfully mapped onto a model of free fermions hopping on the root graph. (c) Choosing an orientation of the root graph corresponds to choosing the sign of the matrix element above the main diagonal in the single-particle Hamiltonian. We choose this orientation such that cycles on the root graph multiply to a sign specified by the eigenspace of the corresponding symmetry. In this example, we choose an eigenspace of $Z_1Z_2Z_3Z_4$, and solve the model over this eigenspace by choosing the appropriate orientation of the single cycle in the free-fermion model. A satisfying orientation can always be chosen. (d) A complete list of obstructions to a free-fermion solution. No model with such a solution can have a subset of terms with frustration graph isomorphic to one of the nine graphs shown here. Conversely, any model whose frustration graph doesn't contain one of these obstructions as an induced subgraph is free-fermion solvable.

Definition 1 (Frustration Graph)**.** *The frustration graph $G(H)$ of a Hamiltonian written in a given Pauli basis has vertex-set V given by Pauli terms in H. Vertices are neighboring in $G(H)$ iff their corresponding Paulis anticommute.*

This graph has been invoked previously in the setting of variational quantum eigensolvers [31–38], commonly under the name "anti-compatibility graph". Notice that it is independent of the specific Pauli representation of the Hamiltonian and so is invariant under Clifford conjugation. The eigenvalues of H, up to multiplicities, are therefore completely determined by this graph and the coupling strengths $\{h_{\boldsymbol{j}}\}$. This graph can also be said to capture the "relevant" spatial structure of the Hamiltonian for the purpose of finding its spectrum.

Our main result requires a simple concept from graph theory:

Definition 2 (Line Graphs)**.** *The line graph $L(R) \equiv (E, F)$ of a root graph $R \equiv (V, E)$ is the graph whose vertex set is the edge set of R and whose edge set is given by*

$$F \equiv \{(e_1, e_2) \mid e_1, e_2 \in E,\ |e_1 \cap e_2| = 1\}\,. \tag{4}$$

That is, vertices are neighboring in $L(R)$ if the corresponding edges in R are incident at a vertex.

See Fig. 1 for an example of a line graph.

Main Results: We seek to recognize spin Hamiltonians H of the form in Eq. (3) for which a mapping to a free-fermion model of the form in Eq. (2) exists, preserving the commutation between terms. Notice that two terms in a free-fermion model only anticommute if they contain a mode in common. Terms in H therefore naturally correspond to *edges* of the fermion-hopping graph. In this talk, we will present two natural theorems and their implications:

Result 1 (Existence of free-fermion solution; Informal version of Thm. 1 in [30])**.** *Given an n-qubit Hamiltonian whose frustration graph G is the line graph of another graph R, then there exists a free-fermion description of H.*

Line-graph recognition can be performed optimally in linear time [39–41]. The root graph constructed in this solution is the *hopping graph* of the free-fermion model, and specifies which elements of $\boldsymbol{h}$ are nonzero. We represent the signs of the elements above the main diagonal in $\boldsymbol{h}$ by an orientation of R. Our next result involves the guaranteed symmetries of free-fermion solvable models, which yield constraints to be satisfied by this orientation.

Result 2 (Graphical symmetries; Informal version of Thm. 2 in [30])**.** *Given an n-qubit Hamiltonian whose frustration graph G is the line graph of another graph R, then Pauli symmetries of H correspond to either:*

(i) Cycles of R;

(ii) A T-join of R, associated to the fermion-parity operator;

(iii) Logically encoded qubits;

and these symmetries generate an abelian group.

Case (i) can be seen from the fact that the product of fermion bilinears around a cycle of the hopping graph will be proportional to the identity, and thus commutes with all other Hamiltonian terms. We solve the model over each eigenspace of its cycle symmetries by choosing an orientation such that these products of bilinears have the correct proportionality constant, and this can always be done. Case (ii) is the product of all Majorana operators in the model, and is only relevant when the number of vertices in the root graph is even. If this product is also generated by a product of cycle symmetries in the qubit model, then we must project onto a fixed-parity subspace of the free-fermion model to obtain the physical solution to H. Finally, case (iii) consists of operators which cannot be constructed by products of Hamiltonian terms, yet commute with the Hamiltonian.

Implications: Though these theorems are simple to state, their implications are manifold. In addition to giving an efficient means for recognizing a free fermion model, these results also yield finitely many small obstructions to the existence of a free-fermion solution, thanks to a structure theorem by Beineke [42]. These subgraphs are shown in Fig. 1(d), and cannot appear as vertex-induced subgraphs for any model with a free-fermion solution of the form we characterize (though some subtleties still apply, as discussed in Ref. [30]). In Ref. [30], we demonstrate how several models with known free-fermion solutions, such as the XY-model and the Kitaev model, fit into our framework. Our characterization will also allow us to find new models with exact free-fermion solutions, such as the Sierpinski-Hanoi model, as described in the main text. This is a 3-local qubit Hamiltonian with terms arranged in a Sierpinski triangle. In particular, we conjecture that the spectrum of this model exhibits a scale symmetry in the infinite limit.

Why QIP? These results provide a systematic way for recognizing the existence of an exact solution to a quantum many-body Hamiltonian. The main result gives an elegant if and only if condition for solvability by a free fermion mapping, one of the most important mappings for both Hamiltonian complexity and (via matchgates) circuit complexity. Moreover, our result leads to a complete classification of the obstructions to such a solution as well as the symmetries that are possible in such systems. The proof itself makes use of familiar objects to the audience, namely graphs, but in a surprising and interesting way. We therefore expect that not just our results but also our techniques will be both interesting and broadly accessible to the QIP audience. Finally, we believe that the frustration graph formalism will find wider applications as a tool for characterizing Hamiltonian complexity, optimizing circuits for variational quantum eigensolvers, and more.

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