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 non-degenerate 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 non-degenerate excited states. In fact, for fermionic systems, it has been conjectured that any non-degenerate 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 non-degenerate 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. It means that correlations in excited states of local Hamiltonians could be dramatically different from those in ground states. We further show that any non-degenerate 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).

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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 kind 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. Especially, 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 $|\psi\rangle$.

As a physical interpretation of irreducible correlations, we note that the non-degenerate ground state of a k-local Hamiltonian contains no irreducible $>k$-party correlation. More concretely, the Hamiltonian H of a real n-particle system usually involves terms of at most k-body interactions, where k is a small number [3]. 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 by the k-RDMs of $|\psi_0\rangle$. Generically, the ground state will be non-degenerate. In this case, $|\psi_0\rangle$ is 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" legitimates, in a very strong sense, the reduced density matrix approach for many-body systems (cf. Ref. [4]).

Similar observation applies for 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 early 1960s [4, 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 non-degenerate excited state of a 2-local fermionic Hamiltonian is simultaneously a unique ground state of another 2-local fermionic Hamiltonian, hence is uniquely determined by its 2-matrix [5]. And a weaker version of this conjecture states that any non-degenerate 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 [4]. The N-representability problem has been studied extensively in the past several decades and significant progresses in studying practical chemical systems have been made [4–6], 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 nice physics phenomena, especially in non-zero temperature situation. Sometimes even the zero temperature physics cannot be characterized by ground states only, for instance, in certain kind of quantum phase transitions [8].

Here we construct explicit counterexamples to show that both conjectures for fermionic systems are false. In more general settings of n-particle systems, not necessarily fermionic, we further show that any non-degenerate 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. This implies, for fermionic systems with 2-local Hamiltonians, that the understanding of some properties of excited states will need the information of their 4-matrices. We also apply our understanding 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 [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:

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

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

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

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 non-degenerate 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 3-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 non-degenerate eigenstate of some 2-local Hamiltonian $H = \sum_i H_i$, where each H_i acts non-trivially on at most two qubits. It is well known that almost all 3-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 non-degenerate eigenstate of some 2-local Hamiltonian, we construct the 2-local Hamiltonian explicitly. We start from a simple case of the GHZ state where $\alpha = \beta = 1/\sqrt{2}$, $|\psi\rangle_{\mathrm{GHZ}} = (|000\rangle + |111\rangle)/\sqrt{2}$. The GHZ state is the eigenstate of the commuting Pauli operators $Z_1Z_2, Z_2Z_3, X_1X_2X_3$ 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], $|\psi\rangle_{\mathrm{GHZ}}$ is stabilized by the group generated by $Z_1Z_2, Z_2Z_3, X_1X_2X_3$.

For the Hamiltonian $H_0 = -Z_1Z_2 - Z_2Z_3$, $|\psi\rangle_{\mathrm{GHZ}}$ is an eigenstate but degenerate with any state in the space spanned by $|000\rangle, |111\rangle$. In order to remove the 2-fold degeneracy and to make $|\psi\rangle_{\mathrm{GHZ}}$ a non-degenerate eigenstate, we note that $X_1X_2X_3|\psi\rangle_{\mathrm{GHZ}} = |\psi\rangle_{\mathrm{GHZ}}$. Therefore, $|\psi\rangle_{\mathrm{GHZ}}$ is an eigenstate of $H_1 = X_1X_2 - X_3$ 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 $|\psi\rangle_{\mathrm{GHZ}}$ is a non-degenerate eigenstate of the 2-local Hamiltonian $H = -Z_1Z_2 - Z_2Z_3 + c(X_1X_2 - X_3)$, for a properly chosen c (for instance, one can choose $c = -1$ then $|\psi\rangle_{\mathrm{GHZ}}$ is the non-degenerate 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 $\mathrm{diag}(a_{11}, a_{22})$, then we have

$$\mathrm{diag}(\frac{\beta}{\alpha}, \frac{\alpha}{\beta})_1 X_1X_2X_3(\alpha|000\rangle + \beta|111\rangle) = \alpha|000\rangle + \beta|111\rangle,$$

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

$$H = aZ_1Z_2 + bZ_2Z_3 + c\,(\mathrm{diag}(\frac{\beta}{\alpha}, \frac{\alpha}{\beta})_1 X_1X_2 - X_3),$$

for some properly chosen a, b, c.

These 3-qubit examples can thus be mapped to fermionic counterexamples of three fermions with six modes, thus disprove the conjecture discussed in [5] and its weaker version in [6].

More counterexamples.— One may think that the existence of the counterexamples from 3-qubit states is due to the fact that almost all (except the GHZ-type) 3-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 3-qubit states provides a systematic way to find a large class of counterexamples.

The idea of constructing the counterexamples from 3-qubit states is the following: start from a 2-local Hamiltonian H_0 whose ground space is degenerate (for simplicity, we assume it is two-fold 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 $M = X_1X_2Z_3Z_4$, one can chose $H_1 = X_1X_2 - Z_3Z_4$), then the Hamiltonian $H = H_0 + cH_1$ will have $|C_0\rangle$ as a non-degenerate 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 case 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 two-fold degenerate, constituting a quantum error-correcting code of distance 3, where $J_x, J_z > 0$, the subscripts j, k refer to the qubit of the j-th row and k-th column and the addition is mod3. 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 non-degenerate 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 non-degenerate 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 of the 3-qubit case, we know that $|\psi^{(n)}\rangle_{\text{GHZ}}$ is a non-degenerate ground state of the $\frac{n}{2}$-local Hamiltonian

$$\begin{aligned} H = &-Z_1Z_2 - Z_2Z_3 - \cdots - Z_{n-1}Z_n \\ &+ c\,(X_1X_2 \cdots X_{n/2} - X_{n/2+1}X_{n/2+2} \cdots X_n), \end{aligned}$$

for a properly chosen c. Using the idea based on quantum error-correcting codes, one can also find other states which are non-degenerate 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' this correlation could be for non-degenerate eigenstates of local Hamiltonians? More concretely, can a non-degenerate eigenstate of a k-local Hamiltonian have non-zero 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 non-degenerate eigenstate of a local Hamiltonian have non-local irreducible correlations?

We show, however, this is not the case—a non-degenerate 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 non-degenerate 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, $|\psi\rangle$ is then uniquely determined by its $2k$-RDMs. This result shows that although correlations in non-degenerate excited states of a local Hamiltonians 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 non-degenerate 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 non-degenerate 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 non-degenerate 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.— We have discussed in a very general setting about 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. As an example, we discuss correlations in n-qubit symmetric Dicke states.

The n-qubit symmetric Dicke state $|W_n(i)\rangle$ ($i = 0, 1, \ldots, n$) is the equal weight superposition of weight-i bit strings [9]. For instance, $|W_n(0)\rangle = |00\cdots 0\rangle$, and $|W_n(1)\rangle = (|10\cdots 0\rangle + |01\cdots 0\rangle + \cdots + |00\cdots 1\rangle)/\sqrt{n}$ 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 $|W_n(i)\rangle$ ($i = 2, 3, \ldots, n-2$) remain open. Here we show that $|W_n(i)\rangle$ is uniquely determined by its 2-RDMs for any i. Note, however, that non-symmetric Dicke states, which are non-equal weight superposition of weight-i bit strings, are in general not uniquely determined by their 2-RDMs [15].

To begin with, 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 $H_0 = S_z + c_i \mathbb{1}$.

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, 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 non-degenerate 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 non-degenerate 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 non-degenerate 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. Moreover, this $2k$ bound is indeed optimal. For a constant k, this result indicates that a non-degenerate excited state cannot have 'non-local' irreducible correlations.

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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