Local entanglement and quantum phase transition in 1D transverse field Ising model

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In this paper, we study the entanglement between two-neighboring sites and the rest of the system in a simple quantum phase transition of 1D transverse field Ising model. We find that the entanglement shows interesting scaling and singular behavior around the critical point, and then can be used as a convenient marker for the transition point.

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Entanglement is one of the most fascinating features of the quantum theory. It roots in the superposition principle of quantum mechanics and the tensor product structure of different Hilbert spaces, and implies the existence nonlocal correlation in quantum world. Since this correlation is absent in the classical world, it is a kind of pure quantum correlation and regarded as crucial resource in many quantum information processing tasks. Actually, similar fascinating property also exists in the classic optics. By recording the interference pattern of two laser beams reflected from one object, the whole image can be recovered from even a small piece of holograph, although the resolution may be reduced. In other words, the superposition of two coherent electromagnetic waves enables us to learn some global information from a localized spatial area. Though it is not a precise analogy, people expect that the entanglement, which roots in the same superposition principle, can enable us to learn some global properties from a small part of the system. This observation may be one of the main motivations in the recent studies on the role of entanglement between a small part, e.g. a block consisting of one or more sites, and the rest of the system in the quantum phase transition.

Conceptually, the single-site and the two-site entanglement, and the block-block entanglement are different notations of the same kind of measurement. They are defined as the von Neumann entropy of the reduced density matrix of a local part in the system. Studies of the block-block entanglement in the one-dimensional spin models have established a close relationship between the conformal field theory and quantum information theory. The block-block entanglement is also generalized in systems other than spin models. Many works are devoted to understand the local entanglement, a limiting case of the block-block entanglement, in the ground state of itinerant fermion systems. For example, in the extended Hubbard model, the global entanglement can be sketched out by the contour map of the single-site local entanglement in the parameter space.

And the entanglement’s scaling behavior is investigated in the one-dimensional Hubbard model at criticality point. In the Hirsch model, the singularity in the first derivative of the single-site entanglement is used to locate the superconductor-insulator transition point. However, in some spin systems with Z2 symmetry, the single-site entanglement usually does not contain enough information to describe the critical behavior, then it is necessary to include more sites, such as two sites in the simplest case, into the block. For example, in 1D XXZ model, the two-site local entanglement reaches maximum at the isotropic transition point.

These results suggest that the local entanglement may be used as a good and convenient marker of quantum phase transition. In a strongly correlated system, the reduced density matrix of a local block involves the bipartite correlation in the system as the consequence of the superposition principle in quantum mechanics. At the quantum critical point, quantum fluctuations extend to all scales, thus it may contribute a singular part in the local entanglement. The idea of using the local entanglement to locate transition point is especially useful in numerical calculations, usually the data obtained from a relative small size lattice is sufficient to detect the quantum phase transitions.

In this paper, we investigate the scaling behavior of the two-site local entanglement near the quantum phase transition point in 1D transverse field Ising model. Since the transition type of the Ising model is different from that in 1D XXZ model, the entanglement shows quite different behavior, such as scaling and singularity. We calculate the entanglement and its first order derivative with respect to the coupling constant numerically. Based on the exact solution, we also obtain explicit expressions which clearly exhibit the logarithmic divergence of local entanglement’s derivative at the critical point. Therefore, by studying the two-site local entanglement, we hope to have a deep understanding on the another type of quantum phase transition, as represented by 1D Ising model.

The Hamiltonian of 1D transverse field Ising model
reads

\[ H_{\text{Ising}} = -\sum_{j=1}^{N} \left[ \lambda \sigma_j^x \sigma_{j+1}^x + \sigma_j^z \right], \]

\[ \sigma_1 = \sigma_{N+1}, \]

where \( \sigma_i(\sigma^x, \sigma^y, \sigma^z) \) are Pauli matrices at site \( i \), \( \lambda \) is an Ising coupling in unit of the transverse field, and the periodic boundary conditions are assumed. In the basis spanned by the eigenstates of \( \{\sigma^z\} \), the Hamiltonian changes the number of down spins by two due to the term \( \sigma_i^z \sigma_{i+1}^z \) in its expression, so the whole space of system can be divided by the parity of the number of down spins. That is the Hamiltonian and the parity operator \( P = \prod_j \sigma_j^z \) can be simultaneously diagonalized and the eigenvalues of \( P \) is \( \pm 1 \). Then it can be proved that for a finite system, the ground state in the whole region of \( \lambda > 0 \) is non-degenerate.

We confine our interest to the entanglement between two neighboring sites and rest of the system, so we need to consider the reduced density matrix of two local sites. According to the parity conservation, the reduced density matrix of two spins in this system takes the form

\[ \rho_{ij} = \begin{pmatrix} u^+ & 0 & 0 & z^- \\ 0 & w_1 & z^+ & 0 \\ 0 & z^+ & w_2 & 0 \\ z^- & 0 & 0 & u^- \end{pmatrix} \]

(2)

in the basis \( \{|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle\} \). The elements in the density matrix \( \rho_{ij} \) can be calculated from the correlation functions

\[ u^\pm = \frac{1}{4}(1 \pm (2\langle \sigma_i^x \rangle + \langle \sigma_i^z \sigma_j^z \rangle)), \]

\[ w_1 = w_2 = \frac{1}{4}(1 - \langle \sigma_i^z \sigma_j^z \rangle), \]

\[ z^\pm = \frac{1}{4}(\langle \sigma_i^z \sigma_j^x \rangle \pm \langle \sigma_i^x \sigma_j^y \rangle). \]

(3)

In a finite system, the ground state is a pure state, so the von Neumann entropy \( E_v \), i.e.

\[ E_v = -\text{tr}[\rho_{ij} \log_2(\rho_{ij})] \]

measures the entanglement between the sites \( i, j \) and the rest \( N - 2 \) sites of the system.

The correlation functions in Eqs (3) can be calculated exactly. The mean magnetization in the ground state is given by [16]

\[ \langle \sigma^z \rangle = \frac{1}{N} \sum_\phi \left( 1 - \lambda \cos \phi \right) / \omega_\phi, \]

(5)

where \( \omega_\phi \) is the dispersion relation,

\[ \omega_\phi = \sqrt{1 + \lambda^2 - 2\lambda \cos(\phi_q)}, \]

\[ \phi_q = 2\pi q/N, \]

(6)

where \( q \) is integer (half-odd integer) for parity \( P = -1(+1) \). The two-point correlation functions are calculated as [17]

\[ \langle \sigma_i^z \sigma_j^z \rangle = \frac{1}{N} \sum_\phi \frac{\lambda - \cos \phi}{\omega_\phi}, \]

\[ \langle \sigma_i^x \sigma_j^y \rangle = \frac{1}{N} \sum_\phi \frac{\lambda \cos(2\phi) - \cos \phi}{\omega_\phi}, \]

\[ \langle \sigma_i^y \sigma_j^x \rangle = \langle \sigma^z \rangle^2 - \langle \sigma_i^z \sigma_j^z \rangle \langle \sigma_i^x \sigma_j^x \rangle \]

(7)

Therefore, we can calculate the two-site local entanglement for arbitrary finite system directly.

As is well known, in a ring with infinite sites, the phase diagram of the transverse field Ising model is divided into two phases by a transition point \( \lambda = 1 \). For \( \lambda < 1 \), the ground state of the system is a paramagnet. Its phys-
Then the first order derivative of the entanglement takes

$$\frac{dE}{d\lambda} = -\log \frac{\epsilon_3}{\epsilon_1} \frac{d\epsilon_4}{d\lambda} - \log \frac{\epsilon_3}{\epsilon_1} \frac{d(\epsilon_3 + \epsilon_4)}{d\lambda} - \log \frac{\epsilon_2}{\epsilon_1} \frac{d\epsilon_2}{d\lambda} \tag{9}$$

Then the first order derivative of the entanglement takes

$$\frac{dE_v}{d\lambda} = -\log \frac{\epsilon_4}{\epsilon_3} \frac{d\epsilon_4}{d\lambda} - \log \frac{\epsilon_3}{\epsilon_1} \frac{d(\epsilon_3 + \epsilon_4)}{d\lambda} - \log \frac{\epsilon_2}{\epsilon_1} \frac{d\epsilon_2}{d\lambda} \tag{9}$$

At the critical point, the eigenvalues $\epsilon_i$ converges quickly as the system size increases

$$\epsilon_{1,2} = \frac{1}{4} + \frac{4}{3\pi^2} \pm \frac{\sqrt{13}}{3\pi}, \quad \epsilon_{3,4} = \frac{1}{4} - \frac{4}{3\pi^2} \pm \frac{1}{3\pi} \tag{10}$$

While for $\lambda > 1$, the strong Ising coupling introduces magnetic long-range order of the order parameter $\langle \sigma^z \rangle$ to the ground state. Therefore, the transition in this model is of type from order-to-disorder, and is quite different from the transition in some other models. In the 1D XXZ model, it has been shown that the two-site local entanglement reaches a local maximum at the transition point $\Delta = 1$ which witnesses a transition of type from order-to-order, and becomes singular at another transition point $\Delta = -1$ due to the ground-state level-crossing. However, in the 1D Ising model, no similar properties can be observed directly from the entanglement, as shown in Fig. 1. As suggested by the classification scheme for the quantum phase transition based on the pairwise entanglement [18], we take the first order derivative of the entanglement with respect to the coupling $\lambda$. The results are shown in Fig. 2. We are happy to notice that the first order derivative around the critical point becomes sharper as the system size increases, and is expected to be divergent in an infinite system.

In the critical phenomena, the most important themes are the scaling and universality. In a finite sample, a physical quantity is a smoothly continuous function if there is no ground-state level-crossing. However, it is expected that the anomalies will become clearer and clearer as the size of sample increases. The relevant study is the finite size scaling. For this system, in order to study the scaling behavior the maximum point of $dE_v/d\lambda$, we locate the maximum point for a given system size numerically and define the corresponding location as $\lambda_m$. From Fig. 2, though there is no divergence when $N$ is finite, the anomalies are obvious. The position of the maximum point $\lambda_m$ scales as $\lambda_c - \lambda_m \propto 1/N^{1/2}$.

The results of $dE_v/d\lambda$ at $\lambda_m$ up to 2000 sites are shown in Fig. 4. Though we can almost conclude logarithmic divergence of $dE_v/d\lambda$ at the transition point from the figure, it is still very difficult to take numerical derivative for a very large system, such as $N = 10^8$. In order to make it more confirmative, we now give a rigorous prove that $dE_v/d\lambda$ obeys a logarithmic behavior at the critical point.

In order to calculate the entanglement, we first need to calculate the eigenvalues of the reduced density matrix

$$\epsilon_{1,2} = \frac{1}{4} \left[ (1 + \langle \sigma^z \rangle^2 - \langle \sigma_0^x \sigma_1^y \rangle \langle \sigma_0^y \sigma_1^x \rangle) \pm \sqrt{4(\langle \sigma^z \rangle^2 + (\langle \sigma_0^x \sigma_1^y \rangle - \langle \sigma_0^y \sigma_1^x \rangle)^2)} \right] \tag{8}$$

$$\epsilon_{3,4} = \frac{1}{4} \left[ (1 - \langle \sigma^z \rangle^2 + \langle \sigma_0^x \sigma_1^y \rangle \langle \sigma_0^y \sigma_1^x \rangle) \pm (\langle \sigma_0^x \sigma_1^y \rangle + \langle \sigma_0^y \sigma_1^x \rangle) \right]$$

FIG. 4: The scaling behavior of the maximum point of $dE_v/d\lambda$. The circle line is obtained by numerical derivative, and the square line by analytical expression directly.
Then after some complicated calculations, one can obtain
\[
\frac{dE_v}{d\lambda} = -\frac{1}{2} \left( \frac{1}{N} \sum_\phi \left| \frac{\cos^2 \frac{\phi}{2}}{\sin \frac{\phi}{2}} \cos \phi \right| \log_2 \frac{\epsilon_4}{\epsilon_3} \right)
+ \left[ -\left( \frac{1}{N} \sum_\phi \left| \frac{\cos^2 \frac{\phi}{2}}{\sin \frac{\phi}{2}} \right| \right) \left( \frac{1}{N} \sum_\phi \left| 2 \sin^2 \frac{\phi}{2} \right| \right) \right]
+ \frac{1}{N^2} \left( \sum_\phi \left| 4 \cos^2 \frac{\phi}{2} \sin \frac{\phi}{2} \right| \right)^2 \frac{1}{2(\epsilon_1 - \epsilon_2)} \log_2 \frac{\epsilon_2}{\epsilon_1}.
\tag{11}
\]

The main contribution to the above expression in the large $N$ limit arise from the summation around zero point of $\phi$. Because
\[
\frac{1}{N} \sum_{\phi \in S} \frac{1}{|\phi|} \simeq -\frac{2}{\pi} \ln \frac{2\pi}{N} \simeq \frac{2}{\pi} \ln N,
\tag{12}
\]
then we obtain, in the large $N$ limit
\[
\frac{dE_v}{d\lambda} \simeq A_1^E \ln N
\tag{13}
\]
where $A_1^E$ is a constant
\[
A_1^E = -\frac{1}{2\pi} \log_2 \frac{3\pi^2 + 4\pi - 16}{3\pi^2 - 4\pi - 16}
+ \frac{3}{2\sqrt{3\pi}} \log_2 \frac{3\pi^2 + 4\sqrt{3}\pi + 16}{3\pi^2 - 4\sqrt{3}\pi + 16}
\tag{14}
\]
as has been shown in Fig. 4. On the other hand, for an infinite system, $dE_v/d\lambda$ diverges on approaching the critical point as
\[
\frac{dE_v}{d\lambda} = A_2^E \ln |\lambda - \lambda_c| + \text{const,}
\tag{15}
\]
as has been shown in Fig. 5. Here $A_2^E$ is not completely independent of $\lambda$, and $A_2^E \approx A_1^E$ at $\lambda = 1$.

According to the scaling ansatz [19], the two-site entanglement, considered as a function of the system size and the coupling, is a function of $N^{1/\nu}(\lambda - \lambda_m)$. In the case of logarithmic divergence, it behaves as $dE_v/d\lambda - dE_v/d\lambda|_{\lambda = \lambda_m} \sim Q|N^{1/\nu}(\lambda - \lambda_m)|$, where $Q(x) \propto \ln x$ for large $x$. In Fig. 6 we perform the scaling analysis and find the entanglement can be approximately collapse to a single curve for $\nu \simeq 0.98$. This behavior is quite different from that of concurrence [20] which diverges as $dC/d\lambda|_{\lambda = \lambda_m} \propto -0.2702 \ln N$ and $dC/d\lambda|_{\lambda = \lambda_c} \propto (8/3\pi^2) \ln |\lambda - \lambda_c|$ respectively. Because of $8/3\pi^2 \approx 0.2702$, the ratio of constants in the ln term is unit. This fact leads to $\nu = 1$ for the concurrence. [20]

Actually, though Osterloh et al only gave a numerical constant 0.2702 for the logarithmic divergence of the concurrence with increasing system size, it also can be exactly obtained that the constant is just $8/3\pi^2$ with the above procedure. However, for the local entanglement,

\[
\text{FIG. 5: Logarithmical divergence of } dE_v/d\lambda \text{ around the critical point of an infinite system.}
\]

\[
\text{FIG. 6: (color online) The finite-size scaling analysis for the case of logarithmic divergence. The local entanglement, considered as a function of system size and the coupling, collapse on a single curve for various system size.}
\]

since $A_2^E$ slightly depends on $\lambda$, we have $\nu \simeq 0.98$ according to numerical analysis.

In summary, we have investigated the scaling behavior of the two-site local entanglement in a quantum phase transition of 1D transverse field Ising model. Different from the entanglement in the transition of 1D XXZ model at $\Delta = 1$ which is of type from order-to-order, the entanglement in 1D transverse field Ising model is not a maximum at the critical point where the quantum phase transition is of the type from order-to-disorder. However, its first order derivative with respect to the coupling becomes singular around the critical point as the system size increases. We show the logarithmic divergence both numerically and analytically.

Note added: During the preparation of the manuscript, we notice that a work on the two-site entanglement in
similar model on the arXiv [21].
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