Complete Characterization of the Ground Space Structure of Two-Body Frustration-Free Hamiltonians for Qubits

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The problem of finding the ground state of a frustration-free Hamiltonian carrying only two-body interactions between qubits is known to be solvable in polynomial time. It is also shown recently that, for any such Hamiltonian, there is always a ground state that is a product of single- or two-qubit states. However, it remains unclear whether the whole ground space is of any succinct structure. Here, we give a complete characterization of the ground space of any two-body frustration-free Hamiltonian of qubits. Namely, it is a span of tree tensor network states of the same tree structure. This characterization allows us to show that the problem of determining the ground state degeneracy is as hard as, but no harder than, its classical analog.

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Quantum spin models are simplified physical models for real materials, but are believed to capture some of their key physical properties, which lie in the heart of modern condensed matter theory [1]. Ground states of strongly correlated spin systems is usually highly entangled, even if the system Hamiltonian carries only local interactions. So in general, finding the ground state of such a system is intractable with traditional techniques, such as mean field theory.

In practical spin systems, different local terms in the Hamiltonian might also compete with each other, a phenomenon called frustration, which makes the system further difficult to analyze [2]. However, frustration is not a necessary factor to cause ground state entanglement. Frustration-free Hamiltonians can carry lots of interesting physics, ranging from gapped spin chains [3] to topological orders [4, 5].

During recently years, the active frontier of quantum information science brings new tools to study quantum spin systems. In particular, local Hamiltonian problems are shown to be in general very hard, i.e., QMA-complete [6]. It is also realized that the study of k-local frustration-free Hamiltonians for qubits is closely related to the quantum k-satisfiability problem (Q-k-SAT) [7], which is the quantum analogy of the classical k-satisfiability (k-SAT), a problem that is of fundamental importance and has been extensively studied in theoretical computer science (see, e.g., [8]).

Spin models with two-body interaction are of the most physical relevance, as two-body interaction, in particular of nearest neighbor or next nearest neighbors on certain type of lattices, are the strongest interaction terms in the real system Hamiltonian. Because two-level systems are most common in nature, spin-1/2 (qubit) systems are of particular importance.

It is realized, however, that certain ground states of a two-body frustration-free (2BFF) Hamiltonian of qubits could be pretty trivial with almost no entanglement at all. Algorithmically, the problem of finding the ground state of a 2BFF Hamiltonian of qubits is known to be solvable in polynomial time [7]. It is also shown recently that for any such Hamiltonian, there is always a ground state that is a product of single- or two-qubit states; and if there is a genuine entangled ground state, the ground space must be degenerate [9]. There are also similar observations of the ground states in random or generic instances [10–13], saying that the entire ground space is of a trivial structure, which is almost always the fully symmetric space, with ground space degeneracy $n+1$, where n is the number of qubits [10, 11, 14].

The main purpose of this work is to characterize the entire ground space in the most general setting. We improve the understanding of the ground space of 2BFF Hamiltonians of qubits by showing that it is always a span of tree tensor network states of the same tree structure. In other words, these states are generated, from products of single qubit states, by the same series of isometries (from single qubit to two qubits). As this characterization holds for the most general case, it implies that computing the degeneracy of 2BFF Hamiltonian (#Q-2-SAT) is in a complexity class called #P [15]. On the other hand, the classical analog #2-SAT of #Q-2-SAT is #P-hard, therefore #P-complete.This answered a question raised in [11].

Two-body frustration-free Hamiltonian.— Consider a system of n qubits labeled by the set $V = \{1, 2, \ldots, n\}$. We will be interested in 2BFF Hamiltonians $H = \sum H_J$ of the system. The Hamiltonian is called two-body if each term H_J acts non-trivially only on two qubits. The index J indicates the two qubits on which H_J acts. The Hamiltonian H is called frustration-free if its ground state also minimizes the energy of each term H_J simultaneously. Without loss of generality, we can assume throughout the paper that the smallest eigenvalue of each term H_J is zero by shifting the energy spectrum. In this convention, the frustration-free Hamiltonian H itself will have zero ground energy. Specifically, we have

$$\mathcal{K}(H) = \bigcap \big(\mathcal{K}(H_J) \otimes \mathcal{H}_{\bar{J}}\big), \qquad (1)$$

where $\mathcal{K}(H)$ is the ground space of H and $\mathcal{H}_{\bar{J}}$ is the Hilbert space of the qubits not in J. From this equation, one easily sees that it is the ground space of each term H_J, not the structures of excited states, that matters for the ground space of a frustration-free Hamiltonian H. In other words, it suffices to consider local terms to be projections Π_J for our purpose.

Closely related to the analysis of 2BFF qubit Hamiltonians is the quantum 2-SAT problem (Q-2-SAT) first considered by Bravyi [7]. Naturally generalizing classical 2-SAT, the Q-2-SAT problem asks whether, for a given set of two-qubit projections $\{\Pi_J\}$ of an n-qubit system, there is a global state $|\Psi\rangle$ such that $\Pi_J|\Psi\rangle = 0$ for all J. Apparently, we answer "yes" to the problem if and only if the Hamiltonian $\sum \Pi_J$ is frustration-free. It was known that Q-2-SAT is decidable in polynomial time on a classical computer [7]. The proof of the statement actually constructs a specific n-qubit state $|\Psi\rangle$ in the ground space of $\sum \Pi_J$ if there is any. Our techniques will be similar to those used by Bravyi, but we will show a stronger result that one can not only find one state in the ground space, but also represent the entire ground space in terms of a span of special states.

A case study of the rank.— Given a 2BFF Hamiltonian $H = \sum H_J$, what can we say about the ground space $\mathcal{K}(H)$? First of all, as argued previously, we only need to consider Hamiltonians of the form $H = \sum \Pi_J$ where Π_J's are projections onto $\mathcal{K}(H_J)^\perp$. We will start our analysis by considering the rank of the projections Π_J.

First, if there is a Π_J of rank 3, the only possible state for the two qubits in J is $I - \Pi_J$ of rank 1, and this reduces to a problem on qubits in $V \setminus J$.

If there is a Π_J of rank 2, the state of qubits in J is restricted to a two-dimensional subspace. Let $|\psi_0\rangle_{a,b}$ and $|\psi_1\rangle_{a,b}$ be two orthogonal states that span the subspace, where a, b are the two qubits in J. One can encode qubits a and b by a single qubit d. For this purpose, we define an isometry U in the following form $U : |0\rangle_d \mapsto |\psi_0\rangle_{a,b},\ |1\rangle_d \mapsto |\psi_1\rangle_{a,b}$. This procedure produces a set of constraints on $n-1$ qubits. It is easy to verify that a state $|\Psi\rangle$ is in the ground space of the reduced problem if and only if $U|\Psi\rangle$ is in the ground space of the original problem [7, 9].

When there is no projection of rank larger than 1, we are dealing with the homogeneous case [7]. It turns out that the homogeneous case is the hardest and we will discuss it two separate sections. As we will see, the ground space of the homogeneous Hamiltonian (more precisely, the simplified homogeneous Hamiltonian defined later) is spanned by single-qubit product states. The above case analysis gives an explicit representation of the ground space of a general 2BFF qubit Hamiltonian, which is given by the following

Main Observation — *The ground space is always a span of tree tensor network states of the same tree structure.*

We illustrate this observation in Fig. 1, where the ground space is viewed as a span of states generated by the isometries (blue triangles) organized in a forest form (a collection of trees) acting on product states (input from the left). In the language of tensor network states [16, 17], one can also represent these states in terms of tree tensor network after combining the input product states and the roots of trees in the forest.

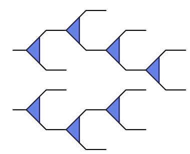


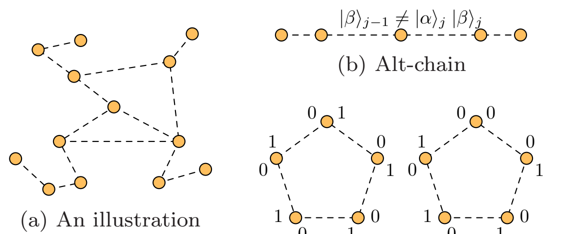
FIG. 1: The general structure of the ground space

Homogeneous case with product constraints.— Consider the Hamiltonian $H = \sum \Pi_J$ where Π_J's are rank-1 projections. One can visualize the interactions in H by a graph G. The graph has n vertices corresponding to the qubits and two vertices are connected when there is a non-trivial interaction Π_J acting on them. We will also distinguish two types of edges in the interaction graph. Let $\Pi = |\phi\rangle\langle\phi|$ be a projection. We will use a solid edge in the graph when $|\phi\rangle$ is entangled and a dashed edge when $|\phi\rangle$ is a product state. Let us first focus on the homogeneous case with product constraints only.

In this case, the interaction graph consists of dashed edges. We will show that the ground space is a span of product of single-qubit states (or, for simplicity, a product span). It will also be useful to know that the states we choose are orthogonal up to a local operation $L = \bigotimes_{j=1}^n L_j$, where L_j is a non-singular local operator acting on the j-th qubit. Note applying L on the 2BFF Hamiltonian $H = \sum H_J$ results in $H^L = \sum L_J^{-1} H_J L_J$, where $L_J = \bigotimes_{j\in J} L_j$. And H^L, which is also 2BFF, has the same ground state degeneracy as H [7, 9]. The relation between the ground space of H and H^L is

$$L^{-1}\mathcal{K}(H) = \mathcal{K}(H^L). \qquad (2)$$

Before we actually give the proof, let us first examine several simple examples. The first example considers a chain of interactions as in Fig. 2b. Let $|\alpha_j\rangle \otimes |\beta_j\rangle$ be the constraint on the j-th edge. We will call it an alternating chain if $|\beta_{j-1}\rangle$ and $|\alpha_j\rangle$ are linearly independent for all j. It is easy to see that the solution space is $k+1$ for an alternating chain of k qubits. The second example shown in Fig. 2c is called the alternating loop. As its name suggests, it is a loop where the two constraints on any vertex are linearly independent. Any alternating loop has solution space of dimension 2, namely the span of $|00\dots0\rangle$ and $|11\dots1\rangle$ up to the local operation that maps $|\alpha_j\rangle$ and $|\beta_{j-1}\rangle$ to $|0\rangle$ and $|1\rangle$. The final example we consider is called the quasi-alternating loop. It is almost the same as the alternating loop except that there is one special vertex on the loop having the same constraint on the two edges adjacent to it. Figure 2d gives such an example where the top vertex is special. It is easy to see that the constraint on the special vertex of a quasi-alternating loop must be satisfied. In particular, for the loop in Fig. 2d, the top vertex must be $|1\rangle$ as otherwise it will be impossible to satisfy all five constraints on the loop.



(a) An illustration of a dashed interaction graph (b) Alt-chain (c) Alt-loop (d) Quasi-loop

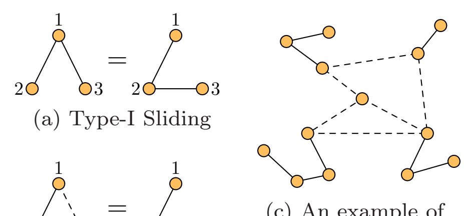
FIG. 2: Dashed interaction graph and three examples

We now start the proof by induction on n, the number of qubits. For $n = 1, 2$, the observation is trivial. If there is a vertex a on which the constraints are the same up to global phases, let the constraints be $|0\rangle_a$ and, more concretely, let the constraints on an edge connects to a be of the form $|0\rangle_a|\alpha\rangle_b$ for some qubit b. We can write any state in the ground space as $|\Phi\rangle = |0\rangle_a|\Phi_0\rangle + |1\rangle_a|\Phi_1\rangle$. Obviously, $|\Phi_0\rangle$ and $|\Phi_1\rangle$ are both in the ground space of the constraints not acting on a. Moreover, $|\Phi_0\rangle$ also needs to be orthogonal to $|\alpha\rangle_b$'s. By the induction hypothesis, both $|\Phi_0\rangle$ and $|\Phi_1\rangle$ are in a product span. Therefore, $|\Phi\rangle$ is also in a product span. On the other hand, if one cannot find any vertex whose constraints are the same, we can find either an alternating loop or a quasi-alternating loop in the graph. If a quasi-alternating loop is found, we know the state for the special vertex of the loop and can use the induction hypothesis on the remaining system. Otherwise, if an alternating loop is found, we can write any state in the ground space as

$$|\Phi\rangle = |00\cdots0\rangle|\Psi_0\rangle + |11\cdots1\rangle|\Psi_1\rangle, \qquad (3)$$

up to local operations on the loop. If a constraint acts on two qubits on the loop, it can only restricts the loop to be exactly $|00\cdots0\rangle$ or $|11\cdots1\rangle$. The analysis is similar to the first case when a constraint $|\alpha\rangle_a|\beta\rangle_b$ acts on one qubit a on the loop and another qubit b outside of the loop. This completes the proof. Notice that the local operations chosen here are determined by the constraints of alternating loops, and that one will never have two alternating loops giving different local operations for a single qubit, the orthogonality of the states up to local operations follows. We note that the orthogonality property only holds for the product constraints. The symmetric subspace, for example, is not a span of *orthogonal* product states up to local operations although it is the span of $|00\rangle, |11\rangle, |{+}{+}\rangle$ where $|+\rangle = (|0\rangle + |1\rangle)/\sqrt{2}$.

General homogeneous case.— Given a general homogeneous Hamiltonian, the interaction graph will consist both solid and dashed edges. The main technique is to simplify the interaction graph in hand without changing the ground space. Two sliding operations as shown in Figs. 3a and 3b will be used in the simplification. The `Type-I` sliding says that if we have entangled interactions between $1,2$ and $1,3$, we can change it to two entangled interactions between $1,2$ and $2,3$ without affecting the ground space. The `Type-II` sliding is of a similar spirit, but involves both entangled and product interactions. We will only prove the validity of `Type-I` sliding as a similar argument holds for the `Type-II` sliding operation.



(a) Type-I Sliding (b) Type-II Sliding (c) An example of simplified interaction graph

FIG. 3: Simplification of the interaction graph

Let $\Pi_{12} = |\phi\rangle\langle\phi|$ and $\Pi_{13} = |\psi\rangle\langle\psi|$ be the two rank-1 operators acting on qubit $1,2$ and $1,3$. We will find a local interaction Π_{23} acting on $2,3$ such that $\Pi_{12} + \Pi_{23}$ has the same ground space as $\Pi_{12} + \Pi_{13}$. As $|\phi\rangle$ and $|\psi\rangle$ are entangled states, one can find local operations L_2 and L_3 acting on qubit 2 and 3 respectively such that $|\phi\rangle = I_1 \otimes L_2|Y\rangle$ and $|\psi\rangle = I_1 \otimes L_3|Y\rangle$ where $|Y\rangle$ is the singlet state $(|01\rangle - |10\rangle)/\sqrt{2}$. The ground space of $\Pi_{12} + \Pi_{13}$ is therefore

$$\begin{aligned} &\mathcal{K}(I \otimes L_2|Y\rangle\langle Y|_{12} I \otimes L_2^\dagger + I \otimes L_3|Y\rangle\langle Y|_{13} I \otimes L_3^\dagger) \\ =\ &(L^\dagger)^{-1}\mathcal{K}(|Y\rangle\langle Y|_{12} + |Y\rangle\langle Y|_{13}) \\ =\ &(L^\dagger)^{-1}\mathcal{K}(|Y\rangle\langle Y|_{12} + |Y\rangle\langle Y|_{23}) \\ =\ &\mathcal{K}(\Pi_{12} + L_2 \otimes L_3|Y\rangle\langle Y|_{23} L_2^\dagger \otimes L_3^\dagger), \end{aligned}$$

where the first equation uses Eq. (2), the second one is obtained by a direct calculation establishing that

$\mathcal{K}(|Y\rangle\langle Y|_{12}+|Y\rangle\langle Y|_{13})$ is the symmetric subspace of the three qubits, and the last step employs Eq. (2) again. This validates the `Type-I` sliding operation.

Repeated applications of the two types of sliding operations can modify an arbitrary graph (a homogeneous Hamiltonian) with solid and dashed edges to the so-called simplified interaction graph (simplified homogeneous Hamiltonian). The simplified graph has a backbone of only dashed edges and several solid-edge tails attached to the backbone. An example of such a graph is shown in Fig. 3c. This simplification can be done in two steps by first changing each connected component of solid edges into a tail, and then sliding all dashed edges connected to a tail to one end of the tail. During the process of the sliding operations, it may happen that there is more than one edge between two vertices. If these multiple edges represent different constraints, one will essentially have a high rank constraint and can deal with it as before in the case study of rank.

Simplified homogeneous case.— Since sliding operations do not change the ground space, we only need to work with simplified interaction graphs. The idea is to build the entire ground space by extending the ground space for the dashed backbone. Let us first consider the case where there is only one tail in the simplified interaction graph. More specifically, let S be the ground space of the dashed constraints in the backbone J, and T be the symmetric subspace confined by the tail of qubit set K, where $J\cap K$ has exactly one qubit a, through which the tail is attached to the backbone. We prove that $R=S\otimes\mathcal{H}_{K\setminus\{a\}}\cap T\otimes\mathcal{H}_{J\setminus\{a\}}$ is again a product span. Write S as the direct sum

$$(S_0\otimes\mathcal{H}_a)\oplus\left(\bigoplus_{j=1}^{d}S_j\otimes|\alpha_j^{\perp}\rangle_a\right),$$

where $|\alpha_j\rangle_a$'s are different dashed constraints on vertex a and d is number of such $|\alpha_j\rangle_a$'s. For the basis of S_0, all the constraints in the backbone are already satisfied, and therefore, the qubit a can be any state. We say that qubit a is free in this case. For the basis of S_j, qubit a has to be $|\alpha_j^{\perp}\rangle$ in order to satisfy all the constraints in the backbone. In this case, the state can only be extended to the tail by copying. In summary, the intersection R contains the space

$$(S_0\otimes T)\oplus\left(\bigoplus_{j=1}^{d}S_j\otimes|\alpha_j^{\perp}\rangle^{\otimes|T|}\right). \qquad (4)$$

We will need to show that this is actually everything in R.

We first claim that the product basis for S_j's all together form a linearly independent set. By orthogonality (up to local operations), S_j and S_k are orthogonal if $|\alpha_j\rangle$ and $|\alpha_k\rangle$ are not. On the other hand, if $|\alpha_j\rangle$ and $|\alpha_k\rangle$ are orthogonal, the basis for S_j and S_k are linearly independent. Otherwise, we will find a state $|\psi\rangle$ in both S_j and S_k, meaning that $|\psi\rangle$ should be in S_0, a contradiction. Now, for any state $|\Psi\rangle$ in R, we can write it as $|\Psi\rangle=\sum_j|\Psi_j\rangle|\Phi_j\rangle$ where $|\Psi_j\rangle$'s are linearly independent product states spanning S. Let $|\hat{\Psi}_j\rangle$ be the state on $J\setminus\{a\}$ when the state on J is $|\Psi_j\rangle$. One can also collect terms according to the state on $J\setminus\{a\}$, that is, $|\Psi\rangle=\sum_k|\hat{\Psi}_k\rangle\sum_l|\Psi\rangle_{k,l}^a|\Phi_{k,l}\rangle$. As shown previously, $|\hat{\Psi}_k\rangle$'s are linearly independent, and we know $\sum_l|\Psi\rangle_{k,l}^a|\Phi_{k,l}\rangle$ is in T for each k. That is, the state $|\psi\rangle$ is indeed in the space of Eq. (4). As the symmetric subspace can always be spanned by product states, we have finished the proof for the case of one tail. For multiple tails, the proof is essentially the same by an induction on the number of tails.

Application to the counting of degeneracy.— The results above actually allow us to prove that counting the ground state degeneracy of a 2BFF Hamiltonian is in #P. The class #P contains functions f if there is a polynomial time algorithm A such that

$$f(x)=|\{y,A(x,y)\text{ accepts.}\}|,$$

where y is usually called a proof to the verifier A.

As indicated by the ground space structure in Fig. 1, the isometries will not change the dimension and we only need to consider the simplified homogeneous case where one can actually replace the solid edges of the tails to be dashed edges forming alternating chains. As long as we choose the constraint of the tail on the vertex connecting to the backbone to be different from all other constraints $|\alpha_j\rangle$ of that vertex, the dimension of the solution space remains unchanged. To understand this, we need to review the extension of the product span with intersection of symmetric subspaces. If the vertex in the intersection is free, we will have the whole symmetric subspace on the tail which is of dimension $k+1$ where k the number of qubits in the tail. This coincides with the dimension of the alternating chain. If the vertex in the intersection is not free, we will have a unique extension in the tail, which again coincides with the case of alternating chain.

It therefore suffices to count the dimension of any dashed graph. To show that it is in #P, one can choose the proof to the verifier to be the non-deterministic $0,1$ choices in the case of (1) all-the-same-constraint vertex and (2) alternating loop.

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[1] B. Nachtergaele, arXiv:math-ph/0603017v2.
[2] H. T. Diep, *Magnetic Systems With Competing Interactions* (World Scientific Publishing Company, 2004).
[3] I. Affleck, T. Kennedy, E. H. Lieb, and H. Tasaki, Phys. Rev. Lett. **59**, 799 (1987).
[4] A. Kitaev and C. Laumann, arXiv:0904.2771.
[5] M. Levin and X.-G. Wen, Phys. Rev. Lett. **96**, 110405 (2006).
[6] A. Y. Kitaev, A. H. Shen, and M. N. Vyalyi, *Classical and Quantum Computation* (American Mathematical Society, 2002).
[7] S. Bravyi, arXiv:quant-ph/0602108.
[8] M. Sipser, *Introduction to the Theory of Computation* (PWS Publishing Company, 2005).
[9] J. Chen, X. Chen, R. Duan, Z. Ji, and B. Zeng, arXiv:1004.3787.
[10] C. Laumann, R. Moessner, A. Scardicchio, and S. Sondhi, Quant. Inf. and Comp. **10**, 0001 (2010).
[11] S. Bravyi, C. Moore, and A. Russell, arXiv:0907.1297.
[12] C. Laumann, A. Läuchli, R. Moessner, A. Scardicchio, and S. Sondhi, arXiv:0910.2058.
[13] A. Ambainis, J. Kempe, and O. Sattath, arXiv:0911.1696.
[14] N. de Beaudrap, M. Ohliger, T. Osborne, and J. Eisert, arXiv:1005.3781.
[15] L. G. Valiant, Theor. Comp. Sci. **8**, 189 (1979), ISSN 0304–3975.
[16] D. Perez-Garcia, F. Verstraete, M. M. Wolf, and J. I. Cirac, Quant. Inf. Comp. **7**, 401 (2007).
[17] Y.-Y. Shi, L.-M. Duan, and G. Vidal, Phys. Rev. A **74**, 022320 (2006).