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Phys. Rev. A **84**, 042338 — Published 27 October 2011

DOI: [10.1103/PhysRevA.84.042338](https://doi.org/10.1103/PhysRevA.84.042338)

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

Zhengfeng Ji,<sup>1,2</sup> Zhaohui Wei,<sup>3</sup> and Bei Zeng<sup>4,5</sup>

<sup>1</sup>*Perimeter Institute for Theoretical Physics, Waterloo, Ontario, Canada*

<sup>2</sup>*State Key Laboratory of Computer Science, Institute of Software, Chinese Academy of Sciences, Beijing, China*

<sup>3</sup>*Centre for Quantum Technologies, National University of Singapore, Singapore 117543, Singapore*

<sup>4</sup>*Department of Mathematics & Statistics, University of Guelph, Guelph, Ontario, Canada*

<sup>5</sup>*Institute for Quantum Computing, University of Waterloo, Waterloo, Ontario, Canada*

(Dated: Dec. 20, 2010)

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.

PACS numbers: 03.67.Lx, 03.67.Mn, 75.10.Jm

## I. INTRODUCTION

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 are 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 interactions are of the most physical relevance, as two-body interactions, in particular of nearest neighbors or next nearest neighbors on certain types 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 on a classical computer [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, 15].

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 can be described as “being generated”, from products of single qubit states, by applying the same series of isometries (from single qubit to two qubits). Tree-like networks of isometries appeared before as a tool of constructing variational ground states for frustrated systems [16], here we show that it provides exact ground states for 2BFF Hamiltonians.

As this characterization holds for the most general case, it implies the problem of determining the ground state degeneracy is as hard as, but no harder than, its classical analog. Putting this in a more formal language of computational complexity theory, our results give a proof that computing the degeneracy of 2BFF Hamiltonian ( $\#Q$ -2-SAT) is in a complexity class called  $\#P$  [17]. On the other hand, the classical analog  $\#2$ -SAT of  $\#Q$ -2-SAT is  $\#P$ -hard, therefore the  $\#Q$ -2-SAT problem is

#P-complete. This answered an open question raised in [11]. Therefore our results further bridge the studies in both quantum many body physics and computer science.

## II. TWO-BODY FRUSTRATION-FREE HAMILTONIAN

Consider a system of  $n$  qubits labeled by the set  $V = \{1, 2, \dots, n\}$ . 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

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

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 structure of excited states, that matters for the ground space of a frustration-free Hamiltonian  $H$ . Denote the projection to the ground space of  $H_J$  by  $\Pi_J$ . Since the ground space of  $\Pi_J$  and that of  $H_J$  are the same, it suffices to consider local terms to be projections  $\Pi_J$  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 simple relation between local operations and frustration-free Hamiltonians turns out to be useful. Let  $L_j$  be a non-singular local operator acting on the  $j$ -th qubit. Note that  $L_j$  might not be a physical operation, which is introduced for the convenience of discussion. Define local operations  $L = \bigotimes_{j=1}^n L_j$ ,  $L_J = \bigotimes_{j \in J} L_j$ . The action of  $L$  on  $H = \sum H_J$  is defined to be the map from

$$H = \sum H_J \text{ to}$$

$$H^L = \sum L_J^\dagger H_J L_J. \quad (2)$$

Notice that  $H^L$  is still a two-body Hamiltonian for qubits. The relation between the ground space of  $H$  and  $H^L$  is

$$L^{-1}\mathcal{K}(H) = \mathcal{K}(H^L). \quad (3)$$

To see this, first let  $|\Psi\rangle \in L^{-1}\mathcal{K}(H)$ . This is equivalent to  $L|\Psi\rangle \in \mathcal{K}(H)$  and, by Eq. (1), to  $H_J L|\Psi\rangle = 0$  for all  $J$ . The last condition holds if and only if  $|\Psi\rangle \in \mathcal{K}(H^L)$  by the non-singularity of  $L_j$ 's.

## III. THE GROUND SPACE STRUCTURE AND THE HOMOGENEOUS CASE

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  $\Pi_J$ 's are projections onto  $\mathcal{K}(H_J)^\perp$ . We will start our analysis by considering the rank of the projections  $\Pi_J$ .

First, if there is a  $\Pi_J$  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  $\Pi_J$  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  $U : |0\rangle_d \mapsto |\psi_0\rangle_{a,b}$ ,  $|1\rangle_d \mapsto |\psi_1\rangle_{a,b}$ . One concern of this encoding is what will happen to other terms of the Hamiltonian that represent interactions between a qubit in  $J$  and one outside  $J$ . Consider, for example, a local term  $\Pi_{a,c}$  between qubits  $a$  and  $c$ . In this case, one can view  $\Pi_{a,c}$  as a term acting on  $a, b, c$  and, after the encoding, it is again an interaction of two qubits, namely  $c$  and  $d$ . More formally, for terms like  $\Pi_{a,c}$ , one can replace it with  $U^\dagger(\Pi_{a,c} \otimes I_b)U$ . 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 in 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. In this figure, every blue triangle is an isometry operation, where the input (the qubit on the left of the triangle) encodes the output (the two qubits on the right of the triangle). By these isometries, the ground space of the original Hamiltonian can be outputted when the input of the whole forest is the ground space of the simplified homogenous Hamiltonian, which is spanned by a set of product states. In the language of tensor network states [18, 19], one can also represent these states in terms of tree tensor networks after combining the input product states and the roots of trees in the forest.

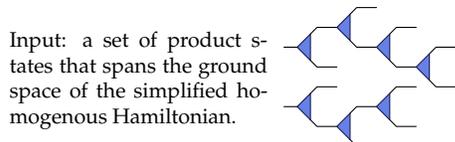


FIG. 1: The general structure of the ground space

Consider the Hamiltonian  $H = \sum \Pi_J$  where  $\Pi_J$ '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  $\Pi_J$  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.

Given a general homogeneous Hamiltonian, the interaction graph will consist of 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. 2a and 2b 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 the **Type-I** sliding as a similar argument holds for the **Type-II** sliding operation.

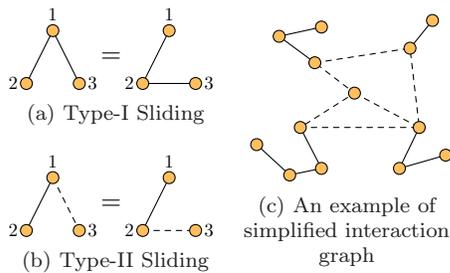


FIG. 2: Simplification of the interaction graph

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  $\Pi_{23}$  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. (3), 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. (3) 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 (denoted by  $S$ ) has a backbone (denoted by  $B$ ) of only dashed edges and several solid-edge tails attached to the backbone. An example of such a graph is shown in Fig. 2c. 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 using the isometry technique discussed in the previous section.

#### IV. THE SIMPLIFIED HOMOGENEOUS CASE

We now study the simplified homogeneous case. The interaction graph has a simple structure which intuitively suggests what the corresponding ground space may look like. We start from analyzing the backbone, where all the edges are dashed lines. We observe the following

**Observation 1.** *For the interaction graph with dotted edges only, the ground space is spanned by orthogonal single-qubit product states.*

To understand this observation, note for an interaction graph with only dotted edges, it contains only product state constraints  $\Pi_{ij} = |\psi\rangle\langle\psi|$  with  $|\psi\rangle = |\alpha_i\rangle \otimes |\alpha_j\rangle$ . Note if we consider the corresponding classical problem in this setting, all the constraints are product states of computational basis states  $|0\rangle$  and  $|1\rangle$ . In this case the solution space is obviously spanned by product states in the computational basis. In the quantum case, however, a general product state constraint  $|\alpha_i\rangle \otimes |\alpha_j\rangle$  may not have  $|\alpha_i\rangle$  and  $|\alpha_j\rangle$  be the computational basis states.

However, given a single product state constraint  $|\alpha_i\rangle \otimes |\alpha_j\rangle$ , one can always transform both  $|\alpha_i\rangle, |\alpha_j\rangle$  to some computational basis states by a local operation  $L = L_i \otimes L_j$ . Note according to Eqs.(2,3), this local operation does not change the ground space dimension and the product state structure. Further more, if an  $n$ -vertex interaction graph with only dotted edges is one dimensional (1D) in geometry, (a straight line or a ring), then one can always find a local operation  $L = \bigotimes_{i=1}^n L_i$  which transforms all the constraints simultaneously to product states of computational basis states. So a 1D backbone is essential ‘classical’.

It turns out this simple 1D analysis is enough to reduce the  $n$ -particle problem to an  $n - 1$  particle problem, which leads to a proof by induction that the ground space of a Hamiltonian (denoted by  $H_B$ ) corresponding to an interaction graph with only dotted edges (the backbone), can be spanned by product states. Indeed, by properly choosing the invertible operators  $L_i$ ’s, we can further show that the ground space can be spanned by orthogonal product states, with the intuitive idea that invertible operators can transform non-orthogonal states to orthogonal states.

Concretely, firstly let us first examine several simple examples. The first example considers a chain of interactions as in Fig. 3b. 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  $k + 1$ -dimensional for an alternating chain of  $k$  qubits. The second example shown in Fig. 3c 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  $|00 \dots 0\rangle$  and  $|11 \dots 1\rangle$  up to the local operation  $L = \bigotimes_j L_j$  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 3d 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. 3d, the top vertex must be  $|1\rangle$  as otherwise it will be impossible to satisfy all five constraints on the loop.

We now start the proof of Observation 1 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.

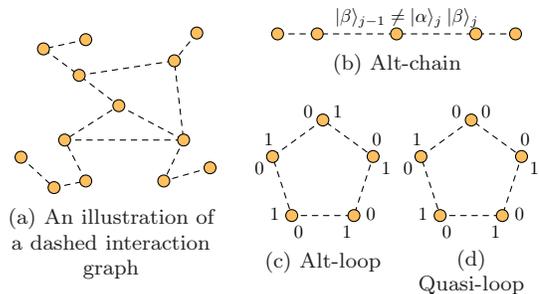


FIG. 3: Dashed interaction graph and three examples

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

$$|\Phi\rangle = |00 \dots 0\rangle |\Psi_0\rangle + |11 \dots 1\rangle |\Psi_1\rangle, \quad (4)$$

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  $|00 \dots 0\rangle$  or  $|11 \dots 1\rangle$ . 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  $|+\rangle = (|0\rangle + |1\rangle)/\sqrt{2}$ .

We now move to discuss the entire simplified homogeneous case, with a interaction graph with both backbone and solid edge tails attached to the backbone. Based on Observation 1, we further have

**Observation 2.** *For the simplified interaction graph, the ground space is spanned by single-qubit product states.*

To understand this observation, denote the homogeneous Hamiltonian corresponding to a simplified interaction graph by  $H_S$ . Note that given the orthogonal product states that span the solution space of  $H_B$ , ground states of  $H_S$  can be obtained in the following way. Recall that the ground space corresponds to each solid edge tail is essentially a symmetric space. Therefore, for any product state  $\bigotimes_{i=1}^{|B|} |\alpha_i\rangle$  on the backbone, and the  $i$ -th qubit connected to the solid tail  $\Gamma_i$ , the state  $\bigotimes_{i=1}^{|B|} |\Gamma_i\rangle$  is a ground state of  $H_S$ , where  $|\Gamma_i\rangle = |\alpha_i\rangle^{\otimes |\Gamma_i|}$ . This is very straightforward as the symmetric space associated with each solid edge tail simply enforces ‘copying’ the

state of the qubit in the backbone to the qubits on the attached tail.

More specifically, let  $\mathcal{B}$  be the ground space of the dashed constraints in the backbone  $B$ , and  $\mathcal{T}$  be the symmetric subspace confined by the tail of qubit set  $T$ , where  $B \cap T$  has exactly one qubit  $a$ , through which the tail is attached to the backbone. We prove that  $\mathcal{S} = \mathcal{T} \otimes \mathcal{H}_{B \setminus \{a\}} \cap \mathcal{B} \otimes \mathcal{H}_{T \setminus \{a\}}$  is again a product span. Write  $\mathcal{B}$  as the direct sum

$$(\mathcal{B}_0 \otimes \mathcal{H}_a) \oplus \left( \bigoplus_{j=1}^d \mathcal{B}_j \otimes |\alpha_j^\perp\rangle_a \right),$$

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  $\mathcal{B}_0$ , 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  $\mathcal{B}_j$ , 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,  $\mathcal{S}$  contains the space

$$(\mathcal{B}_0 \otimes \mathcal{T}) \oplus \left( \bigoplus_{j=1}^d \mathcal{B}_j \otimes |\alpha_j^\perp\rangle^{\otimes |T|} \right). \quad (5)$$

We will need to show that this is actually everything in  $\mathcal{S}$ .

We first claim that the product basis for  $\mathcal{B}_j$ 's all together form a linearly independent set. By orthogonality (up to local operations),  $\mathcal{B}_j$  and  $\mathcal{B}_k$  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  $\mathcal{B}_j$  and  $\mathcal{B}_k$  are linearly independent. Otherwise, we will find a state  $|\psi\rangle$  in both  $\mathcal{B}_j$  and  $\mathcal{B}_k$ , meaning that  $|\psi\rangle$  should be in  $\mathcal{B}_0$ , a contradiction. Now, for any state  $|\Psi\rangle$  in  $\mathcal{S}$ , 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  $\mathcal{B}$ . Let  $|\hat{\Psi}_j\rangle$  be the state on  $B \setminus \{a\}$  when the state on  $B$  is  $|\Psi_j\rangle$ . One can also collect terms according to the state on  $B \setminus \{a\}$ , 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. (5). 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.

## V. APPLICATION

One important application of our results is to analyze the computational complexity of the problem of counting the ground degeneracy of two-body frustration-free qubit Hamiltonians. Previously, this problem was considered to be hard due to the possible entanglement structure in

the ground space [11]. Our complete characterization of the ground space shows that the ground space does have simple structure where entanglement plays no essential role. Therefore, determining the ground state degeneracy is as hard as, but no harder than, its classical analog. In a more formal language of computational complexity theory, our results can lead to a proof that computing the degeneracy of 2BFF Hamiltonian ( $\#Q$ -2-SAT) is in a complexity class called  $\#P$  [17]. 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  $|S|$  means the cardinality of set  $S$ , and  $y$  is usually called a proof to the verifier  $A$ .

In order to count the ground state degeneracy of 2BFF Hamiltonian, we should note the following two facts. Firstly, as indicated by the ground space structure in Fig. 1, the isometries will not change the dimension, so we only need to consider the simplified homogeneous case. Secondly, actually if one replaces the solid edges of the tails to be dashed edges forming alternating chains, the dimension of the ground space does not change either, 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. 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 cases of (1) all-the-same-constraint vertex and (2) alternating loop.

On the other hand, the classical analog  $\#2$ -SAT or  $\#Q$ -2-SAT is  $\#P$ -hard, therefore the  $\#Q$ -2-SAT is  $\#P$ -complete.

## VI. SUMMARY

In this paper, we give a complete characterization of the ground space of two-body frustration-free qubit Hamiltonians. The entire ground space is shown to be a span of tree tensor network states. This proof contains two major steps. First, we reduce the problem to the homogeneous case by isometries. Second, we reduce the homogeneous case to the simplified homogeneous case by two types of sliding operations which do not change the ground space, giving a much more intuitive picture to analyze the problem.

Our results sharpen the understanding of quantum spin-1/2 systems, and hopefully, provide ideas for the further research of quantum many-body systems, as well as further bridges between the studies in quantum many body physics and computer science.

### Acknowledgments

We thank S. Bravyi and X.G. Wen for valuable discussions. ZJ acknowledges support from NSF of China

(Grant No. 60736011); his research at Perimeter Institute is supported by the Government of Canada through Industry Canada and by the Province of Ontario through the Ministry of Research & Innovation. ZW is supported by the grant from the Centre for Quantum Technologies, the WBS grant under contract no. R-710-000-007-271 and R-710-000-008-271. BZ is supported by NSERC and CIFAR.

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