Classification of entanglement and quantum phase transition in $XX$ Model

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Abstract. We study the relation between entanglement and quantum phase transition (QPT) from a new perspective. Motivated by one’s intuition: QPT is characterized by the change of the ground-state structure, while entangled states belong to different classes have different structures, we conjecture that QPT occurs as the class of ground-state entanglement changes and prove it in $XX$ model. Despite the classification of multipartite entanglement is yet unresolved, we proposed a new method to judge whether two many-body states belong to the same entanglement class.

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1. Introduction

Quantum phase transition (QPT) is a phase transition that occurs at absolute zero temperature, and means nonanalyticity of the ground-state properties. The singularity may be a discontinuity in the first or higher-order derivative of the ground-state energy, respectively referred as first-order or continuous QPT[1].

QPT is usually accompanied by a qualitative change in the nature of the correlation in the ground state, and quantum fluctuation is the ultimate reason leading to QPT, so it is certainly of major interest in both condensed matter physics and quantum information science to describe the connection between QPT and quantum entanglement[2]. Various entanglement measures are calculated and hoped to exhibit singular behavior at quantum critical point. Some bipartite entanglement measurements such as concurrence[3, 4, 5], entanglement entropy[6, 7], can indeed identify particular QPT. There even a general theory of the relation between QPT and bipartite entanglement was developed under certain conditions[8]. However, counterexample was soon found[9]. Therefore, QPT in terms of multipartite entanglement began drawing attentions[10, 11]. It is also a noteworthy problem whether multipartite or bipartite entanglement being favored at QPT[12, 13].

So far there is not a universal conclusion of the relation between entanglement (bipartite or multipartite) and QPT (first-order or continuous). Considering that the intrinsic character of QPT is the change of the ground-state structure, so the problem is probably due to that the singularities of entanglement measures aren’t essential to the change of the ground-state structure. Geometric phase[14] or fidelity[15, 16, 17] may be a good indication of QPT. But concerning entanglement, we think that inequivalent entanglement class can appropriately reflect the change of ground-state structure, since two inequivalently entangled states have different structures. So a promising way to reveal the deep connection between QPT and entanglement is to study the classification of ground-state entanglement around QPT. Our focus in the paper is to investigate the classification of entangled ground states in the vicinity of QPT in one-dimensional XX model[18]. It is shown that, no matter the model length $N$ is arbitrary or tends to infinity, the change of ground-state entanglement class always indicates the occurrence of QPT.

2. SLOCC classification of entanglement

As concerning the classification of entangled states, stochastic local operation and classical communications (SLOCC) are usually used to define equivalent classes. That is, two states are said to belong to the same entanglement class if both of them can be obtained from the other with nonzero probability by means of local operation assisted by classical communications. Many researchers have investigated the SLOCC-inequivalent classes of pure entangled states[19, 20, 21].

The complete classification of pure entangled states is indeed an intricate task.
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However, if we only need to judge whether two states are SLOCC-inequivalent, there is a simple criterion by virtue of Schmidt decomposition [2]. As well known, for any bipartite pure state $|\Psi\rangle \in \mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$, there exist local orthonormal bases $\{|u_i\rangle\} \in \mathcal{H}_A$ and $\{|v_i\rangle\} \in \mathcal{H}_B$ such that

$$|\Psi\rangle = \sum_i a_i |u_i\rangle \otimes |v_i\rangle,$$  

(1)

$a_i$ are nonnegative real numbers satisfying $\sum_i a_i^2 = 1$, referred to as Schmidt coefficients. The number of nonzero $a_i$ is known as the Schmidt rank, here denoted by $\text{Sch}(|\Psi\rangle)$. It can be easily deduced that any two SLOCC-equivalent states must have the same Schmidt rank [22, 23]. In other words, two bipartite states with different Schmidt rank are SLOCC-inequivalent. It provides a clue to judge the SLOCC-inequivalence of multipartite state. Given two $N$-party states, we can calculate its Schmidt rank based on a particular bipartition. A bipartition means a division of $N$-party system into two nonempty and disjoint parts, i.e., one part including $M (1 \leq M < N)$ bodies and the other $(N - M)$ bodies. If two $N$-party states have different Schmidt rank based on the same bipartition, they necessarily belong to different entanglement class. This method bypasses the involved issue of complete classification of multipartite states and may be crucial in the researches of QPT in many-body system.

3. First-order and continuous QPT in XX model

The Hamiltonian of XX model is

$$\mathcal{H} = \frac{J}{4} \sum_{i=1}^{N} (\sigma_x^i \sigma_x^{i+1} + \sigma_y^i \sigma_y^{i+1}) - B \sum_{i=1}^{N} \sigma_z^i. $$  

(2)

where $\sigma_{x/y/z}^i$ are the usual Pauli matrices of the $i$th spin (cyclic boundary condition $N + 1 \equiv 1$ is assumed). The external magnetic field $B$ could always be supposed positive without loss of generality. The model can be analytically solved by Jordan-Wigner transformation [18]. Using the operators

$$\sigma_{\pm} = \frac{1}{2} (\sigma_x \pm i \sigma_y) , \quad c_k^\dagger = \sigma_{z}^{\frac{k-1}{2}} \prod_{i=1}^{k-1} \sigma_{z}^i,$$

the Hamiltonian (2) is transformed into

$$\mathcal{H} = - \frac{J}{2} \sum_{i=1}^{N-1} (c_{i+1}^\dagger c_i + c_i^\dagger c_{i+1}) + \frac{J}{2} \alpha (c_1^\dagger c_N + c_N^\dagger c_1) - BN + 2B \sum_{i=1}^{N} c_i^\dagger c_i$$

where $\alpha \equiv \prod_{k=1}^{N}(1 - 2c_k^\dagger c_k) = \prod_{k=1}^{N} \sigma_z^k = (-1)^r$. $r$ is the total number of spin-downs which is a constant. Introducing the Fourier transformation of $c_k^\dagger$:

$$C_q^\dagger = \frac{1}{\sqrt{N}} \sum_{k=1}^{N} \exp(iqk)c_k^\dagger, \quad q = \frac{2\pi n}{N}$$  

(3)

where $n$ is integer (half-odd integer) for odd (even) $r$, the Hamiltonian is that of one-dimensional spinless fermions

$$\mathcal{H} = -BN + \sum_q (2B - J \cos q) C_q^\dagger C_q.$$
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The lowest energy eigenstate with fixed $r$ can be expressed as
\[ |\psi_r^0\rangle = \prod_{l=1}^{r} C_{\pi(r+1-2l)/N}^l |0\cdots0\rangle, \]
and its energy is
\[ E_r^0 = -J \sum_{l=1}^{r} \cos[\pi(r + 1 - 2l)/N] - B(N - 2r) \]
\[ = -J \csc \left( \frac{\pi}{N} \right) \sin \left( \frac{\pi r}{N} \right) - B(N - 2r) \]
\[ \approx -D^r J - B(N - 2r). \]
Obviously, $D^r = D^{N-r}$. Thus when $J$ is fixed and $B$ is tuned,
\[ \mathcal{G} = \{|\psi_0^0\rangle, |\psi_1^0\rangle, \ldots, |\psi_{\lfloor N/2 \rfloor}^0\rangle\} \]
includes all of the possible ground states of the XX model. With the modulation of the external magnetic field, each state in $\mathcal{G}$ becomes the ground state in turn, while the energy of the system changes abruptly. The first-order derivative of the energy with the magnetic field $B$ is discontinuous. A first-order QPT occurs.

For $N$-limited XX model, the first-order QPT occur at $[\frac{N}{2}]$ critical values of magnetic field, which can be achieved from the eigenenergy corresponding to each state in $\mathcal{G}$. That is, the energy of $|\psi_r^0\rangle$ is $-D^r J - B(N - 2r)$, then the transition from $|\psi_r^0\rangle$ to $|\psi_{r+1}^0\rangle$ occurs at
\[ -D^r J + 2Br = -D^{r+1} J + 2B(r + 1), \]
i.e.,
\[ B_c^r = \frac{J}{2} \sec \left( \frac{\pi}{2N} \right) \cos \left[ \frac{\pi(r + \frac{1}{2})}{N} \right], \quad r = 0, \ldots, \lfloor \frac{N}{2} \rfloor - 1. \]

For $N \to \infty$, it is already known that at $B_c = J/2$, there occurs a continuous QPT, i.e., a superfluid-Mott insulator phase transition\[1\].

4. SLOCC classification of ground-state around QPT in XX model

Now we begin to investigate the ground-state entanglement class around QPT in XX model.

When $N \to \infty$, there is only one continuous QPT. At $B_c = J/2$, the system transits from Mott-insulator phase to superfluid phase or vice versa. The ground state of Mott-insulator phase is a separable state with all spins pointing to the same direction, while the ground state of superfluid phase is sure to be an entangled state\[1\]. Therefore, the class of ground-state entanglement changes when QPT happens.

When $N$ is limited, since every stats in $\mathcal{G}$ could be ground state with the adjustment of magnetic field, we need to prove that all states in $\mathcal{G}$ is inequivalently entangled.

To complete this tough task for arbitrary $N$, we calculate the Schmidt rank of every element in $\mathcal{G}$, based on $[\frac{N}{2}] \otimes N - [\frac{N}{2}]$ bipartition. We will show that $\text{Sch}(|\psi_0^r\rangle) = 2^r$ holds for arbitrary $r$ and $N$. For simplicity, $[\frac{N}{2}] \equiv M$ henceforth.
Notice that
\[
c_i^j c_i^l |0\cdots0\rangle_N = \begin{cases} 
|mn\rangle, & \text{if } m < n, \\
-|mn\rangle, & \text{if } m > n, \\
0, & \text{if } m = n,
\end{cases}
\]
where \(|mn\rangle\) corresponds to spin configuration in which all spins are up, except the spin at the site \(m\) and \(n\) are down. Replacing Eq. (3) into (4), the ground state with \(r\) spin-downs can be expressed as
\[
|\psi_0^r\rangle = \frac{1}{\sqrt{N^r}} \prod_{l=1}^{N} \sum_{k_1 < \cdots < k_r \leq N} \left[ \prod_{1 \leq i < j \leq r} \sin \left( \frac{(k_i - k_j)\pi}{N} \right) \right] |k_1 \cdots k_r\rangle.
\]

The last step is achieved using \(e^{ix} - e^{-ix} = 2i \sin x\).

Next we calculate the Schmidt rank of \(|\psi_0^r\rangle\) based on \(M \otimes N - M\) bipartition. The constant \((2i)^{C^2_r}/\sqrt{N^r}\) can be omitted. \(|\psi_0^r\rangle\) is a weighted superposition of all possible \(|k_1 \cdots k_r\rangle\) where the value range of all \(k_i\) are \([1, N]\) and \(k_1 < \cdots < k_r\) must be satisfied, so we rewrite \(|\psi_0^r\rangle\) as
\[
|\psi_0^r\rangle = |0\cdots0\rangle_M \otimes \left[ \sum_{M<k_1 < \cdots < k_r \leq N} \prod_{1 \leq i < j \leq r} \sin \left( \frac{(k_i - k_j)\pi}{N} \right) |k_1 \cdots k_r\rangle \right] \\
+ \cdots + \left[ \sum_{1 \leq k_1 < \cdots < k_l \leq M} |k_1 \cdots k_l\rangle \otimes \sum_{M<k_{l+1} < \cdots < k_r \leq N} \prod_{1 \leq i < j \leq r} \sin \left( \frac{(k_i - k_j)\pi}{N} \right) |k_{l+1} \cdots k_r\rangle \right] \\
+ \cdots + \left[ \sum_{1 \leq k_1 < \cdots < k_r \leq M} \prod_{1 \leq i < j \leq r} \sin \left( \frac{(k_i - k_j)\pi}{N} \right) |k_1 \cdots k_r\rangle \right] \otimes |0\cdots0\rangle_{N-M}.
\]

That is, we first carry out a preliminary Schmidt decomposition by divide all possible \(|k_1 \cdots k_r\rangle\) into \(r + 1\) groups, according to the number of spin-downs that locate in the former \(M\) qubits, i.e.,
\[
|\psi_0^r\rangle = \sum_{l=0}^{r} \sum_i a_i^l |u_i^l\rangle \otimes |v_i^l\rangle,
\]
(6)

Obviously, when \(k \neq l\), \(\forall i, j\), \(\langle u^k_i | u^l_j \rangle = \langle u^k_i | v^l_j \rangle = 0\) always hold. If \(\text{Sch}(|\psi_0^{r(l)}\rangle)\) represents the number of nonzero \(a_i^l\), then
\[
\text{Sch}(|\psi_0^r\rangle) = \sum_{l=0}^{r} \text{Sch}(|\psi_0^{r(l)}\rangle).
\]
(7)

We will explain that
\[
\text{Sch}(|\psi_0^{r(l)}\rangle) = C^l_r,
\]
(8)
thereby

$$\text{Sch}(\psi_0^r)) = \sum_{l=0}^{r} C_r^l = 2^r.$$  (9)

Notice that the maximum value of \( r \) is \( M \), so the Schmidt rank of \( |\psi_0^r\rangle \) will never exceed \( 2^M \).

First it is easily found \( \text{Sch}(|\psi_0^{r(0)}\rangle) = \text{Sch}(|\psi_0^{r(r)}\rangle) = 1 \). Eq. (9) holds for \( l = 0, r \).

Next remembering that if \( \{\alpha_1, \cdots, \alpha_l\} \) is a set of linear independent vectors, then we can achieve an equivalent set of orthogonal vectors \( \{\beta_1, \cdots, \beta_l\} \) by Schmidt orthogonalization. Thereby, \( \text{Sch}(|\psi_0^{r(l)}\rangle) \) is the rank of such a \( C_M \otimes C_{N-M}^l \)-dimensional matrix \( A^{(l)} \). Every element of \( A^{(l)} \) can be uniformly expressed as \( \prod_{1 \leq i \leq j \leq r} \sin[(k_i - k_j)\pi/N] \), i.e., a product of \( C_r^2 \) sine functions. For each row \( 1 \leq k_1 < \cdots < k_l \leq M \) are fixed and \( M < k_{l+1} < \cdots < k_r \leq N \) vary, while for each column the situation is just the reverse. We find the rank of \( A^{(l)} \) by elementary row(column) transformation. So every element can first be simplified as \( \prod_{1 \leq i \leq l, l+1 \leq j \leq r} \sin[(k_i - k_j)\pi/N] \), i.e., a product of \( l(r-l) \) sine functions, as for each row of \( A^{(l)} \), \( \prod_{1 \leq i \leq j \leq l} \sin[(k_i - k_j)\pi/N] \) is a constant, and for each column \( \prod_{l+1 \leq i \leq j \leq r} \sin[(k_i - k_j)\pi/N] \) is a constant. Furthermore, \( \text{Sch}(|\psi_0^{r(l)}\rangle) = \text{Sch}(|\psi_0^{r(r-l)}\rangle) \) should hold. The reason is that the elementary row and column transformation of \( A^{(l)} \) and \( A^{(r-l)} \) will yield similar simplest form. Then we only need to calculate \( \text{Sch}(|\psi_0^{r(l)}\rangle) \) by elementary row transformation for \( l = 1, \cdots, \lfloor \frac{r}{2} \rfloor \).

Take \( r = 2, l = 1 \) as an example, every element can be expressed as \( \sin[(k_1 - k_2)\pi/N] \), and for each column \( 1 \leq k_1 \leq M \) varies while for each row \( M < k_2 \leq N \) varies. So the the matrix is (overall minus sign is omitted)

$$A^{(1)} = \begin{bmatrix}
\sin(\frac{\pi}{N}) & \sin(\frac{2\pi}{N}) & \cdots & \sin(\frac{N-M}{N}\pi) \\
\sin(\frac{2\pi}{N}) & \sin(\frac{3\pi}{N}) & \cdots & \sin(\frac{N-M+1}{N}\pi) \\
\vdots & \vdots & \ddots & \vdots \\
\sin(\frac{M-N}{N}\pi) & \sin(\frac{M+1}{N}\pi) & \cdots & \sin(\frac{N-1}{N}\pi)
\end{bmatrix}$$

Let the \( i \)th row vector of \( A^{(1)} \) is denoted as \( \mathbf{a}_i \), because

$$\sin\left(\frac{m\pi}{N}\right) + \sin\left(\frac{(m+2)\pi}{N}\right) = 2\cos\left(\frac{\pi}{N}\right)\sin\left(\frac{(m+1)\pi}{N}\right)$$,

so for \( i = 1, \cdots, M - 2 \),

$$\mathbf{a}_i + \mathbf{a}_{i+2} = 2\cos\left(\frac{\pi}{N}\right)\mathbf{a}_{i+1}$$

always holds. Then by elementary row transformation \( \mathbf{a}_{i+2} = \mathbf{a}_{i+2} + \mathbf{a}_i - 2\cos\left(\frac{\pi}{N}\right)\mathbf{a}_{i+1} \) for \( i = 1, \cdots, M - 2 \), \( A^{(1)} \) can be transformed into

$$A^{(1)} = \begin{bmatrix}
0 & 0 & \cdots & 0 \\
0 & 0 & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
\sin(\frac{M-N}{N}\pi) & \sin(\frac{M}{N}\pi) & \cdots & \sin(\frac{N-2}{N}\pi) \\
\sin(\frac{M-N}{N}\pi) & \sin(\frac{M+1}{N}\pi) & \cdots & \sin(\frac{N-1}{N}\pi)
\end{bmatrix}$$
So the rank of $A^{(1)}$ is 2. Elementary column transformation apparently yields the same result.

For bigger $r$ and $l$, although the matrix $A^{(l)}$ becomes complicated rapidly, the knack used to find the rank of $A^{(l)}$ is analogous, however, much more intricate. We will expatiate step by step.

First consider $A^{(1)}$, every element is in the simplified form of $\prod_{2 \leq j \leq r} \sin((k_1 - k_j)\pi/N)$, i.e., a product of $r - 1$ sine functions. It can be transformed into a linear sum of a series of sine functions like $\sin\{[p k_1 + f_p(2, \ldots, k_r)]\pi/N\}$, where $p = r - 1, r - 3, \ldots, 1(0)$ for even (odd) $r$. After elementary row transformation like above, there are two rows left for every nonzero $p$ and only one row left when $p = 0$. Then the simplest expression of $A^{(1)}$ is

$$A^{(1)} = \begin{bmatrix} \Pi_{2 \leq j \leq r} \sin \left( \frac{(M-r+1-k_1)\pi}{N} \right) & \cdots & \cdots \\ \vdots & \ddots & \vdots \\ \Pi_{2 \leq j \leq r} \sin \left( \frac{(M-k_2)\pi}{N} \right) & \cdots & \cdots \end{bmatrix},$$

so the rank of $A^{(1)} = r = C_r^1$.

Next consider $A^{(2)}$, the element is simplified as $\prod_{3 \leq j \leq r} \sin((k_1 - k_j)\pi/N)\sin((k_2 - k_j)\pi/N)$, which is a product of $2(r - 2)$ sine functions. When we simplify $A^{(2)}$ by similar strategy, we must bear in mind that both $k_1$ and $k_2$ vary in the value range $[1, M]$ and $k_1 < k_2$ must be satisfied. So the simplest form of $A^{(2)}$ is

$$A^{(2)} = \begin{bmatrix} \cdots & \Pi_{3 \leq j \leq r} \sin \left( \frac{(M-r+1-k_1)\pi}{N} \right) \sin \left( \frac{(M-r+2-k_1)\pi}{N} \right) & \cdots \\ \vdots & \ddots & \vdots \\ \Pi_{3 \leq j \leq r} \sin \left( \frac{(M-r+1-k_2)\pi}{N} \right) \sin \left( \frac{(M-k_2)\pi}{N} \right) & \cdots & \cdots \\ \vdots & \ddots & \vdots \\ \cdots & \Pi_{3 \leq j \leq r} \sin \left( \frac{(M-1-k_1)\pi}{N} \right) \sin \left( \frac{(M-k_1)\pi}{N} \right) & \cdots & \cdots \end{bmatrix},$$

the rank of $A^{(2)} = 1 + 2 + \cdots + r - 1 = C_r^2$.

Finally, analogous but involved generalization yields the ultimate expression of $A^{(l)}$ is

$$A^{(l)} = \begin{bmatrix} \cdots & \Pi_{l+1 \leq j \leq r} \sin \left( \frac{(M-r+1-k_l)\pi}{N} \right) & \cdots & \cdots \\ \vdots & \ddots & \vdots & \ddots \\ \Pi_{l+1 \leq j \leq r} \sin \left( \frac{(M-l+1-k_l)\pi}{N} \right) & \cdots & \cdots & \cdots \end{bmatrix},$$

and its rank is

$$\begin{align*}
(r - l + 1) + (r - l)(1 + 2) + (r - l - 1)(1 + 2 + 3) \\
+ \cdots + (1 + 2 + \cdots r - l + 1) \\
= \sum_{j=1}^{r-l+1} [r - (l - 2 + j)] \left\lceil \sum_{i=1}^{j} i \right\rceil \\
= C_r^d.
\end{align*}$$

So far we have explained Eq. (8), accordingly Eq. (9) is proved for arbitrary $r$ and $N$. So we have proved that in arbitrary $N$-qubit XX model, no matter $N$ is infinite or
The occurrence of all QPT, first-order and continuous, can be witnessed by the change of ground-state entanglement class.

5. Conclusion

In conclusion, we have studied the relation between classification of ground-state entanglement and QPT in $N$-qubit XX model. For arbitrary $N$, when the exchange constant $J$ is kept invariable and the external magnetic field $B$ is tuned, QPT occurs. For $N \to \infty$ or limited $N$, the QPT is continuous or first-order respectively. No matter what the type of QPT is, we find that the occurrence of QPT is always indicated by the change of class of entangled ground state. Although the conclusion obtained in the XX model seems too particular, we think it is indeed a reasonable conclusion that the entangled ground states in the vicinity of the transition are SLOCC-inequivalent. Because the intrinsic feature of QPT is the change of the structure of the ground state, and inequivalently entangled states have different structure. We believe our results grasp the essence of the relevance of entanglement in QPT and hope it can be verified broadly in the future. Besides, the proof based on the Schmidt rank provides a partial solution to judge SLOCC-inequivalent entanglement. Although it works only if Schmidt rank indeed changes at the QPT, since the coincidence of the Schmidt rank does not ensure the same entanglement class for three or more components, it develops a new method regardlessly the complete classification of multipartite entangled is far to be resolved nowadays.

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