Characterizing Ground and Thermal States of Few-Body Hamiltonians

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The question whether a given quantum state is a ground or thermal state of a few-body Hamiltonian can be used to characterize the complexity of the state and is important for possible experimental implementations. We provide methods to characterize the states generated by two- and, more generally, k-body Hamiltonians as well as the convex hull of these sets. This leads to new insights into the question of which states are uniquely determined by their marginals and to a generalization of the concept of entanglement. Finally, certification methods for quantum simulation can be derived.

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Introduction.—Interactions in quantum mechanics are described by Hamilton operators. The study of their properties, such as their symmetries, eigenvalues, and ground states, is central for several fields of physics. Physically relevant Hamiltonians, however, are often restricted to few-body interactions, as the relevant interaction mechanisms are local. But the characterization of generic few-body Hamiltonians is not well explored, since in most cases one starts with a given Hamiltonian and tries to find out its properties.

In quantum information processing, ground and thermal states of local Hamiltonians are of interest for several reasons: First, if a desired state is the ground or thermal state of a sufficiently local Hamiltonian, it might be experimentally prepared by engineering the required interactions and cooling down or letting thermalize the physical system [1]. For example, one may try to prepare a cluster state, the resource for measurement-based quantum computation, as a ground state of a local Hamiltonian [2]. Second, on a more theoretical side, ground states of k-body Hamiltonians are completely characterized by their reduced k-body density matrices. The question of which states are uniquely determined by their marginals has been repeatedly studied and is a variation of the representability problem, which asks whether given marginals can be represented by a global state [3]. It has turned out that many pure states have the property to be uniquely determined by a small set of their marginals [4,5], and, for practical purposes, it is relevant that often entanglement or nonlocality can be inferred by considering the marginals only [6].

In this Letter we present a general approach to characterize ground and thermal states of few-body Hamiltonians. We use the formalism of exponential families, a concept first introduced for classical probability distributions by Amari [7] and extended to the quantum setting in Refs. [8–11]. This offers a systematic characterization of the complexity of quantum states in a conceptionally pleasing way. We derive two methods that can be used to compute various distances to thermal states of k-body Hamiltonians: The first method is general and uses semidefinite programming, while the second method is especially tailored to cluster and, more generally, graph states. In previous approaches it was only shown that some special states are far away from the eigenstates of local Hamiltonians [12], but no general method for estimating the distance is known.

Our approach leads to new insights in various directions. First, it has been shown that cluster and graph states can, in general, not be exact ground states of two-body Hamiltonians [2], but it was unclear whether they still can be approximated sufficiently well. Our method shows that this is not the case and allows us to bound the distance to ground and thermal states. Second, as shown in Ref. [4], almost all pure states of three qubits are completely determined by their two-party reduced density matrices. As we prove, for $N \geq 5$ qubits or four qutrits this is not the case, but we present some evidence that the fact might still be true for four qubits. Finally, our method results in witnesses, which can be used in a quantum simulation experiment to certify that a three-body Hamiltonian or a Hamiltonian having long-range interactions was generated.

The setting.—A two-local (or two-body) Hamiltonian of a system consisting of N spin-$1/2$ particles can be written as

$$H = \sum_{i,j=1}^{N} \sum_{\alpha\beta} \lambda_{\alpha\beta}^{(ij)} \sigma_\alpha^{(i)} \otimes \sigma_\beta^{(j)}, \qquad (1)$$

where $\sigma_\alpha^{(i)}$ denotes a Pauli matrix $\{\mathbb{1}, \sigma_x, \sigma_y, \sigma_z\}$ acting on the ith particle, etc. Note that the identity matrix is included, so H can also contain single particle terms. We denote the set of all possible two-local Hamiltonians by $\mathcal{H}_2$ and in an analogous manner the set of k-local Hamiltonians by $\mathcal{H}_k$. An example for a two-local Hamiltonian is the Heisenberg model having nearest-neighbor interactions. However, our approach generally ignores any geometrical arrangement of the particles. Finally, for an arbitrary multiqubit operator A we call the number of qubits where it acts on nontrivially the *weight* of A. In practice, this can be determined by expanding A in terms of tensor products of Pauli operators and looking for the largest nontrivial product.

The set we aim to characterize is the so-called exponential family $\mathcal{Q}_2$, consisting of thermal states of two-local Hamiltonians

$$\mathcal{Q}_2 = \left\{ \tau | \tau = \frac{e^{-\beta H}}{\mathrm{tr}[e^{-\beta H}]}, H \in \mathcal{H}_2 \right\}. \quad (2)$$

Ground states can be reached in the limit of infinite inverse temperature β. For any k, the exponential families $\mathcal{Q}_k$ can be defined in a similar fashion. The set $\mathcal{Q}_1$ consists of mixed product states, the set $\mathcal{Q}_N$ of the full state space. The exponential families form the hierarchy $\mathcal{Q}_1 \subseteq \mathcal{Q}_2 \subseteq \cdots \subseteq \mathcal{Q}_N$, and a suitable βH can be seen as a way of parametrizing a specific density matrix $\tau = e^{-\beta H}/\mathrm{tr}[e^{-\beta H}]$. The question arises, what states are in $\mathcal{Q}_k$? And for those which are not, what is their best approximation by states in $\mathcal{Q}_k$?

It turns out to be fruitful to consider the convex hull

$$\mathrm{conv}(\mathcal{Q}_2) = \left\{ \sum_i p_i \tau_i | \tau_i \in \mathcal{Q}_2, \sum_i p_i = 1, p_i \geq 0 \right\},$$

and ask whether a state is in this convex hull or not (see also Fig. 1). The convex hull has a clear physical interpretation as it contains all states that can be generated by preparing thermal states of two-body Hamiltonians stochastically with probabilities p_i. In this way, taking the convex hull can be seen as a natural extension of the concept of entanglement: The thermal states of one-body Hamiltonians are just the mixed product states and their convex hull are the fully separable states of N particles [13]. In this framework, the result of Linden *et al.* [4] can be rephrased as stating that all three-qubit states are in the closure of the convex hull $\mathrm{conv}(\mathcal{Q}_2)$, since nearly all pure states are ground states of two-body Hamiltonians.

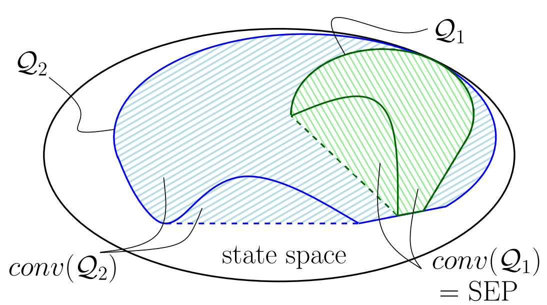

FIG. 1. Schematic view of the state space, the exponential families $\mathcal{Q}_1$ and $\mathcal{Q}_2$, and their convex hulls. While the whole space of mixed states is convex, the exponential families are nonconvex low-dimensional manifolds. The convex hull of $\mathcal{Q}_1$ are the fully separable states and our approach allows us to characterize the convex hull for arbitrary $\mathcal{Q}_k$.

Finally, the characterization of the convex hull leads to the concept of witnesses that can be used for the *experimental* detection of correlations [13]. Witnesses are observables that have positive expectation values for states inside a given convex set. Consequently, the observation of a negative expectation value proves that a state is outside of the set. We will see below that such witnesses can be used to certify quantum simulation.

Quantum exponential families.—We recall some results on the characterization of quantum exponential families [10,11]. Given a state ϱ, consider its distance from the exponential family $\mathcal{Q}_2$ in terms of the relative entropy (or divergence) $S(\varrho||\tau) = \mathrm{tr}[\varrho(\log(\varrho) - \log(\tau))]$. As the closest state to ϱ in $\mathcal{Q}_2$, one obtains the so-called information projection $\tilde{\varrho}_2$. It has been shown that the following three characterizations for the information projection $\tilde{\varrho}_2 \in \mathcal{Q}_2$ are equivalent [10]: (a) $\tilde{\varrho}_2$ is the unique minimizer of the relative entropy of ϱ from the set $\mathcal{Q}_2$,

$$\tilde{\varrho}_2 = \mathrm{argmin}_{\tau \in \mathcal{Q}_2} S(\varrho||\tau). \quad (3)$$

(b) Of the set of states having the same two-body reduced density matrices (2-RDMs) as ϱ, denoted by $\mathcal{M}_2(\varrho)$, $\tilde{\varrho}_2$ has a maximal von Neumann entropy

$$\tilde{\varrho}_2 = \mathrm{argmax}_{\mu \in \mathcal{M}_2(\varrho)} S(\mu). \quad (4)$$

(c) Finally, $\tilde{\varrho}_2$ is the unique intersection of $\mathcal{Q}_2$ and $\mathcal{M}_2(\varrho)$. From (b) it follows that if for a state σ another state ϱ of higher entropy but having the same 2-RDMs can be found, then σ must lie outside of $\mathcal{Q}_2$. A further discussion can be found in the Supplemental Material, Appendix A [14].

States not in $\mathcal{Q}_2$ are said to have irreducible correlations of order 3 or higher, because they contain information which is not already present in their 2-RDMs, if one wishes to reconstruct the global state from its marginals according to Jaynes' maximum entropy principle [15]. This is conceptionally nice, but also has certain drawbacks. Importantly, the irreducible correlation as quantified by the relative entropy is not continuous, as shown in Ref. [16]. In addition, the relative entropy is difficult to estimate experimentally without doing state reconstruction, so other distances such as the fidelity are preferable. These properties make the relative entropy somewhat problematic and give further reasons why we consider the convex hull.

Characterization via semidefinite programming.—Our first method to estimate the distance of a given state to the convex hull of $\mathcal{Q}_2$ relies on semidefinite programming [17]. This optimization method is insofar useful, as semidefinite programs are efficiently solvable and their solutions can be certified to be optimal. Moreover, ready-to-use packages for their implementation are available.

As a first step we formulate a semidefinite program to test if a given pure $|\psi\rangle$ state is outside of $\mathcal{Q}_2$. From the characterization in Eq. (4) it follows that it suffices to find a different state ϱ having the same 2-RDMs as $|\psi\rangle$. If ϱ is mixed, its entropy is higher than that of $|\psi\rangle$, meaning that $|\psi\rangle$ cannot be its own information projection and therefore lies outside of $\mathcal{Q}_2$. If ϱ is pure, consider the convex combination $(|\psi\rangle\langle\psi| + \varrho)/2$, again having a higher entropy. To simplify notation we define for an arbitrary N-qubit operator X the operator $R_k(X)$ as the projection of X onto those operators, which can be decomposed into terms having at most weight k. In practice, $R_k(X)$ can be computed by expanding X in Pauli matrices, and removing all terms of weight larger than k. Note that $R_k(\varrho)$ may have negative eigenvalues.

The following semidefinite program finds a state with the same k-body marginals as a given state $|\psi\rangle$:

$$\begin{aligned} \min_{\varrho}: \ & \mathrm{tr}[\varrho|\psi\rangle\langle\psi|] \\ \text{subject to} \quad & R_k(\varrho) = R_k(|\psi\rangle\langle\psi|), \\ & \mathrm{tr}[\varrho] = 1, \qquad \varrho = \varrho^\dagger, \qquad \varrho \geq \delta\mathbb{1}. \end{aligned} \tag{5}$$

While this program can be run with $\delta = 0$, it is useful to choose δ to be strictly positive. Then, a strictly positive ϱ may be found, which is guaranteed to be distant from the state space boundary. Consequently, if $|\psi\rangle$ is disturbed, one can still expect to find a state with the same reduced density matrices in the vicinity of ϱ. This can be used to prove that the distance to $\mathcal{Q}_2$ is finite, and will allow us to construct witnesses for proving irreducible correlations in $|\psi\rangle$. We make this rigorous in the following observation. For that, let $\mathcal{B}(|\psi\rangle)$ be the ball in trace distance $D_{\mathrm{tr}}(\mu, \eta) = \frac{1}{2}\mathrm{tr}(|\mu - \eta|)$ centered at $|\psi\rangle$.

Observation 1.—Consider a pure state $|\psi\rangle$ and a mixed state $\varrho \geq \delta\mathbb{1}$ with $R_k(\varrho) = R_k(|\psi\rangle\langle\psi|)$. Then, for any state σ in the ball $\mathcal{B}_\delta(|\psi\rangle)$ a valid state $\tilde{\varrho}$ in $\mathcal{B}_\delta(\varrho)$ can be found, such that their k-party reduced density matrices match. Moreover, the entropy of $\tilde{\varrho}$ is larger than or equal to the entropy of σ. This implies that the ball $\mathcal{B}_\delta(|\psi\rangle)$ contains no thermal states of k-body Hamiltonians.

The proof is given in the Supplemental Material, Appendix B [14].

In the observation, we considered the trace distance, but a ball in fidelity instead of trace distance can be obtained: Consider a state σ near $|\psi\rangle$, having the fidelity $F(\sigma, \psi) = \alpha \geq 1 - \delta^2$, where $F(\varrho, \psi) = \mathrm{tr}[\varrho|\psi\rangle\langle\psi|] = \langle\psi|\varrho|\psi\rangle$. Then from the Fuchs–Van de Graaf inequality follows $D_{\mathrm{tr}}(\sigma, |\psi\rangle\langle\psi|) \leq \sqrt{1 - F(\sigma, \psi)} \leq \delta$, and observation 1 is applicable [18].

The usage of the fidelity as a distance measure has a clear advantage from the experimental point of view, as it allows the construction of witnesses for multiparticle correlations. Indeed, the observable

$$\mathcal{W} = (1 - \delta^2)\mathbb{1} - |\psi\rangle\langle\psi| \tag{6}$$

has a positive expectation value on all states in $\mathcal{Q}_k$ and, due to the linearity of the fidelity, also on all states within the convex hull $\mathrm{conv}(\mathcal{Q}_k)$. So, a negative expectation value signals the presence of k-body correlations. Witnesses for entanglement have already found widespread applications in experiments [13].

Equipped with a method to test whether a pure state is in $\mathrm{conv}(\mathcal{Q}_2)$ or not we are able to tackle the question whether the results of Ref. [4] can be generalized. Recall that in this reference it was shown that nearly all pure states of three qubits are uniquely determined (among all mixed states) by their reduced two-body density matrices. This means that they are ground states of two-body Hamiltonians. Consequently, the closure of the convex hull $\mathrm{conv}(\mathcal{Q}_2)$ contains all pure states and therefore also all mixed states, and the semidefinite program in Eq. (5) will not be feasible for δ strictly positive. The question is whether this result holds for more qubits too.

Concerning pure five-qubit states, we numerically found a fraction of 40% to be outside of $\mathrm{conv}(\mathcal{Q}_2)$. In the case of pure four-qubit states, however, no tested random state has been found to lie outside of $\mathrm{conv}(\mathcal{Q}_2)$. Given the fact that the test works well in the cases of five and six qubits, this leads us to conjecture that nearly all pure four qubit states are in $\mathrm{conv}(\mathcal{Q}_2)$, and hence also in $\mathcal{Q}_2$. This would imply that a similar result as the one obtained by Ref. [4] holds in the case of four qubits: almost every pure state of four qubits is completely determined by its two-particle reduced density matrix. More details are given in the Supplemental Material, Appendix C [14].

Characterization via the graph state formalism.—The family of graph states includes cluster states and GHZ states and has turned out to be important for measurement-based quantum computation and quantum error correction [19]. Because of their importance, the question whether graph states can be prepared as ground states of two-body Hamiltonians has been discussed before [2]. Generally, graph states have shown to not be obtainable as unique nondegenerate ground states of two-local Hamiltonians. Further, any ground state of a k-local Hamiltonian H can only be ϵ-close to a graph state $|G\rangle$ with $m(|G\rangle) > k$ at the cost of H having an ϵ-small energy gap relative to the total energy in the system [2]. Here, $m(|G\rangle)$ is the minimal weight of any element in the stabilizer S of state $|G\rangle$ (see also below). But as pointed out in Ref. [2], this does not imply that graph states cannot be approximated in general, as ϵ is a relative gap only.

Let us introduce some facts about graph states. A graph consists of vertices and edges (see Fig. 2). This defines the generators

$$g_a = \sigma_x^{(a)} \prod_{b \in N(a)} \sigma_z^{(b)}, \tag{7}$$

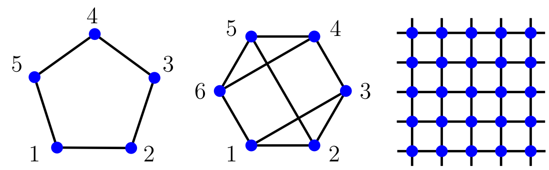

FIG. 2. Examples of graphs discussed in this Letter. Left: The five-qubit ring-cluster graph. The corresponding ring-cluster state $|C_5\rangle$ has a finite distance to the exponential family $\mathcal{Q}_2$. Middle: The maximally entangled six-qubit $|M_6\rangle$ state is not in the convex hull of $\mathcal{Q}_3$. Right: The 2D periodic 5×5 cluster state $|C_{5\times 5}\rangle$ is not in $\mathrm{conv}(\mathcal{Q}_4)$.

where the product of the $\sigma_z^{(b)}$ runs over all vertices connected to vertex a, called neighborhood $N(a)$. The graph state $|G\rangle$ can be defined as the unique eigenstate of all the g_a, that is $|G\rangle = g_a|G\rangle$. This can be rewritten with the help of the stabilizer. The stabilizer S is the commutative group consisting of all possible 2^N products of g_a, that is, $S = \{s_i = \prod_{a\in I} g_a\}$. Then, the graph state can be written as $|G\rangle\langle G| = 2^{-N}\sum_{s_i\in S} s_i$ [19]. This formula allows us to determine the reduced density matrices of graph states easily, since one only has to look at the products of the generators g_a.

For instance, all stabilizer elements of the five-qubit ring cluster state $|C_5\rangle$ have at least weight three, and, therefore, the 2-RDMs of $|C_5\rangle$ are maximally mixed. By choosing $\delta = 2^{-5}$ in observation 1, the maximum overlap to $\mathrm{conv}(\mathcal{Q}_2)$ is bounded by $F_{\tau\in\mathcal{Q}_2}(|C_5\rangle,\tau) \le 1-\delta^2 \approx 0.999\,02$. Note that Ref. [20] has demonstrated a slightly better bound $F(|C_5\rangle,\tau) \le 1/32 + \sqrt{899/960} \approx 0.998\,96$. However, both bounds are by far not reachable in current experiments. In fact, one can do significantly better. In the following, we will formulate a stricter bound by first considering $\mathcal{Q}_2$ and the ring cluster state $|C_N\rangle$ for an arbitrary number of qubits $N \ge 5$, but the result is general.

Observation 2.—The maximum overlap between the N-qubit ring cluster state $|C_N\rangle$ and an N-qubit state $\tau \in \mathcal{Q}_2$ is bounded by

$$\sup_{\tau\in\mathcal{Q}_2} \langle C_N|\tau|C_N\rangle \le \frac{D-1}{D}, \tag{8}$$

where $D = 2^N$ is the dimension of the system. More generally, for an arbitrary pure state with maximally mixed reduced k-party states in a $d^{\otimes N}$ system, the overlap with $\mathcal{Q}_k$ is bounded by $(d^N-1)/d^N$.

The proof is given in the Supplemental Material, Appendix D [14].

In the case of five qubits, $F_{\tau\in\mathcal{Q}_2}(|C_5\rangle,\tau) \le 31/32 \approx 0.968\,75$, which improves the bound on the distance to $\mathrm{conv}(\mathcal{Q}_2)$ by more than 2 orders of magnitude [21]. From observation 2, we can construct the witness

$$\mathcal{W} = \frac{D-1}{D}\mathbb{1} - |C_N\rangle\langle C_N|, \tag{9}$$

which detects states outside of $\mathrm{conv}(\mathcal{Q}_2)$. In a similar fashion, any state having the maximally mixed state as k-particle RDMs can be used to construct a witness for $\mathrm{conv}(\mathcal{Q}_k)$. First, there is a four-qutrit state with maximally mixed 2-RDMs [22], which can be used to derive a witness for $\mathrm{conv}(\mathcal{Q}_2)$. The highly entangled six-qubit state $|M_6\rangle$ (see the graph in Fig. 2) has maximally mixed 3-RDMs, so $\mathcal{W} = \frac{63}{64}\mathbb{1} - |M_6\rangle\langle M_6|$ is a witness to exclude thermal states of three-body Hamiltonians. Third, consider a 5×5 2D cluster state with periodic boundary conditions (see Fig. 2). This state has $m(|C_{5\times 5}\rangle) = 5$ [2], and can, therefore, serve as a witness $\mathcal{W} = \alpha\mathbb{1} - |C_{5\times 5}\rangle\langle C_{5\times 5}|$ for $\mathrm{conv}(\mathcal{Q}_4)$, where $\alpha = (2^{25}-1)/2^{25}$. It should be noted that this witness can also be used for $\mathrm{conv}(\mathcal{Q}_2)$, for which the value α might be improved [23]. Finally, the minimal distance D_k in terms of the relative entropy from $\mathcal{Q}_k$ can be lower bounded by the fidelity distance from its convex hull $\mathrm{conv}(\mathcal{Q}_k)$, see the Supplemental Material, Appendix D for details [14].

Quantum simulation as an application.—The aim of quantum simulation is to simulate a physical system of interest by another well-controllable one. Naturally, it is crucial to ascertain that the interactions really perform as intended. Different proposals have recently come forward to engineer sizable three-body interactions in systems of cold polar molecules [24], trapped ions [25], ultracold atoms in triangular lattices [26], Rydberg atoms [27], and circuit QED systems [28]. Using the ring cluster state witness $\mathcal{W} = \alpha\mathbb{1} - |C_N\rangle\langle C_N|$ derived above, it is possible to certify that three- or higher-body interactions have been engineered. This is done by letting the system under control thermalize. If then $\langle\mathcal{W}\rangle < 0$ is measured, one has certified that interactions of weight three or higher are present. At least five qubits are generally required for this, but by further restricting the interaction structure, four qubits can be enough for demonstration purposes. This can already be done with a fidelity of 93.75%, which is within reach of current technologies. Further details can be found in the Supplemental Material, Appendix E [14].

As an outlook, one may try to extend this idea of interaction certification to the unitary time evolution under local Hamiltonians. For instance, digital quantum simulation can efficiently approximate the time evolution of a time-independent local Hamiltonian and in Ref. [29] an effective 6-particle interaction has been engineered by applying a stroboscopic sequence of universal quantum gates. The process fidelity was quantified using quantum process tomography; however, it would be of interest to prove that the same time evolution cannot be generated by 5-particle interactions only.

Conclusion.—We have provided methods to characterize thermal and ground states of few-body Hamiltonians. Our results can be used to test experimentally whether three-body or higher-order interactions are present. For future work, it would be desirable to characterize the entanglement properties of $\mathcal{Q}_2$, e.g., to determine whether the entanglement in these states is bounded, or whether they can be simulated classically in an efficient manner. Furthermore, it is of significant experimental relevance to develop schemes to certify that a unitary time evolution was generated by a k-body Hamiltonian.

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