

Correlations in excited states of local Hamiltonians

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Physical properties of the ground and excited states of a k -local Hamiltonian are largely determined by the k -particle reduced density matrices (k -RDMs), or simply the k -matrix for fermionic systems—they are at least enough for the calculation of the ground-state and excited-state energies. Moreover, for a nondegenerate ground state of a k -local Hamiltonian, even the state itself is completely determined by its k -RDMs, and therefore contains no genuine $>k$ -particle correlations, as they can be inferred from k -particle correlation functions. It is natural to ask whether a similar result holds for nondegenerate excited states. In fact, for fermionic systems, it has been conjectured that any nondegenerate excited state of a 2-local Hamiltonian is simultaneously a unique ground state of another 2-local Hamiltonian, hence is uniquely determined by its 2-matrix. And a weaker version of this conjecture states that any nondegenerate excited state of a 2-local Hamiltonian is uniquely determined by its 2-matrix among all the pure n -particle states. We construct explicit counterexamples to show that both conjectures are false. We further show that any nondegenerate excited state of a k -local Hamiltonian is a unique ground state of another $2k$ -local Hamiltonian, hence is uniquely determined by its $2k$ -RDMs (or $2k$ -matrix). These results set up a solid framework for the study of excited-state properties of many-body systems.

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In many-body quantum systems, correlations in quantum states, both ground states and excited states, play an important role for many interesting physics phenomena, ranging from high-temperature superconductivity, fractional quantum Hall effect to various kinds of quantum phase transitions. Traditionally, correlation is characterized by correlation functions of local physical observables. To better understand the structure of many-body correlations, however, we need a method to separate out the contribution of the amount that comes from essentially fewer-body correlations. Irreducible k -party correlation [1,2], a concept originating from information theoretical ideas, provides such a method to quantify many-body correlations. In particular, an n -particle pure state $|\psi\rangle$ contains no irreducible $>k$ -party correlation if it is uniquely determined by its k -particle reduced density matrices (k -RDMs), meaning that there does not exist any other n -particle state, pure or mixed, which has the same k -RDMs as those of $|\psi\rangle$.

This definition of irreducible multiparty correlation relates the study of many-body correlation itself, the reduced density matrix approach for many-body systems (cf. Ref. [3]), and the ground-state properties of a local Hamiltonian as we will elaborate in the following paragraph. The main contribution of this Rapid Communication is to show the dramatic difference between many-body corrections of excited states and those of ground states, and to establish a framework for the study of excited-state properties based on the reduced density matrix approach.

The Hamiltonian H of a real n -particle system usually involves terms of at most k -body interactions, where k is a small number [4]. This kind of Hamiltonian is called k -local and for most physical systems $k = 2$. If $|\psi_0\rangle$ is a ground state of H , then the ground-state energy $E_0 = \langle\psi_0|H|\psi_0\rangle$ is determined only by the k -RDMs of $|\psi_0\rangle$. This observation

implies that, when $|\psi_0\rangle$ is nondegenerate, the state must be uniquely determined by its k -RDMs, because if there exists any other n -particle state, pure or mixed, which has the same k -RDMs as those of $|\psi_0\rangle$, then there must be another pure state which has the same energy as $|\psi_0\rangle$, making the ground space degenerate. This kind of “unique determination” legitimately, in a very strong sense, the reduced density matrix approach for many-body systems.

Similar observation applies to fermionic systems, namely, the unique ground state of a k -local fermionic Hamiltonian is uniquely determined by its k -matrix. Indeed, related studies for fermionic systems in quantum chemistry date back to the early 1960s [3,5], where the properties of both ground states and excited states of 2-local fermionic Hamiltonians were studied. For excited states, it is conjectured that any nondegenerate excited state of a 2-local fermionic Hamiltonian is simultaneously a unique ground state of another 2-local fermionic Hamiltonian, and hence is uniquely determined by its 2-matrix [5]. A weaker version of this conjecture states that any nondegenerate excited state of a 2-local fermionic Hamiltonian is uniquely determined by its 2-matrix among all the pure n -particle fermionic states [6].

If these conjectures were true, then understanding the excited-state properties of a system of N fermions could be restricted in studying the set of all the 2-matrices, whose characterization is called the N -representability problem in quantum chemistry [3]. The N -representability problem has been studied extensively in the past several decades and significant progress in studying practical chemical systems has been made [3,5,6], though this problem is shown to be difficult in the most general settings [7]. Meanwhile, it is also natural to ask whether similar conjectures may hold for excited states of k -local spin Hamiltonians, as excited states are also

important for characterizing interesting physics phenomena, especially in nonzero temperature situations. Sometimes even zero-temperature physics cannot be characterized by ground states only, for instance, in certain kinds of quantum phase transitions [8].

Here we construct explicit counterexamples to show that both conjectures for fermionic systems are false. In the more general settings of n -particle systems, not necessarily fermionic, we further show that any nondegenerate excited state of a k -local Hamiltonian is a unique ground state of another $2k$ -local Hamiltonian, and hence is uniquely determined by its $2k$ -RDMs. For fermionic systems with 2-local Hamiltonians, our results imply that the understanding of some properties of excited states will need the information of their 4-matrices, and that 4-matrices are also enough for all purposes. In addition, we also apply our techniques to the study of correlations in n -qubit symmetric Dicke states [9] and show that they are uniquely determined by their 2-RDMs. We believe that our result sets a good starting point for studying excited-state properties of many-body systems based on the reduced density matrix approach, and will lead to fruitful results in related areas, including quantum information science, quantum chemistry, and many-body physics.

From spin systems to fermion systems. To relate the fermionic problem to known results in quantum information theory, we need a map from a qubit system to a fermionic system. We now show how to map an n -qubit system to a fermionic system, with $N = n$ fermions and $M = 2N$ modes. This map has been already discussed in Refs. [7,10], so we briefly review the construction here. The idea is to represent each qubit s as a single fermion that can be in two different modes a_i, b_i , so each n -qubit basis state corresponds to the following N -fermion state:

$$|z_1, \dots, z_n\rangle \mapsto (a_1^\dagger)^{1-z_1} (b_1^\dagger)^{z_1} \dots (a_n^\dagger)^{1-z_n} (b_n^\dagger)^{z_n} |\Omega\rangle,$$

where $z_i = 0, 1$ and $|\Omega\rangle$ is the vacuum state. Also, all the relevant single-qubit Pauli operators can be mapped via

$$X_i \mapsto a_i^\dagger b_i + b_i^\dagger a_i, \quad Y_i \mapsto i(b_i^\dagger a_i - a_i^\dagger b_i), \quad Z_i \mapsto \mathbb{1} - 2b_i^\dagger b_i.$$

In addition, one needs to add the following projectors as extra terms in the fermionic Hamiltonian:

$$P_i = (2a_i^\dagger a_i - \mathbb{1})(2b_i^\dagger b_i - \mathbb{1}).$$

As all the P_i 's are biquadratic and commute with all the single-qubit Pauli operators, the complete Hamiltonian will be block diagonal. By making the weights of these projectors large enough, we can always guarantee that the ground state of the full Hamiltonian will have exactly one fermion per site.

Therefore, to disprove both conjectures for fermionic systems, one only needs to find counterexamples in n -qubit systems. In other words, we will need to find an n -qubit pure state $|\psi\rangle$ which is a nondegenerate eigenstate of some 2-local Hamiltonian, but there exists another pure state $|\psi'\rangle$ which has the same 2-RDMs as those of $|\psi\rangle$. Therefore, $|\psi\rangle$ cannot be a unique ground state of any 2-local Hamiltonian. Then by applying the spin-to-fermion map discussed above, one can result in a counterexample for the fermionic case.

Simple counterexamples from three-qubit states. To construct explicit counterexamples, we start from the simplest

case of $n = 3$. First of all, we need a state $|\psi\rangle$ which is not uniquely determined by its 2-RDMs and then further show that $|\psi\rangle$ is a nondegenerate eigenstate of some 2-local Hamiltonian $H = \sum_i H_i$, where each H_i acts nontrivially on at most two qubits. It is well known that almost all three-qubit states are uniquely determined by their 2-RDMs except those locally equivalent to the GHZ-type states $\alpha|000\rangle + \beta|111\rangle$, for $\alpha, \beta \neq 0$ [1,11]. Up to local unitary operations, one only needs to consider the case where α, β are real. Apparently, the pure state $\alpha|000\rangle + \beta e^{i\theta}|111\rangle$ has the same 2-RDMs as those of $\alpha|000\rangle + \beta|111\rangle$, so $\alpha|000\rangle + \beta|111\rangle$ is not uniquely determined by its 2-RDMs, even among pure states.

To show that $\alpha|000\rangle + \beta|111\rangle$ can be a nondegenerate eigenstate of some 2-local Hamiltonian, we construct the 2-local Hamiltonian explicitly. We start from a simple case of the GHZ state where $\alpha = \beta = 1/\sqrt{2}$, $|\psi\rangle_{\text{GHZ}} = (|000\rangle + |111\rangle)/\sqrt{2}$. The GHZ state is the eigenstate of the commuting Pauli operators $Z_1 Z_2, Z_2 Z_3, X_1 X_2 X_3$ with eigenvalue 1, where X_i, Y_i, Z_i stands for the Pauli X, Y, Z operators acting on the i th qubit. In the language of stabilizers [12], $|\psi\rangle_{\text{GHZ}}$ is stabilized by the group generated by $Z_1 Z_2, Z_2 Z_3, X_1 X_2 X_3$.

For the Hamiltonian $H_0 = -Z_1 Z_2 - Z_2 Z_3$, $|\psi\rangle_{\text{GHZ}}$ is an eigenstate but degenerate with any state in the space spanned by $|000\rangle, |111\rangle$. In order to remove the twofold degeneracy and to make $|\psi\rangle_{\text{GHZ}}$ a nondegenerate eigenstate, we note that $X_1 X_2 X_3 |\psi\rangle_{\text{GHZ}} = |\psi\rangle_{\text{GHZ}}$. Therefore, $|\psi\rangle_{\text{GHZ}}$ is an eigenstate of $H_1 = X_1 X_2 - X_3$ with eigenvalue 0, which is not the case for any other state in the space spanned by $|000\rangle, |111\rangle$. Finally, one concludes that $|\psi\rangle_{\text{GHZ}}$ is a nondegenerate eigenstate of the 2-local Hamiltonian $H = -Z_1 Z_2 - Z_2 Z_3 + c(X_1 X_2 - X_3)$, for a properly chosen c (for instance, one can choose $c = -1$, then $|\psi\rangle_{\text{GHZ}}$ is the nondegenerate first excited state of H , with energy -2 .)

For the state $\alpha|000\rangle + \beta|111\rangle$, similar ideas apply. Denote a 2×2 diagonal matrix with diagonal elements a_{11}, a_{22} by $\text{diag}(a_{11}, a_{22})$, then we have

$$\text{diag}\left(\frac{\beta}{\alpha}, \frac{\alpha}{\beta}\right)_1 X_1 X_2 X_3 (\alpha|000\rangle + \beta|111\rangle) = \alpha|000\rangle + \beta|111\rangle,$$

where the operator $\text{diag}\left(\frac{\beta}{\alpha}, \frac{\alpha}{\beta}\right)_i$ acts on the i th qubit. Therefore, $\alpha|000\rangle + \beta|111\rangle$ is a nondegenerate eigenstate of the 2-local Hamiltonian

$$H = aZ_1 Z_2 + bZ_2 Z_3 + c \left[\text{diag}\left(\frac{\beta}{\alpha}, \frac{\alpha}{\beta}\right)_1 X_1 X_2 - X_3 \right],$$

for some properly chosen a, b, c .

These three-qubit examples can thus be mapped to fermionic counterexamples of three fermions with six modes, thus disproving the conjecture discussed in Ref. [5] and its weaker version in Ref. [6].

More counterexamples. One may think that the existence of the counterexamples from three-qubit states is due to the fact that almost all (except the GHZ-type) three-qubit states are uniquely determined by their 2-RDMs, and hope that these conjectures could actually hold for most of the other cases. Here we show that the above discussion of the counterexamples from three-qubit states provides a systematic way to find a large class of counterexamples.

The idea of constructing the counterexamples from three-qubit states is the following: start from a 2-local Hamiltonian H_0 whose ground space is degenerate (for simplicity, we assume it is twofold degenerate). Choose a basis $|C_0\rangle$ and $|C_1\rangle$ for the ground space of H_0 such that (1) $|C_0\rangle$ and $|C_1\rangle$ have the same 2-RDMs; (2) there exists a weight 3 or 4 operator M such that $M|C_0\rangle = |C_0\rangle$ but $M|C_1\rangle \neq |C_1\rangle$. Then one can “decompose” the operator M into a 2-local one, H_1 , such that $|C_0\rangle$ is an eigenvector with eigenvalue zero (for instance, if $M = X_1 X_2 Z_3 Z_4$, one can choose $H_1 = X_1 X_2 - Z_3 Z_4$), then the Hamiltonian $H = H_0 + cH_1$ will have $|C_0\rangle$ as a nondegenerate eigenstate for a properly chosen c . Thus $|C_0\rangle$ gives a counterexample after applying the spin-to-fermion map.

In general, for a given H_0 one cannot guarantee the existence of such $|C_0\rangle$, $|C_1\rangle$, and M . However, in certain cases of quantum error-correcting codes [12], they are easy to find. Consider a quantum error-correcting code of dimension >1 which is a ground state of a 2-local Hamiltonian, with distance 3 or 4. Then any state in the code space has the same 2-RDMs [10,13], so one can easily find $|C_0\rangle$ and $|C_1\rangle$ which are orthogonal. If the code is a stabilizer or stabilizer subsystem code, then the logical operator M which satisfies $M|C_0\rangle = |C_0\rangle$ and $M|C_1\rangle = -|C_1\rangle$ will be a Pauli operator of weight 3 (if the code distance is 3) or 4 (if the code distance is 4).

One simple example is the Bacon-Shor code on a 3×3 (or 4×4) square lattice [14]. We discuss the 3×3 case for simplicity. The system consists of $n = 9$ qubits arranged on a 3×3 square lattice, and the Hamiltonian is given by

$$H_0 = -J_x \sum_{j,k} X_{j,k} X_{j+1,k} - J_z \sum_{k,j} Z_{j,k} Z_{j,k+1},$$

whose ground space is twofold degenerate, constituting a quantum error-correcting code of distance 3, where $J_x, J_z > 0$, and the subscripts j, k refer to the qubit of the j th row and k th column and the addition is modulo 3. An orthonormal basis of the code space can be chosen as $|C_0\rangle$ and $|C_1\rangle$ such that the logical Z operator \bar{Z} , satisfying $\bar{Z}|C_0\rangle = |C_0\rangle$ and $\bar{Z}|C_1\rangle = -|C_1\rangle$, is given by $\bar{Z} = Z_{1,1} Z_{2,1} Z_{3,1}$ [14]. Therefore, $|C_0\rangle$ is a nondegenerate eigenstate of the 2-local Hamiltonian

$$H = H_0 + c(Z_{1,1} Z_{2,1} - Z_{3,1})$$

for a properly chosen c .

Correlations in excited states. We would like to consider this problem in more general settings of n -particle states which are not necessarily fermionic, or do not have any kind of symmetry. Our method directly generalizes to the case of $k > 2$, showing that a nondegenerate eigenstate of a k -local Hamiltonian may not be uniquely determined by its k -RDMs, even among pure states. A simple example could be the n -particle GHZ state

$$|\psi^{(n)}\rangle_{\text{GHZ}} = \frac{1}{\sqrt{2}}(|0\rangle^{\otimes n} + |1\rangle^{\otimes n}).$$

For simplicity we take n even (the odd cases can be dealt with similarly). Note the GHZ state is not uniquely determined by its $(n-1)$ -RDMs, as the state $\frac{1}{\sqrt{2}}(|0\rangle^{\otimes n} + e^{i\theta}|1\rangle^{\otimes n})$ has the same $(n-1)$ -RDMs.

Using similar ideas as in the three-qubit case, we know that $|\psi^{(n)}\rangle_{\text{GHZ}}$ is a nondegenerate ground state of the $\frac{n}{2}$ -local

Hamiltonian

$$H = -Z_1 Z_2 - Z_2 Z_3 - \dots - Z_{n-1} Z_n \\ + c(X_1 X_2 \dots X_{n/2} - X_{n/2+1} X_{n/2+2} \dots X_n),$$

for a properly chosen c . Using the idea based on quantum error-correcting codes, one can also find other states which are nondegenerate eigenstates of a k -local Hamiltonian but are not uniquely determined by their k -RDMs, even among pure states.

Given that a unique ground state of a k -local Hamiltonian is uniquely determined by its k -RDMs, these examples show that correlations in excited states of local Hamiltonians could be dramatically different from correlations in the ground states. Then an interesting question arises: How “dramatic” could this correlation be for nondegenerate eigenstates of local Hamiltonians? More concretely, can a nondegenerate eigenstate of a k -local Hamiltonian have nonzero irreducible r -party correlations for any $r \leq n$? This question becomes more intriguing when k is a constant independent of n . That is, can a nondegenerate eigenstate of a local Hamiltonian have nonlocal irreducible correlations?

We show, however, this is not the case—a nondegenerate eigenstate of a k -local Hamiltonian is uniquely determined by its $2k$ -RDMs and, therefore, cannot have $>2k$ -party irreducible correlation. To see this, let us consider a nondegenerate eigenstate $|\psi\rangle$ of a k -local Hamiltonian H with $H|\psi\rangle = h|\psi\rangle$, and without loss of generality, assume $h = 0$. Then, $H^2|\psi\rangle = 0$, and $|\psi\rangle$ becomes the ground state of H^2 . Because H is k -local, H^2 is at most $2k$ -local, and $|\psi\rangle$ is then uniquely determined by its $2k$ -RDMs. This result shows that although correlations in nondegenerate excited states of a local Hamiltonian are different from those in ground states, they are still “local” irreducible correlations.

We mention that the $2k$ bound is tight, as there exists a nondegenerate excited state of a k -local Hamiltonian that is not uniquely determined by its $(2k-1)$ -RDMs. One simple example is the GHZ state of $2k$ qubits, which is a nondegenerate excited state of a k -local Hamiltonian, but is not uniquely determined by its $(2k-1)$ -RDMs.

It is also easy to see that the discussion here about nondegenerate eigenstates can be directly extended to the degenerate case. That is, if V is an eigenspace of a k -local Hamiltonian, then V is a ground space of a $2k$ -local Hamiltonian.

Applications. In a very general setting, we have investigated the correlations in excited states of local Hamiltonians. It turns out that our techniques can also help to understand correlations in certain quantum states in a relatively simple way. Let us now look at the correlations in n -qubit symmetric Dicke states.

The n -qubit symmetric Dicke state $|W_n(i)\rangle$ ($i = 0, 1, \dots, n$) is the equal weight superposition of weight- i bit strings [9]. For instance, $|W_n(0)\rangle = |00 \dots 0\rangle$, and $|W_n(1)\rangle = (|10 \dots 0\rangle + |01 \dots 0\rangle + \dots + |00 \dots 1\rangle)/\sqrt{n}$ is the n -qubit W state.

As $|W_n(0)\rangle$ and $|W_n(n)\rangle$ are product states, they are uniquely determined by their 1-RDMs. We know that $|W_n(1)\rangle$ is uniquely determined by its 2-RDMs [15], and the case for $|W_n(i)\rangle$ ($i = 2, 3, \dots, n-2$) remains open. Here we show that $|W_n(i)\rangle$ is uniquely determined by its 2-RDMs for any i . Note, however, that nonsymmetric Dicke states, which are nonequal

weight superposition of weight- i bit strings, are in general not uniquely determined by their 2-RDMs [15].

To begin, we define a collective operator $S_z = \sum_{i=j}^n Z_j$, the Z component of the total angular momentum of the system. Obviously for a given i , $|W_n(i)\rangle$ is an eigenstate of S_z , which is in general degenerate. For a properly chosen constant c_i , $|W_n(i)\rangle$ could be an eigenvalue zero eigenstate of $H_0 = S_z + c_i \mathbb{1}$.

We now employ the squaring technique. For a given i , $|W_n(i)\rangle$ is then the ground state of the 2-local Hamiltonian H_0^2 . The ground space is in general degenerate, however, $|W_n(i)\rangle$ is the only state in the ground space which is invariant under the permutation of any two qubits. To split the degeneracy and to make $|W_n(i)\rangle$ the unique ground state, note the two-qubit SWAP operator $\text{SWAP}_{jk}|x\rangle_j|y\rangle_k = |y\rangle_j|x\rangle_k$ has eigenvalues 1 and -1 . For any $j \neq k$, $\text{SWAP}_{jk}|W_n(i)\rangle = |W_n(i)\rangle$. Therefore, $|W_n(i)\rangle$ is the unique ground state of the 2-local Hamiltonian

$$H = H_0^2 - c \sum_{j < k} \text{SWAP}_{jk}$$

for small enough $c > 0$, hence $|W_n(i)\rangle$ is uniquely determined by its 2-RDMs.

Conclusion. We have discussed the correlations in excited states of local Hamiltonians. Explicit examples are constructed to show that, a nondegenerate excited state of a k -local Hamiltonian may not be uniquely determined by its k -RDMs, even among pure states. By applying a spin-to-fermion map, these examples disprove a conjecture in quantum chemistry, as well as a weaker version, regarding nondegenerate excited states of 2-local Hamiltonians in fermionic systems. Therefore,

to understand the properties of the excited states of a 2-local fermionic system, the information in 2-matrices may not be enough and one has to resort to 4-matrices in some cases.

We further showed that any nondegenerate excited state of a k -local Hamiltonian is a unique ground state of another $2k$ -local Hamiltonian, and hence is uniquely determined by its $2k$ -RDMs. Moreover, this $2k$ bound is indeed optimal. For a constant k , this result indicates that a nondegenerate excited state cannot have “nonlocal” irreducible correlations. It is worth noting that the squaring construction does not preserve the geometrically local structure that the original Hamiltonian may have. It is not clear to us whether there exists a general construction that preserves geometrically local structure, and we leave it to future research.

Our techniques also helped us to understand correlations in certain quantum states in a relatively simple way. As an example, we have shown that all the n -qubit symmetric Dicke states are uniquely determined by their 2-RDMs.

In conclusion, our work corrects some misconceptions about the excited states of k -local Hamiltonians and provides the basis for further investigation of excited-state properties of many-body quantum systems. We hope that our investigations will help to build new connections between quantum information science, quantum chemistry, and many-body physics.

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