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Gapped Two-Body Hamiltonian Whose Unique Ground State Is Universal for One-Way Quantum Computation

Xie Chen, Bei Zeng, Zheng-Cheng Gu, Beni Yoshida, and Isaac L. Chuang

Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA

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Many-body entangled quantum states studied in condensed matter physics can be primary resources for quantum information, allowing any quantum computation to be realized using measurements alone, on the state. Such a universal state would be remarkably valuable, if only it were thermodynamically stable and experimentally accessible, by virtue of being the unique ground state of a physically reasonable Hamiltonian made of two-body, nearest-neighbor interactions. We introduce such a state, composed of six-state particles on a hexagonal lattice, and describe a general method for analyzing its properties based on its projected entangled pair state representation.

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Many-body entanglement is fundamental to the understanding of complex condensed matter systems, as well as a primary resource for quantum computation. A surprising result in quantum computation is that certain entangled states can be employed to perform arbitrary quantum information processing tasks, merely by measuring single sites in different bases, in a method known as “one-way” quantum computation [1]. If such universal resource states are available, this approach potentially simplifies experimental requirements by employing only measurements and not multiqubit gates normally needed. Exotic physical properties may arise in these states due to their large amount of entanglement; many methods have been developed in condensed matter theory to study such systems, including the matrix product state formalism [2] or more generally the projected entangled pair states (PEPS) representation [3].

The special entangled states which make arbitrary one-way quantum computation possible unfortunately seem to be difficult to realize naturally. Ideally, such universal resource states could be obtained as the unique ground state of a naturally occurring Hamiltonian, one with only nearest-neighbor two-body interactions. If this were the case, especially if an energy gap existed between the ground and first excited states, the one-way quantum computation could be robust against noise. However, no such Hamiltonian exists for any of the presently known resource states of one-way quantum computation.

Many efforts have been made to construct the desired many-body entangled state such that it could be the ground state of a naturally occurring Hamiltonian. The first and best known resource state is the cluster state, a simple entangled state on a two-dimensional (2D) square lattice; unfortunately, it cannot be the exact ground state of any naturally occurring Hamiltonian [4,5]. Perturbative approaches providing a Hamiltonian whose ground state approximates that desired have been developed [4,6–8]. A nice scheme for constructing universal resource states

has been proposed and has yielded many interesting examples [9]. Based on this, a mixed approach can be taken, using a one-dimensional (1D) Hamiltonian to create chains, which are then coupled by two-body unitary operations [9,10] to form a 2D resource state. Matrix product state [2] techniques allow any measurement of these 1D chains to be computed efficiently, on a classical computer, however, implying that they alone are insufficient for quantum computation. Two-dimensional many-body entangled states are thus likely to be essential for arbitrary quantum computations, but few techniques are presently known for finding local 2D Hamiltonians with the desired ground states. Properties of such states generally remain intrinsically hard to determine [11].

Here, we present results from a new approach to studying the quantum informational and physical properties of 2D many-body entangled states using the PEPS representation. On the one hand, this representation naturally includes many-body entanglement in its state description [3] and hence facilitates understanding of one-way quantum computation schemes [9,12]. On the other hand, methods have been developed to study the physical properties of PEPS states as ground state of parent Hamiltonians [13]. Combining these insights, we are able to construct the first examples of a system which is both the exact unique ground state of a gapped two-body nearest-neighbor Hamiltonian and a universal resource state for one-way quantum computation. Moreover, we aim at reducing the dimension of local Hilbert space in the state as much as possible for experimental convenience, and we arrive at the “tricluster” state which is composed of 6-dimensional particles.

Building on PEPS.—We start with an example which illustrates the challenge. Consider the state $|\psi_{\text{PEPS}}^{\text{Sqr}}\rangle$ defined on a square lattice [Fig. 1(a)] where each pair of nearest-neighbor sites are connected by singlets $|\varphi\rangle = |00\rangle + |01\rangle + |10\rangle - |11\rangle$ (suppressing normalization). On sufficiently large lattices, starting with $|\psi_{\text{PEPS}}^{\text{Sqr}}\rangle$, any

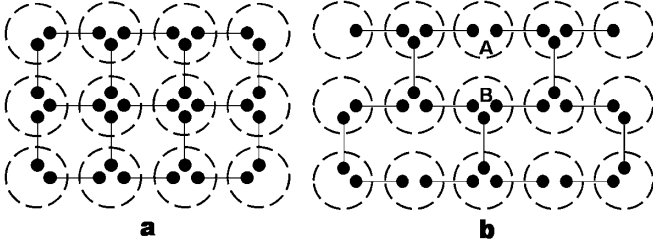


FIG. 1. PEPS representation of 2D (a) square $|\psi_{\text{PEPS}}^{\text{Sqr}}\rangle$ and (b) hexagonal $|\psi_{\text{PEPS}}^{\text{Hex}}\rangle$ lattice states. Filled circles connected by solid lines denote virtual singlet pairs $|\varphi\rangle$. Dashed circles denote projection of virtual qubits into physical states.

quantum circuit can be efficiently simulated by measuring all four qubits at each site (on the boundary, two or three) in appropriate time sequences and measurement bases [12].

$|\psi_{\text{PEPS}}^{\text{Sqr}}\rangle$ is the unique ground state of a gapped two-body Hamiltonian, as it is simply a tensor product of two-body entangled states. However, the multiparticle measurement required to make this state universal [12] is generally disallowed in one-way quantum computation models. Still, if the four qubits at each site were treated as a single 16-dimensional particle, the model could be interpreted as giving the desired result, a universal resource state for one-way quantum computation and also the unique ground state of a gapped two-body Hamiltonian. While use of 16-dimensional particles is experimentally unrealistic, this model does provide a good starting point for constructing simpler states.

Specifically, consider the set of states given by projecting lattices of singlets into smaller subspaces. For example, the projector $P_{\text{Cluster}}^{\text{Sqr}} = |\tilde{0}\rangle\langle 0000| + |\tilde{1}\rangle\langle 1111|$ applied to all sites of the square lattice state gives the cluster state on a square lattice [12] $|\Psi_{\text{Cluster}}\rangle \propto P_{\text{Cluster}}^{\text{Sqr}} |\psi_{\text{PEPS}}^{\text{Sqr}}\rangle$, where $|\tilde{0}\rangle$ and $|\tilde{1}\rangle$ are the physical qubits in the cluster state model. In this ‘‘PEPS representation’’ picture, the physical PEPS state is defined by two elements, a lattice of ‘‘virtual’’ singlets (connecting neighboring sites in the lattice) and a set of projectors which act on lattice sites. Not all PEPS states are universal for quantum computation; only a few, such as $|\Psi_{\text{Cluster}}\rangle$, are known to be universal.

Compared with $|\psi_{\text{PEPS}}^{\text{Sqr}}\rangle$ with 16-dimensional particles, $|\Psi_{\text{Cluster}}\rangle$ employs only qubits at each site, and hence is more experimentally accessible. Unfortunately it cannot occur as the exact ground state of nearest-neighbor interactions [4], and the gapped Hamiltonian having it as a unique ground state involves at least five-body interactions. Moreover, it is known that PEPS states composed of lower dimensional particles generally require larger interaction range in their parent Hamiltonian [13]. Nevertheless, this line of thought, using PEPS states, can indeed lead to a universal resource state which is the unique ground state of a gapped nearest-neighbor Hamiltonian, while also being composed of particles of relatively low dimension, as we now show.

The tricluster state.—The structure of the lattice of singlets, and the choice of projectors, in the construction of PEPS states, provide powerful degrees of freedom for exploring interesting new states. Two specific insights from the above examples illustrate this freedom: (1) Instead of on a square lattice, a cluster state defined on a hexagonal lattice $|\Psi_{\text{Cluster}}^{\text{Hex}}\rangle$ is also universal [14]. On a hexagonal lattice of singlet pairs [Fig. 1(b)], the projector defining this cluster state is $P_{\text{Cluster}}^{\text{Hex}} = |\tilde{0}\rangle\langle 000| + |\tilde{1}\rangle\langle 111|$, giving $|\Psi_{\text{Cluster}}^{\text{Hex}}\rangle \propto P_{\text{Cluster}}^{\text{Hex}} |\psi_{\text{PEPS}}^{\text{Hex}}\rangle$, where the labels denote left-right-up and left-right-down virtual qubits on sites in sublattices A and B, respectively. (2) PEPS states defined with projectors $P' = |\tilde{0}\rangle\langle 100| + |\tilde{1}\rangle\langle 011|$ or $P'' = |\tilde{0}\rangle\langle 010| + |\tilde{1}\rangle\langle 101|$ only differ from $|\Psi_{\text{Cluster}}^{\text{Hex}}\rangle$ by local Pauli \tilde{Z} operations, as $\tilde{Z}P = P'(x \otimes z \otimes I) = P''(z \otimes x \otimes I)$ and $|\psi_{\text{PEPS}}^{\text{Hex}}\rangle$ is invariant with $(x \otimes z \otimes I)$ or $(z \otimes x \otimes I)$ applied to every site. Hence, a modified local measurement scheme still exists, allowing these states to also be universal.

We now introduce a new state, the tricluster state $|\Psi_{\text{Tric}}\rangle$, which is motivated by these two insights, and has properties we desire. This is defined in the PEPS representation on a two-dimensional hexagonal lattice [Fig. 1(b)], with projectors

$$P_{\text{Tric}} = |\tilde{0}\rangle\langle 000| + |\tilde{1}\rangle\langle 111| + |\tilde{2}\rangle\langle 100| + |\tilde{3}\rangle\langle 011| + |\tilde{4}\rangle\langle 010| + |\tilde{5}\rangle\langle 101|, \quad (1)$$

using the same labeling scheme as above, such that $|\Psi_{\text{Tric}}\rangle \propto P_{\text{Tric}} |\psi_{\text{PEPS}}^{\text{Hex}}\rangle$. Hence, at each lattice site there lives a 6-dimensional particle.

Intuitively, $|\Psi_{\text{Tric}}\rangle$ is universal because it is closely related to the standard cluster state. Specifically, $|\Psi_{\text{Tric}}\rangle$ projected into the subspace spanned by $\{|\tilde{0}\rangle, |\tilde{1}\rangle\}$ is the same as $|\Psi_{\text{Cluster}}\rangle$, as are also the states given by $|\Psi_{\text{Tric}}\rangle$ projected into $\{|\tilde{2}\rangle, |\tilde{3}\rangle\}$ and $\{|\tilde{4}\rangle, |\tilde{5}\rangle\}$, up to local Pauli errors. Thus, $|\Psi_{\text{Tric}}\rangle$ is like a ‘‘superposition’’ of three cluster states. Computational qubits are encoded in the virtual qubits and operated upon by measuring the physical particles. Although the three subspaces of $|\Psi_{\text{Tric}}\rangle$ cannot be decoupled physically, they may be employed independently in processing encoded qubits with a suitable choice of measurement basis, as detailed later.

The most interesting nontrivial feature of $|\Psi_{\text{Tric}}\rangle$ is that it is the unique ground state of a gapped two-body Hamiltonian, and we begin with that.

Uniqueness and gap.—The fact that $|\Psi_{\text{Tric}}\rangle$ occurs as the unique ground state of a gapped two-body Hamiltonian is very surprising, as on the one hand the ground states of two-body Hamiltonians are rarely exactly known and on the other hand simply constructed states are not always ground states of simple Hamiltonians. Even the one-dimensional cluster state requires three-body interactions in its parent Hamiltonian. Below, we give a two-body nearest-neighbor Hamiltonian H_{Tric} which has $|\Psi_{\text{Tric}}\rangle$ as its ground state. Furthermore, we prove that $|\Psi_{\text{Tric}}\rangle$ is the

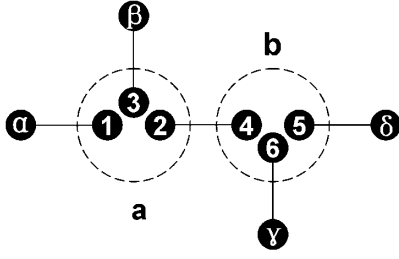


FIG. 2. Two representative sites a , b , and neighboring boundary, in the hexagonal lattice of $|\psi_{\text{PEPS}}^{\text{Hex}}\rangle$. Filled circles connected by solid lines represent virtual singlets $|\varphi\rangle$, and dashed circles indicate sites projected to obtain the physical state.

only ground state of H_{Tric} and the Hamiltonian has a constant gap independent of system size.

The central step in constructing H_{Tric} and studying its properties is to find the support space S_{ab} of the reduced density matrix of any two nearest-neighbor particles a and b in the state (a , b are in two sublattices, A , B , respectively). This is accomplished by first finding the corresponding support space S_{ab}^{PEPS} of the six virtual qubits on sites a and b , in the PEPS picture, and then computing $S_{ab} \propto P_{\text{Tric}} S_{ab}^{\text{PEPS}}$. For example, when a is to the left of b (Fig. 2), virtual qubits 1 to 6 on those sites are only connected to virtual qubits α to δ elsewhere. By tracing out α to δ from the 5 singlet pairs, we find S_{ab}^{PEPS} for virtual qubits 1 to 6 to be spanned by $|\pm\rangle_1|\pm\rangle_3|\varphi\rangle_{24}|\pm\rangle_5|\pm\rangle_6$, where $|\pm\rangle = (|0\rangle \pm |1\rangle)/\sqrt{2}$ and $|\varphi\rangle$ is the singlet state. This 16-dimensional space is then projected to give S_{ab} for the depicted lattice site. S_{ab} is different for the three bond directions in a hexagonal lattice, i.e., a to the left of, to the right of, and below b .

Providing a two-body Hamiltonian with $|\Psi_{\text{Tric}}\rangle$ being a ground state is straightforward. The Hilbert space of two neighboring sites a , b is 36-dimensional, larger than the dimension of S_{ab} . Therefore we may choose any non-negative Hermitian operator h_{ab} on the two sites that has S_{ab} as its null space, such that $h_{ab}|\Psi_{\text{Tric}}\rangle = 0$ for every h_{ab} . Thus, $|\Psi_{\text{Tric}}\rangle$ is a ground state of the two-body Hamiltonian $H_{\text{Tric}} = \sum_{ab} h_{ab}$, where the summation is over all nearest-neighbor pairs. However, the key is to construct H_{Tric} such that $|\Psi_{\text{Tric}}\rangle$ is the unique ground state, and it turns out the above procedure does work.

Specifically, let h_{ab} be the projection operator h_{ab}^p which projects onto the $36 - 16 = 20$ dimensional subspace orthogonal to S_{ab} , giving the total Hamiltonian

$$H_{\text{Tric}} = \sum_{a \in A} (h_{ab}^p + h_{ba}^p + h_a^p). \quad (2)$$

The summation is over sites a in sublattice A and the three terms h_{ab}^p , h_{ba}^p , h_a^p correspond, respectively, to three bond directions. The Hamiltonian is hence invariant under translation along sublattice A . An explicit expression for H_{Tric} in terms of spin operators is given in [15].

The specific H_{Tric} we have presented has $|\Psi_{\text{Tric}}\rangle$ as its unique ground state. This is shown by verifying the condition [13] that for any region R of spins in $|\Psi_{\text{Tric}}\rangle$, the support space S_R of the reduced density matrix on R satisfies $S_R = \bigcap_{(ab)} S_{ab} \otimes I_{R \setminus ab}$ where the intersection is taken over all neighboring pairs ab and $I_{R \setminus ab}$ is the full Hilbert space of all spins in region R except a and b . For every possible configuration containing three or four connected sites in $|\Psi_{\text{Tric}}\rangle$ the condition is confirmed by direct calculation. To check the condition for larger regions, it is useful to notice that any region in $|\Psi_{\text{Tric}}\rangle$ containing more than one site is injective [13]. By Lemma 2 of [13], (1) if regions R_1 and R_3 are not connected and R_2 and R_3 are injective, then $S_{R_1 \cup R_2 \cup R_3} = (S_{R_1 \cup R_2} \otimes I_{R_3}) \cap (S_{R_2 \cup R_3} \otimes I_{R_1})$, and (2) if regions R_1 , R_2 , R_3 are all injective, then $S_{R_1 \cup R_2 \cup R_3} = (S_{R_1 \cup R_2} \otimes I_{R_3}) \cap (S_{R_2 \cup R_3} \otimes I_{R_1}) \cap (S_{R_1 \cup R_3} \otimes I_{R_2})$. Hence for a region R containing more than 4 sites in $|\Psi_{\text{Tric}}\rangle$, S_R is the intersection of all four-body support spaces in R . By induction, it follows that the required condition is satisfied on $|\Psi_{\text{Tric}}\rangle$ for any R . Therefore, $|\Psi_{\text{Tric}}\rangle$ is the unique ground state of H_{Tric} .

H_{Tric} is also gapped; an energy gap η above the ground state exists, which is constant as the system size goes to infinity. The existence of this gap guarantees protection of $|\Psi_{\text{Tric}}\rangle$ against thermal noise. η can be bounded. First, we show that η is greater than λ , the gap of another Hamiltonian K which also has $|\Psi_{\text{Tric}}\rangle$ as its unique ground state, but has four-body terms instead of only two-body terms. We then bound λ above a positive constant value.

Consider the Hamiltonian K for a relabeled version of $|\Psi_{\text{Tric}}\rangle$, in which particles are regrouped into disjoint blocks each containing two nearest neighbors (Fig. 3). Let $K = \sum_{mn} k_{mn}$, where m, n denote two connected blocks, each containing two particles $m^{[l]}$, $m^{[r]}$ and $n^{[l]}$, $n^{[r]}$, respectively, and k_{mn} is the projection onto the orthogonal space of the four-body reduced density matrix on $m^{[l]}$, $m^{[r]}$, $n^{[l]}$, $n^{[r]}$ (assuming $m^{[r]}$ and $n^{[l]}$ are connected). Then
$$H_{\text{Tric}} = \sum_{ab} h_{ab}^p \geq \frac{1}{4} \sum_{mn} (h_{m^{[l]}m^{[r]}n^{[l]}n^{[r]}}^p + h_{n^{[l]}n^{[r]}m^{[l]}m^{[r]}}^p) \geq \frac{1}{4} \sum_{mn} \mu k_{mn} = \frac{1}{4} \mu K. \quad (h_{m^{[l]}m^{[r]}n^{[l]}n^{[r]}}^p + h_{n^{[l]}n^{[r]}m^{[l]}m^{[r]}}^p)$$
 and k_{mn} are both non-negative operators with the same null space, so the last inequality holds for some positive number μ . Assume that the gaps of the projectors h_{ab}^p and k_{mn} are both 1. Direct calculation gives $\mu = \frac{1}{2}$. As

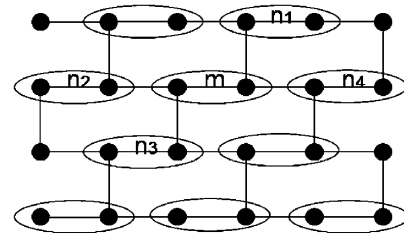


FIG. 3. Regrouping of lattice sites in tricluster state into disjoint blocks, each containing two sites.

discussed in the uniqueness proof, K also has $|\Psi_{\text{Tric}}\rangle$ as its unique ground state. Using this, we find $\eta \geq \frac{1}{4}\mu\lambda = \frac{1}{8}\lambda$. The gap λ can be bounded by showing that $K^2 \geq cK$ for some positive constant c . $K^2 = (\sum_{mn} k_{mn})^2 = K + \sum_{mn, m'n'} (k_{mn}k_{m'n'} + k_{m'n'}k_{mn}) \geq K + \sum_{n_i, m, n_j} k_{mn_i}k_{mn_j} + k_{mn_j}k_{mn_i}$, and n_i and n_j are blocks connected to m . The last inequality holds because when region mn and region $m'n'$ do not intersect $k_{mn}k_{m'n'} + k_{m'n'}k_{mn} \geq 0$. Direct calculation shows that (Fig. 3) $k_{mn_i}k_{mn_j} + k_{mn_j}k_{mn_i} \geq 0$ for $(i, j) = (1, 2), (1, 3), (2, 4),$ or $(3, 4)$, and $k_{mn_i}k_{mn_j} + k_{mn_j}k_{mn_i} \geq -\frac{1}{3}k_{mn_i} - \frac{1}{3}k_{mn_j}$ for $(i, j) = (1, 4)$ or $(2, 3)$. Summing over all consecutive $n_i, m,$ and n_j gives $\sum_{n_i, m, n_j} k_{mn_i}k_{mn_j} + k_{mn_j}k_{mn_i} \geq -\frac{2}{3}\sum_{mn} k_{mn}$. Therefore $K^2 \geq \frac{1}{3}K$, giving $\lambda \geq \frac{1}{3}$. Finally, we find a lower bound on the gap η of H_{Tric} of $\eta \geq \frac{1}{8}\lambda \geq \frac{1}{24}$.

Universality.— $|\Psi_{\text{Tric}}\rangle$ is a universal resource state. Similar to a cluster state, computational qubits are encoded in the virtual qubits, and the active computational state flows along the lattice as measurements on the physical states are performed. In contrast, however, with $|\Psi_{\text{Tric}}\rangle$ extra Pauli errors occur, thus necessitating additional analysis. Below, we describe the steps necessary, focusing on initialization and readout, one-qubit gates, and a two-qubit gate sufficient for universality.

1. Initialization and readout: Just as with the cluster state, with $|\Psi_{\text{Tric}}\rangle$, measurement in the six-state basis $\{|\tilde{0}\rangle \cdots |\tilde{5}\rangle\}$ accomplishes several tasks. First, such measurement detaches unnecessary sites from their neighbors (up to a known Pauli error). Next for state initialization, it gives a postmeasurement state with an encoded qubit projected into $|+\rangle$ (when the outcome is $\tilde{0}, \tilde{3},$ or $\tilde{4}$) and $|-\rangle$ (for outcomes $\tilde{1}, \tilde{2},$ or $\tilde{5}$). At the end of computation, the encoded qubit can also be read out in this way, giving 0 (for $\tilde{0}, \tilde{2},$ or $\tilde{5}$) and 1 (for $\tilde{1}, \tilde{3},$ or $\tilde{4}$).

2. One-qubit gates: Similar to gate implementations with the cluster state, once a line in the lattice has been detached from the rest, appropriately measuring a site in the line performs a single qubit rotation, up to a known Pauli error. Specifically, measuring in the basis $\{|\tilde{0}\rangle \pm e^{i\theta}|\tilde{1}\rangle, |\tilde{2}\rangle \pm e^{i\theta}|\tilde{3}\rangle, |\tilde{4}\rangle \pm e^{-i\theta}|\tilde{5}\rangle\}$ implements operation $\{HZ(\theta), XHZ(\theta), ZHZ(\theta), YHZ(\theta), ZHZ(\theta), YHZ(\theta)\}$, respectively, on the encoded qubit [using standard notation for qubit gates, with $Z(\theta)$ denoting a rotation about \hat{z} by angle θ], up to preexisting Pauli frame errors from detaching the line.

3. Two-qubit controlled-Z gate: Measurement of two vertically connected particles a and b implements the final

ingredient needed for universality, a controlled-Z gate CZ_{ab} . Specifically, measuring in basis $\{\hat{0} \dots \hat{5}\} = \{|\tilde{0}\rangle \pm |\tilde{1}\rangle, |\tilde{2}\rangle \pm |\tilde{3}\rangle, |\tilde{4}\rangle \pm |\tilde{5}\rangle\}$ implements the two-qubit operation $(X_a^{u_a} Z_a^{v_a} H_a)(X_b^{u_b} Z_b^{v_b} H_b) \otimes (X_a^{w_a} X_b^{w_b} CZ_{ab} X_a^{w_a} X_b^{w_b})$ on the two adjacent encoded qubits. For $x \in \{a, b\}$, $u_x = 1$ for x measurement outcomes $\hat{1}, \hat{3},$ or $\hat{5}$; $v_x = 1$ for outcomes $\hat{2}, \hat{3}, \hat{4},$ or $\hat{5}$; $w_x = 1$ for $\hat{4}, \hat{5}$; and u_x, v_x, w_x are 0 otherwise. More complicated configuration for use in a larger circuit is given in [15].

Conclusion.— $|\Psi_{\text{Tric}}\rangle$ is a remarkable entangled many-body state which is universal for both one-way quantum computation and the unique ground state of a gapped Hamiltonian H_{Tric} , made of local two-body terms. While imperfect, due to the use of six-state spins, the tricluster model steps closer to physical realizability than previous models. Moreover, the methods introduced here, based on the PEPS representation, are very general. These analysis methods lead directly to a number of additional universal states, and deepen connections between the study of complex condensed matter systems and quantum information science.

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