

**No-go theorem for one-way quantum computing on naturally occurring two-level systems**Jianxin Chen,<sup>1</sup> Xie Chen,<sup>2</sup> Runyao Duan,<sup>1,3</sup> Zhengfeng Ji,<sup>4,5</sup> and Bei Zeng<sup>6</sup><sup>1</sup>*Department of Computer Science and Technology, Tsinghua National Laboratory for Information Science and Technology, Tsinghua University, Beijing, China*<sup>2</sup>*Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts, USA*<sup>3</sup>*Centre for Quantum Computation and Intelligent Systems (QCIS), Faculty of Engineering and Information Technology, University of Technology, Sydney, New South Wales, Australia*<sup>4</sup>*Perimeter Institute for Theoretical Physics, Waterloo, Ontario, Canada*<sup>5</sup>*State Key Laboratory of Computer Science, Institute of Software, Chinese Academy of Sciences, Beijing, China*<sup>6</sup>*Institute for Quantum Computing and Department of Combinatorics and Optimization, University of Waterloo, Waterloo, Ontario, Canada*

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The ground states of some many-body quantum systems can serve as resource states for the one-way quantum computing model, achieving the full power of quantum computation. Such resource states are found, for example, in spin- $\frac{5}{2}$  and spin- $\frac{3}{2}$  systems. It is, of course, desirable to have a natural resource state in a spin- $\frac{1}{2}$ , that is, qubit system. Here, we give a negative answer to this question for frustration-free systems with two-body interactions. In fact, it is shown to be impossible for any genuinely entangled qubit state to be a nondegenerate ground state of any two-body frustration-free Hamiltonian. What is more, we also prove that every spin- $\frac{1}{2}$  frustration-free Hamiltonian with two-body interaction always has a ground state that is a product of single- or two-qubit states. In other words, there cannot be any interesting entanglement features in the ground state of such a qubit Hamiltonian.

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Quantum computers are distinct from classical ones, not only in that they can solve hard problems that are intractable on classical computers, factoring large numbers for example [1], but also in that they can be implemented in architectures such as one-way quantum computing [2–4] that have no evident classical analogs at all. Unlike the quantum circuit model [5–7], which employs entangling gates during the computation, one-way quantum computation requires only single-particle measurements on some prepared entangled state, also known as the resource state. This quantum computation scheme sheds light on the role of entanglement in quantum computation and provides possible advantages in physical implementation of quantum computers. Moreover, from the theoretical computer science perspective, although one-way quantum computations are polynomial-time equivalent to the unitary circuit model, they may have advantages over the circuit model in terms of parallelizability [3, 8, 9]. For example, the quantum Fourier transform [10], the key quantum part of Shor’s factoring algorithm, is approximately implementable in constant depth in the one-way model [11]. All these nice facts about the one-way computing model make it a worthy topic to pursue both theoretically [12–19] and experimentally [4].

Quantum entanglement is believed to be a necessary ingredient of quantum computation [20–22]. This is also the case in the one-way quantum computing [23–26]. However, the entanglement used in a one-way quantum computer is cleanly separated in the initial preparation step from the whole computation. Moreover, it usually has a regular structure and is independent of the computation problem and inputs. This allows us to focus on the preparation of some specific entangled resource state.

An appealing idea is to obtain the resource state in some strongly correlated quantum many-body system at low

temperature. This approach requires the resource state to be the nondegenerate ground state of some gapped Hamiltonian, which involves only two-body nearest-neighbor interactions. In this way, the resource state can be effectively created via cooling, and the procedure is robust against thermal noises. We also want the Hamiltonian to be frustration free; that is, the ground state minimizes the energy of each local term of the Hamiltonian simultaneously, so that measurements in the course of the computation leave the remaining particles in the ground space.

The canonical resource state for one-way quantum computing, known as the cluster state [2], does not naturally occur as a ground state of a physical system [27]. As a result, there have been significant efforts to identify alternative resource states that appear naturally as ground states in spin lattices [13, 14, 28–30]. In Ref. [29], a natural resource state called triCluster is found in a spin- $\frac{5}{2}$  system. Very recently, a two-body spin- $\frac{3}{2}$  Hamiltonian from a quantum magnet was found whose unique ground state is also a universal resource state for one-way quantum computing [30]. As two-level systems are more widely available in practice than higher-level systems, it is natural to ask whether there exists a universal resource state in spin- $\frac{1}{2}$  (qubit) system that naturally occurs.

In this Rapid Communication, however, we show that it is not the case. Namely, a genuinely entangled qubit state cannot be a nondegenerate ground state of any two-body frustration-free Hamiltonian, as there is always a product of single qubit states in the ground space. This indicates that one-way computing with naturally occurring resource states cannot be done with qubits. Therefore, the best one can hope for is to find natural a resource state in spin-1 systems, the existence of which remains an open question, or one needs to resort to some other techniques, such as the perturbation approaches [31, 32].

We also show that any two-body frustration-free Hamiltonian has a ground state that is a product of single- or two-qubit states. This leads to a deeper understanding of the relationship between frustration in the Hamiltonian and entanglement in the ground state of qubit systems. Namely, frustration is necessary for qubit systems to have nontrivial entanglement ground states, and it is necessary only for qubit systems because it is well known that the spin-1 Affleck-Kennedy-Lieb-Tasaki (AKLT) state [33] is a unique ground state of a two-body frustration-free Hamiltonian on a chain. We also emphasize that our result is general as we do not require the interactions to be nearest-neighbor on some lattice or require the system to be gapped.

It is worth noting that our discussion is also closely related to a problem in quantum computational complexity theory, the quantum analog of 2-satisfiability (abbreviated as quantum 2-SAT [34]). We discuss the relation in detail in the next section.

*The frustration-free Hamiltonian.* We start our proof by assuming that there does exist such a naturally occurring state of  $n$  qubits, denoted by  $|\Psi\rangle$ . We also assume for simplicity that the state is genuinely entangled, meaning that it is not a product state with respect to any bipartition of the  $n$ -qubit system.

Given any density matrix  $\rho$ , we define its support  $\text{supp}(\rho)$  to be the subspace spanned by the eigenvectors of nonzero eigenvalues of  $\rho$ . For any two qubits  $i, j$ , the two-particle reduced density matrix of these two qubits of state  $|\Psi\rangle$  is denoted as  $\rho_{ij}$ .

For any state  $|\Psi\rangle$ , define a two-body frustration-free Hamiltonian  $H_\Psi$  that has  $|\Psi\rangle$  in its ground space to be the sum of projections  $\Pi_{ij}$  onto the orthogonal space of the  $\text{supp}(\rho_{ij})$ . That is,

$$H_\Psi = \sum_{ij} \Pi_{ij}. \quad (1)$$

As  $H_\Psi$  is constructed from state  $|\Psi\rangle$ , we call it the two-body frustration-free Hamiltonian of  $|\Psi\rangle$ .

Clearly  $H_\Psi$  is two-body and frustration-free, as  $|\Psi\rangle$  is in the ground space and minimizes the energy of each local term. Note that the ground space of  $H_\Psi$  is given by

$$\mathcal{S}(|\Psi\rangle) = \bigcap_{ij} \text{supp}(\rho_{ij} \otimes I_{\bar{ij}}), \quad (2)$$

where  $I_{\bar{ij}}$  is the identity operator on qubits other than  $i, j$ .

Generally, a frustration-free Hamiltonian  $H = \sum H_k$  needs not to be a summation of projections. However, we can always find one whose local terms are indeed projections and has the same ground space as  $H$ . More specifically, one can choose  $\Pi_k$  to be the projection onto the orthogonal space of the ground space of  $H_k$  and consider  $\sum \Pi_k$  instead. Therefore, we only consider frustration-free Hamiltonians that are summations of projections in this Rapid Communication. It is also not hard to see that any two-body frustration-free Hamiltonian  $H'$  that has  $|\Psi\rangle$  as a ground state also contains  $\mathcal{S}(|\Psi\rangle)$  in its ground space. In other words,  $H_\Psi$  has the smallest possible ground space among all frustration-free Hamiltonians having  $|\Psi\rangle$  as a ground state.

There is a natural correspondence between a two-body frustration-free Hamiltonian  $H$  and the quantum 2-SAT

problem. Classically, a 2-SAT problem asks whether a logical expression in the conjunctive normal form with two variables per clause, for example,  $(x_0 \vee x_1) \wedge (\neg x_1 \vee x_2) \wedge (x_2 \vee \neg x_0)$ , is satisfiable, where  $x_i$  are Boolean variables and  $\wedge, \vee, \neg$  are logical AND, OR, NOT operations, respectively. There is a well-known polynomial time classical algorithm that solves 2-SAT while the related 3-SAT problem is believed to be much harder (NP-Complete [35]). In Ref. [34], it was proved that the quantum analog of the 2-SAT problem, which asks whether a set of projections on two-qubit subsystems has a simultaneous ground state, is also efficiently solvable on a classical computer. It was also shown there that quantum 4-SAT is one of the hardest problems in  $\text{QMA}_1$  (a quantum analog of NP [35]), meaning that it is probably hard even for quantum computers. The relation between a frustration-free Hamiltonian and its corresponding quantum SAT problem is evident. The Hamiltonian  $H$  is indeed frustration-free, thereby having 0 ground energy, if and only if the quantum SAT problem defined by the set of projections in the Hamiltonian  $H$  is satisfiable. In the case of two-body Hamiltonian  $H_\Psi$ , the corresponding Quantum 2-SAT problem is defined by  $\Pi_{ij}$ 's. If for each term  $\Pi_{ij}$ , the rank of it is either 0 or 1, the corresponding quantum 2-SAT problem is called homogeneous [34], a concept that is used in the following.

Now we go back to the Hamiltonian problem and show that  $|\Psi\rangle$  cannot be a unique ground state of any two-body frustration-free Hamiltonian by proving the following theorem.

*Theorem 1.* Given an  $n$ -qubit state  $|\Psi\rangle$  that is genuinely entangled and any two-body frustration-free Hamiltonian  $H$  having  $|\Psi\rangle$  as its ground state, there always exists a product state of single qubits also in the ground space of  $H$  for  $n \geq 3$ .

As  $H_\Psi$  has the smallest ground space, we only need to prove the theorem for  $H_\Psi$  instead of the general  $H$ . Also, it is equivalent to prove that  $\mathcal{S}(|\Psi\rangle)$  is of dimension at least 2 and contains a product state of single qubits.

*Proof of the theorem.* We prove this theorem by induction. Before doing so, we examine the following fact. Let  $|\Psi\rangle$  and  $|\Phi\rangle$  be two  $n$ -qubit states that can be transformed into each other by invertible local operations. That is, there are  $2 \times 2$  nonsingular linear operators  $L_1, \dots, L_n$ , such that  $|\Psi\rangle = \mathcal{L}|\Phi\rangle$ , where  $\mathcal{L} = L_1 \otimes \dots \otimes L_n$ . This is equivalent to saying that  $|\Psi\rangle$  and  $|\Phi\rangle$  can be transformed to each other via stochastic local operation and classical communication (SLOCC) [36,37]. Noticing the fact [38] that  $|\Psi\rangle$  is a ground state of  $H$  if and only if  $|\Phi\rangle$  is a ground state of

$$H' = \sum_{ij} (L_i \otimes L_j)^\dagger \Pi_{ij} (L_i \otimes L_j), \quad (3)$$

and the trivial fact that  $\mathcal{L}$  maps product states to product states, we only need to discuss states that are representatives of equivalent classes induced by such local transforms  $\mathcal{L}$ . Equivalently, it suffices to consider SLOCC equivalent classes.

For three-qubit genuinely entangled states, there are only two different SLOCC equivalent classes [37], represented by the  $|W\rangle$  and  $|\text{GHZ}\rangle$ , respectively, where  $|W\rangle = (|001\rangle + |010\rangle + |100\rangle)/\sqrt{3}$ , and  $|\text{GHZ}\rangle = (|000\rangle + |111\rangle)/\sqrt{2}$ . For the  $|W\rangle$  state, one has

$$\mathcal{S}(|W\rangle) = \text{span}\{|W\rangle, |000\rangle\}; \quad (4)$$

therefore, the product state  $|000\rangle$  is in the ground space. While for  $|\text{GHZ}\rangle$ ,

$$\mathcal{S}(|\text{GHZ}\rangle) = \text{span}\{|000\rangle, |111\rangle\}, \quad (5)$$

both product states  $|000\rangle$  and  $|111\rangle$  are in the ground space. This then proves the theorem for the three-qubit case.

Now we proceed to the four-qubit case. Note that  $|\Psi\rangle$  is genuinely entangled, meaning all  $\rho_{ij}$  must be of rank at least 2; that is, the dimension of the  $\text{supp}(\rho_{ij})$  is at least 2 and the rank of  $\Pi_{ij}$  is at most 2. We discuss two cases here.

*Case 1.* If for some pair of qubits, say (3,4), the rank of their reduced density matrix  $\rho_{34}$  is 2, then the pair of qubits 3,4 can be encoded as a single qubit. Therefore, we can reduce our problem to a similar one of smaller system size.

To be more precise, suppose  $\rho_{34}$  is supported on two orthogonal states  $|\psi_0\rangle_{34}$  and  $|\psi_1\rangle_{34}$ . Define an isometry

$$V : |0\rangle_{3'} \rightarrow |\psi_0\rangle_{34}, |1\rangle_{3'} \rightarrow |\psi_1\rangle_{34}, \quad (6)$$

which maps a single qubit to two qubits. That is, we have used qubit  $3'$  to encode the two qubits 3,4. Define  $|\Phi\rangle = V^\dagger|\Psi\rangle$  so that  $|\Psi\rangle$  is a ground state of  $H$  if and only if  $|\Phi\rangle$  is a ground state of  $H' = V^\dagger H V$ . One can easily verify that  $H'$  is still a two-body frustration-free Hamiltonian and  $|\Phi\rangle$  is a genuinely entangled state of three qubits. This reduces to a case already proved and there is product state  $|\alpha_1\rangle \otimes |\alpha_2\rangle \otimes |\alpha_3\rangle$  which is also a ground state of  $H'$ .

Let  $|\beta_{34}\rangle$  be  $V|\alpha_3\rangle$ , a two-qubit state of qubits 3,4. If it is a product state, then we are done. If it is entangled, as  $\rho_{34}$  is supported on a two-dimensional space, there always exists a product state  $|\beta_3\rangle \otimes |\beta_4\rangle \in \text{supp}(\rho_{34})$  [39]. Consider now the bipartition between qubits 1,2 and qubits 3,4. As  $|\beta_{34}\rangle$  is entangled, any projection term that concerns two qubits from different partitions will have trivial constraints on qubits 3 and 4. Therefore, the product state  $|\alpha_1\rangle \otimes |\alpha_2\rangle \otimes |\beta_3\rangle \otimes |\beta_4\rangle$  is also a ground state of  $H$ .

*Case 2.* If all of the  $\text{supp}(\rho_{ij})$  are of rank 3 or 4, we employ the homogeneous 2-SAT and completion techniques in Ref. [34] to finish the proof. The completion procedure adds possibly new projection terms to the frustration-free Hamiltonian without changing the ground space. For any three qubits, say 1,2,3, the procedure takes two rank-1 Hamiltonian terms, say  $\Pi_{12}$  and  $\Pi_{23}$ , and generates a possibly new constraint  $\Omega_{13}$ . See Fig. 1 for an illustration. We briefly review the specific rule for obtaining  $\Omega_{13}$  from  $\Pi_{12}$  and  $\Pi_{23}$  and refer the interested readers to Ref. [34] for the proof and details. Let  $\Pi_{12} = |\phi\rangle\langle\phi|$ ,  $\Pi_{23} = |\theta\rangle\langle\theta|$ , and  $\Omega_{13} = |\omega\rangle\langle\omega|$ , where  $|\phi\rangle, |\theta\rangle, |\omega\rangle$  are two-qubit pure states. Denote, for example,  $\phi_{\alpha,\beta}$  as the amplitude  $\langle\alpha, \beta|\phi\rangle$ . Then relation is given by  $\omega_{\alpha,\gamma} = \phi_{\alpha,\beta} \epsilon_{\beta,\delta} \theta_{\delta,\gamma}$ , where  $\epsilon = |0\rangle\langle 1| - |1\rangle\langle 0|$  and the summation of repeated indices is implicit [34].

The key point here is that the construction of  $H_\Psi$  guarantees that no new constraint could ever be added during the completion procedure. Therefore,  $H_\Psi$  corresponds to a quantum 2-SAT that satisfies all the conditions (homogeneous and completed) in Lemma 2 of Ref. [34] and it follows from the lemma that there is a product of single-qubit states in the ground space of  $H_\Psi$ .

This proves the theorem for the four-qubit case and the general  $n$ -qubit case can be proved by the same induction.

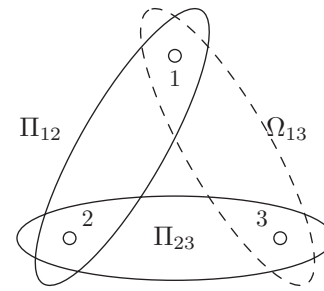


FIG. 1. An illustration of completion procedure.

*Entanglement versus frustration for a qubit system.* We have shown a no-go theorem for one-way quantum computing, which says that in order to do one-way quantum computing with a natural ground state, one has to go to higher-dimensional particle systems other than two-level systems. Interestingly, little extra work will give a better understanding for the relationship of entanglement and frustration for qubit systems, which we now show.

*Theorem 2.* For any two-body frustration-free Hamiltonian  $H$  of a qubit system, there always exists a ground state, which is a product of single- or two-qubit states.

Let  $\bigotimes_{i=1}^m |\Psi_i\rangle$  be a ground state. If  $|\Psi_i\rangle$  is a genuinely entangled state of more than two qubits, there cannot be any nontrivial constraint interacting the qubits of  $|\Psi_i\rangle$  and the remaining qubits in the system. We can therefore apply Theorem 1 to that part of the system and replace  $|\Psi_i\rangle$  with a product state to get another ground state.

This theorem indicates that frustration is a necessary condition for genuine many-body ground-state entanglement in any qubit system.

In the language of quantum 2-SAT, the above theorem states that if a quantum 2-SAT is satisfiable, there will be a ground state that is the product of single- or two-qubit states. This is a much simpler form than the recursive construction in Ref. [34].

If we further require some symmetry of the Hamiltonian, say, a certain kind of translational invariance, there could be only two phases for a nondegenerate frustration-free system with qubits at zero temperature: One is a product state phase, and the other is a dimer phase [40]. This relationship of entanglement and frustration is not true in a spin-1 (qutrit) system. For instance, the famous AKLT state [33] is a nondegenerate ground state of a two-body frustration-free Hamiltonian on a chain. Interestingly, the AKLT state and some of its variants on a chain are indeed powerful enough to process single-qubit information in the one-way quantum computing model [13,19,28,41].

*Summary and discussion.* We have shown that it is impossible for a genuinely entangled qubit state to be a unique ground state of any two-body frustration-free Hamiltonian  $H$ , because there is always a product state of single qubits also in the ground space of  $H$ . This indicates that one-way computing cannot be done on naturally occurring qubit systems. Furthermore, we use a similar technique to prove that every spin- $\frac{1}{2}$  frustration-free Hamiltonian with two-body interaction always has a ground state that is a product of single- or two-qubit states. These results are strong in the sense that they are independent of the lattice structure and therefore

valid for any lattice geometry with natural nearest-neighbor interactions in the Hamiltonian.

A direct consequence also follows for condensed-matter theory. Namely, without frustration, there is no genuine many-body entanglement in a spin- $\frac{1}{2}$  system with two-body interaction. This is not the case for frustration-free higher spin systems or spin- $\frac{1}{2}$  systems with more than two-body interactions. These observations are also closely related to the study of quantum computational complexity theory, which shows that quantum 2-SAT is easy, but quantum 2-SAT with large-enough local dimensions or quantum 3-SAT might be much more difficult [34,42]. Our result also simplifies the structure of the solution space of quantum 2-SAT given in Ref. [34]. However, a full characterization of the solution-space structure needs further investigation. We

hope that our result helps in further investigations of local Hamiltonian problems and in linking the fields of condensed matter, quantum information, and computer science.

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