Block-block entanglement and quantum phase transitions in one-dimensional extended Hubbard model

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In this paper, we study block-block entanglement in the ground state of one-dimensional extended Hubbard model. Our results show that the phase diagram derived from the block-block entanglement manifests richer structure than that of the local (single site) entanglement because it comprises nonlocal correlation. Besides phases characterized by the charge-density-wave, the spin-density-wave, and phase-separation, which can be sketched out by the local entanglement, singlet superconductivity phase could be identified on the contour map of the block-block entanglement. Scaling analysis shows that log$_2(l)$ behavior of the block-block entanglement may exist in both noncritical and the critical regions, while some local extremum are induced by the finite-size effect. We also study the block-block entanglement defined in the momentum space and discuss its relation to the phase transition from singlet superconducting state to the charge-density-wave state.

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I. INTRODUCTION

Entanglement, as one of the most intriguing feature of quantum mechanics and a crucial resource in quantum information theory, has been a subject of much study in recent years. For the purpose of practical application, to realize quantum information processing, such as quantum state transfer, based on the condensed matter physics is of great importance. Such potential prospect in the application now has motivated many theoretical investigations on the entanglement in spin and fermionic systems. On the other hand, quantum phase transitions (QPTs), which are characterized by change in the properties of the ground state of a many-body system, are generally driven by quantum fluctuation at zero temperature. One therefore expects that the entanglement, as a term of pure quantum correlation, should closely relate to QPTs. Indeed, some observed relationships between the entanglement and QPTs now have not only deepened our understanding on the QPTs, but also strengthened the connection between the quantum information theory and condensed matter physics. For example, Osterloh et al. reported that the pairwise entanglement of two nearest neighbors shows scaling behavior in the vicinity of quantum phase transition point of the transverse-field Ising model. For other models, such as the XXZ model, spin model with mutual exchanges, etc., the pairwise entanglement also manifests various interesting properties, such as being maximum at transition point, exhibits singularity, and shows scaling behavior.

Besides the pairwise entanglement between two sites, for a non-degenerate ground state, the block-block entanglement also provides a good quantity to describe the pure quantum correlation at zero temperature. The scaling property of the block-block entanglement establishes an interesting connection between concepts of quantum information and quantum field theory. Moreover, unlike the concurrence, a measurement of the entanglement of formation, which is computable only for spin-$1/2$ system, the block-block entanglement can be generalized to high-spin and fermionic systems. There are some works which studied the entanglement in fermionic systems. However, the investigations on the entanglement in relation to QPTs are still on an early stage.

In the extended Hubbard model, it has been shown that the global phase diagram can be sketched out by the contour map of a quantity called the local entanglement. However, the local entanglement fails to identify phases which are related to the off-diagonal-long-range order, such as the superconducting phase. In this paper, we extend our previous investigation on the local entanglement in the extended Hubbard model to the block-block entanglement. We show that the block-block entanglement with block size larger than one can provide more useful information than the local entanglement since it comprises the nonlocal correlation in its expression. The paper is organized as follows. In Sec. II we first briefly review some basic knowledge of the extended Hubbard model and then introduce the definition of the block-block entanglement. In Sec. III we address the problem of the global phase diagram on the $U-V$ plane by introducing the contour map of the block-block entanglement. In Sec. IV we study the scaling behavior of the block-block entanglement by changing the system size. One of the interesting results obtained in this work is that the log$_2(l)$ behavior ($l$ is the block size) of the block-block entanglement also shows in noncritical region. In Sec. V we study the finite-size effect and clarify some unaccustomed behaviors of the block-block entanglement. A simple expression of the local entanglement is obtained. In Sec. VI we try other measure of the block-block entanglement in order to explore the phase boundary which may not be identified by the extremum of the local entanglement. Finally, a brief summary is
given in Sec. VII

II. THE MODEL AND FORMULISM

The one-dimensional extended Hubbard model is defined by the Hamiltonian

$$H = - \sum_{\sigma,j,\delta} c_{j,\sigma}^\dagger c_{j+\delta,\sigma} + U \sum_j n_{j\uparrow} n_{j\downarrow} + V \sum_j n_{j} n_{j+1},$$

where $\sigma = \uparrow, \downarrow; j = 1, \ldots, L; \delta = \pm 1$, $c_{j,\sigma}$ and $c_{j,\sigma}^\dagger$ are creation and annihilation operators at site $j$, and $U$ and $V$ define the on-site and nearest-neighbor Coulomb interactions, respectively. On each site the local states have four possible configurations, denoted by

$$|\phi(l = 1, 2, 3, 4)\rangle = |0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle.$$

The Hilbert space associated with $L$-site system, known as the Fock space $\mathcal{H}_F(L)$, is spanned by $4^L$ basis vectors $|j_1, \ldots, j_L\rangle = \prod_{j=1}^L |\phi_j(t_j)\rangle$. Any state in such a system can be expressed as a superposition of these basis. If we choose periodic boundary condition for $L = 4n + 2$ and anti-periodic boundary condition for $L = 4n$, where $n$ is an arbitrary integer, the ground state is non-degenerate. Therefore, considering the reduced density matrix of a block of 1 successive site of the ground state $\rho_l = \text{tr}_r |\Psi\rangle\langle |\Psi|$, the von Neumann entropy $E_v(l)$, i.e.

$$E_v(l) = -\text{tr}[\rho_l \log_2(\rho_l)]$$

measures the entanglement between the $l$ sites and the rest $L - l$ sites of the system, as shown in the following figure for 10-site system with $l = 4$.

![block diagram](image)

A simple case of the block-block entanglement is when only one site is taken into account. Then the reduced density matrix can be written into a simple form

$$\rho_1 = z |0\rangle\langle 0| + u^+ |\uparrow\rangle\langle \uparrow| + u^- |\downarrow\rangle\langle \downarrow| + w |\uparrow\downarrow\rangle\langle \uparrow\downarrow|,$$

in which

$$w = \langle n_\uparrow n_\downarrow \rangle - \langle n_\uparrow \rangle \langle n_\downarrow \rangle,$$

$$u^+ = \langle n_\uparrow \rangle - w,$$

$$u^- = \langle n_\downarrow \rangle - w,$$

$$z = 1 - u^+ - u^- - w = 1 - \langle n_\uparrow \rangle - \langle n_\downarrow \rangle + w.$$

Here $\langle n_\uparrow \rangle$ and $\langle n_\downarrow \rangle$ are electron densities with spin up and spin down respectively. The corresponding von Neumann entropy then takes the form

$$E_v = -z \log_2 z - u^+ \log_2 u^+ - u^- \log_2 u^- - w \log_2 w.$$

If $l > 1$, the reduced density matrix can not be written into a simple expression. However, since the Hamiltonian $H$ has $U(1)\times SU(2)$ symmetry: $c_{j,\sigma} \rightarrow e^{i\theta} c_{j,\sigma}$; $c_{j,\sigma} \rightarrow U_{\sigma}^c c_{j,\delta}$, which manifests the charge conservation and invariance under spin rotation $U_{\sigma}$. Therefore, any eigenstate of the Hamiltonian $H$ can be both the eigenstate of $z$ component of total spins and of particle number. This fact leads to that, for arbitrary block size $l$, there is no coherent superposition of local state with different value of $S^z(l) = \sum_j (n_{j\uparrow} - n_{j\downarrow})$ and $N(l) = \sum_j (n_{j\uparrow} + n_{j\downarrow})$ in the reduced density matrix. That is, the reduced density matrix must have the diagonal form classified by both $S^z(l)$ and $N(l)$. In this paper, we apply exact diagonalization technique to get the ground state and then exactly diagonalize the reduced density matrix to calculate the block-block entanglement.

III. ENTANGLEMENT AND THE PHASE DIAGRAM

The extended Hubbard model is a prototype model in condensed matter theory for it exhibits a rich phase diagram where various quantum phase transitions occur among symmetry broken states. The corresponding symmetry broken states typically include the charge-density-wave (CDW), the spin-density-wave (SDW), phase separation (PS), singlet (SS) and triplet superconducting phase(TS), and bond-order wave (BOW). Many efforts have been made to obtain the phase diagram of the extended Hubbard model at different band fillings on the $U$-$V$ plane. In our previous work on the local entanglement, it is remarkable to see that the skeleton of the phase diagram of the extended Hubbard model can be directly obtained from the contour map of the local entanglement. This is by no means trivial. In the conventional approach to obtain the phase diagram of the extended Hubbard model, one has to study behaviors of different order parameters in different regions, either by comparing the ground-state energy or the critical exponent of correlation functions associated with broken symmetry. While using a single quantity, $E_v$, the global picture of the system at zero temperature can be observed. This is not a coincident, for the non-vanishing order parameter means the existence of non-local corresponding correlation, whose quantum part is just the entanglement, so the competitions between different orders may lead to changes in the entanglement. When a QPT occurs, entanglement will also behave distinctively in different phases. Therefore, this result reflects the underlying relation between the entanglement and QPTs beyond the superposition principle of quantum mechanics. However, there are some limitations. For example, the local entanglement can not be used to identify superconducting phases, due to the fact that the broken symmetry is associated with off-diagonal-long-range-order, whereas the local reduced density matrix is diagonal. To identify such phase is a challenge, and it is one of our motivations to include the off-diagonal correlation in the study of the entanglement and QPTs.
In Fig. 1 we show a three-dimensional diagram, as well as its contour map of the block-block entanglement for 8 sites system with block size \( l = 3 \). Obviously the structure of the contour map is richer than that of the local entanglement, especially at the region near \( U < 0, -1 < V < 0 \). The contour lines should be similar in the same phase region, because the entanglement should behave in a similar way in the same phase. So the distinct change of the contour lines suggests the existence of a new phase. Compare this contour map with the phase diagram of the extended Hubbard model at half-filling, this region corresponds to SS phase. For the transition from CDW to SDW, the block-block entanglement, including the local entanglement, exhibits maximal value. This fact can be understood by noting that, at the QPT point from CDW to SDW, the weights for different component in the reduced-density matrix are closer due to the higher symmetry in the critical region. Take the local entanglement as an example, we have equally valued \( w, u^+, u^- \), and \( z \) at the transition point. From this point of view, the extremum behavior of the entanglement at the transition point manifests that the QPTs are induced by symmetry broken. For the transition from SS to CDW, the contour lines have an inflexion, which suggests the existence of other types of phase transitions.

In Fig. 2 we show the block-block entanglement as a function of \( V \) for various block size. Here \( L = 10, U = -2 \).

IV. ENTANGLEMENT CHANGE WITH BLOCK SIZE

In Fig. 2 we show the block-block entanglement as a function of \( V \) for various block size at fixed \( U = -2 \), \( L = 10 \). In the cross section of \( U = -2 \), there are three phases. If \( V \ll -1 \), the ground state is phase separated.
That is almost half of sites are doubly occupied and congregate together, while another half of sites are empty. The corresponding wavefunction is dominated by the following configuration, e.g. for the 10-sites system,

\[ \text{PS(a)} : \uparrow \downarrow \uparrow \downarrow \uparrow \downarrow \uparrow \downarrow \uparrow \downarrow \ 0 \ 0 \ 0 \ 0 \ 0, \]

which is in fact an eigenstate of the Hamiltonian with \( t = 0 \). Obviously, this state is separable and has no entanglement. However, in the presence of the hoping term, the ground state becomes a superposition of all possible configurations transformed from the above one through an arbitrary translation operation. This process introduces entanglement into the ground state. If we take the reduced-density matrix with block size \( l \), the number of block matrix corresponding to different particle numbers, \( N(l) = 0, 2, \cdots, 2l \) is \( l + 1 \). The dimension of the block matrix with a given nonzero \( N(l) = 2n, n \leq l, \) is \( l-n+1 \), then the number of nonzero eigenvalues of the reduced density matrix \( \rho_l \) is \( (l^2 + l + 2)/2 \). This result implies a \( \log(l) \) behavior of the block-block entanglement in the phase-separated region. That is, the block-block entanglement will not tend to a constant with the increasing of block size, as shown in Fig. 2. This phenomenon is quite different from previous studies of spin chains, where the \( \log(l) \) behavior of the block-block entanglement only exists at the critical region, while at noncritical region, it will tend to a constant as \( l \) increases.

When the absolute value of negative \( V \) becomes smaller, the effect of the hoping term and the on-site interaction can not be neglected. Though the later still try to maintain the number of doubly occupied sites, the former really want to diffuse the cumulated electron pairs. Then the configuration PS(a) will not be the dominant one, and the weights of the following configurations

\[ \text{PS(b)} : \uparrow \uparrow \uparrow \uparrow \uparrow \downarrow \ 0 \ 0 \ 0 \ 0 \ 0 \]

\[ \text{PS(c)} : \uparrow \downarrow \uparrow \downarrow \uparrow \downarrow \downarrow \ 0 \ 0 \ 0 \ 0 \ 0 \]

will increase. Obviously the configuration PS(b) will introduce block matrices with odd number of particles into the reduced-density matrix, and thus increase the entanglement. So the ordered phase is destroyed gradually as \( V \) increases, and finally the system has maximum entanglement and transits to the SS phase. In the SS phase, the ground state is characterized by an off-diagonal-long-range order. If \( V \to 0 \), the off-diagonal correlation functions in the reduced-density matrix will cause a decrease in entanglement which is consistent with the figure. If \( V \geq 0 \), the hoping process will be suppressed, and the off-diagonal-long-range order will be destroyed. This fact leads to further decrease of the block-block entanglement. Moreover, with the increasing of \( V \), the weight of CDW will increase almost to 1, so that the reduced density matrix is composed of \( 1/2 \uparrow \downarrow \) and \( 0 \) each, and the corresponding entanglement can be calculated exactly:

\[
E_{\nu}(l) = - \sum_{i=1,2} \frac{1}{2} \log_2 \frac{1}{2} = 1
\]

This result is consistent with the previous work on the spin model, which says that the block-block entanglement will tend to a constant in the noncritical region as the block size increases.

In Fig. 3 we show the block-block entanglement as a function of \( V \) for various block size at fixed \( U = 0, l = 10 \). Similar analysis for Fig. 2 can be applied to Fig. 3. The main difference is that in the nearby region of \( V = 0 \), it seems to be a flat area. As SDW, CDW, SS and TS all exist in this region, it is not easy to divide them clearly by using the block-block entanglement only. We also take more detailed calculation in this region. It is surprising that for \( L = 10, U = 0 \), the block-block entanglement get a minimum value at \( V = 0.0 \), and a maximum value at \( V = 0.09 \). It seems that the minimum point is a transition point, just like the appearance of a maximum in the local entanglement at this point. However, whether these points witness phase transitions needs further investigation on longer chains.

*From the above investigations, we find that the block-block entanglement is an increasing function of \( l \) in the region \( l \in [0, L/2] \). In our study, in order to obtain the entropy of reduced density matrix, we need to diagonalize density matrix by the standard QR algorithm. Limited by the computer power, the largest size we have studied is 12, then the block size varies from 1 to 6. It has been argued that the behavior of the entanglement in a critical spin chain matches the result of the conformal field theory, where the geometry entropy is analogs to the spin block entropy. Although we can not give the exact result of scaling on the EHM, we can still see from Fig. 4 that the block-block entanglement grows logarithmically with the block size in some critical regions. Moreover, as we pointed out in the above, such a logarithmic behavior of the block-block entanglement can also exist in the noncritical region for the extended Hubbard model.*
V. ENTANGLEMENT CHANGE WITH SYSTEM SIZE

In this section, we study the dependence of the block-block entanglement on the system size. In our previous work on the local entanglement of the Hubbard model, the local entanglement in some regions (CDW and SDW, for example) obtained from the Bethe Ansatz method (for \( L = \infty \) and \( L = 70 \)) and by the exact diagonalization technique (\( L = 10 \)) agree with each other excellently. However, if one wants to study phases such as phase separation, entanglement will show strong finite size dependence. For simplicity, we look at the local entanglement of the Hubbard model, the local entanglement has a strong finite size dependence:

\[
E_1 = \frac{2}{L} \log_2 \frac{L - \left(1 - \frac{2}{L}\right) \log_2 \left(\frac{1}{2} - \frac{1}{L}\right)}{L - 1}\,.
\]

(7)

Though it will tend to 1 in the thermodynamic limit, it develops a jump in the 3D figure of the local entanglement for a small system. Such a jump in a finite chain signals a crossover from one PS configurations to another.

We now address the problem for the case of \( l > 1 \). We show the block-block entanglement change with the value of \( V \) for fixed \( l = 4 \) and vary system size in Fig. 4. From the figure, we first notice a jump around \( U = 5 \), which is the critical point for the transition from PS to SDW. We also see that there are seemly jumps of the block-block entanglement around \( U = 0.6 \). However, it is not a critical point. It is just a result of finite-size effect, as we found in the local entanglement. Because in both \( U < 0.6 \) and \( 0.6 < U < 4 \) regions, the ground state is dominated by phase separation configurations. The difference is that in the region \( U < 0.6 \), the dominant configuration is PS(a). As \( U \) increases, one doubly occupied site tends to be singly occupied. So the configuration PS(d) becomes the dominating configuration. Therefore the jump here does not correspond to a true critical point and will be suppressed to zero in the thermodynamic limit.

Another finite-size effect is shown in Fig 6. There are two obviously close apexes for both \( L = 10 \) and \( L = 12 \). For \( L = 8 \), there are two close apexes for smaller value of \( U \). Actually, the first apex is not a critical point. It is also caused by the crossover between two PSs. Take \( L = 10 \) as an example, for \( V < -2.8 \), the ground state is dominated by configuration PS(d), while for \( -2.8 < V < -2.2 \), it is dominated by configuration PS(a). At first glance, this result seems unreasonable, because when \( V > -2.2 \), the ground state is dominated by SDW. Why the ground state tends to be doubly occupied before it becomes a SDW phase? A second order perturbation analysis will help us to understand the complication here. In the strong coupling limit, \(|t/U| \ll 1\) and/or \(|t/V| \ll 1\), we have the energy for the configuration PS(d) and PS(a), respectively, \(5U+16V+4t^2/V\) and \(4U+16V+(3/2)t^2/V\). For small \( |U|\), the system prefers to be phase separated due to attractive Coulomb potential \( V\), and the hopping process prefers the configuration PS(a). Thus the effect of hopping process is stronger than that of the on-site Coulomb interaction when the absolute values of \( V\) decreases, and the dominating configuration changes from PS(d) to PS(a). Similar to the argument for Fig. 5, this unexpected apex is also a finite size effect. Because when the block size is fixed, we vary system size to \( \infty \), the change from one pair of separate \( \uparrow \) and \( \downarrow \) to a doubly occupied will cause no weight change in the reduced-density matrix.

FIG. 5: The block-block entanglement change with different values of \( V \) for fixed block size \( l = 4 \) and various system size. Here \( V = -4 \).

FIG. 4: The block-block entanglement change with log \( l \) for fixed block size \( V = 4 \) and various system size.
VI. DISCUSSIONS

An important observation in our study is that in order to reveal phase transition by the block-block entanglement, the choice of block type is essential. Sometimes, the block-block entanglement could be a smoothly continuous function and shows no obvious structure at the transition point. As a result, finding the phase boundaries of some transitions is not an easy job, when the block-block entanglement at the critical point behaves neither singular nor extremum. Extremal values or discontinuities shown at some parameters is only suggestive. One must do more detailed analysis to identity where there exists true QPT and its nature. A typical example is the transition from SS to CDW, as shown in Fig. 2. When such situation arises, one may ask oneself these questions: (i) What is the behavior of the block-block entanglement in the critical region, i.e. its derivatives? (ii) How about choose different block, such as the “block” in the momentum space instead of in real space due to off-diagonal-long-range order?

Regarding the first question, Osterloh et.al.\(^\text{11}\) found out that in the one-dimensional transverse-field Ising model, the first derivative of the concurrence with respect to the coupling diverges at the critical point, even though the concurrence itself does not show maximum value at that point. This approach was also applied to other quantum spin models\(^\text{13}\) and they found similar results. In Fig. 7, we show the first derivative of the block-block entanglement with respect to the nearest-neighbor interaction \(V\): \(\partial E/\partial V\). At the point \(V = -0.2\), the derivative of the block-block entanglement achieves a extreme value, which is very close to the phase transition point for the infinite chain at \(V = 0\). Therefore, besides its extremum behavior in the QPT process, the derivative of the entanglement may show extremum at critical point.

Regarding the second question, we choose the “block” in the momentum space. The choice came from the nature of superconducting paring, for the order parameter is

\[
\Delta_x = \frac{1}{\sqrt{N}} \sum_i c_{i,\uparrow}^\dagger c_{i+x,\downarrow}^\dagger, \quad (8)
\]

thus, in the momentum space, one has, for singlet superconducting phase,

\[
\Delta_x + \Delta_{-x} = \frac{2}{N} \sum_k \cos kxc_{k,\uparrow}^\dagger c_{-k,\downarrow}^\dagger, \quad (9)
\]

while for triplet superconducting phase,

\[
\Delta_x - \Delta_{-x} = \frac{2i}{N} \sum_k \sin kxc_{k,\uparrow}^\dagger c_{-k,\downarrow}^\dagger. \quad (10)
\]

So if we choose the block in the momentum space, i.e. ±\(k\), the creating operator of cooper pairs, which is indeed
a superposition of the superconducting order parameter, is naturally included in the reduced density matrix.

We compute the block-block entanglement in the momentum space for the $L = 8$ system. Using the anti-periodic boundary conditions, the bases we choose are $K = \pm 1/8\pi, \pm 3/8\pi, \pm 5/8\pi, \pm 7/8\pi$. The results of the block-block entanglement between $K = \pm 1/8\pi$ and the rest of the momenta are shown in Fig. 5. From the figure we observe that the block-block entanglement in the momentum space shows a minimum value at the point $V = -0.2$. This minimum value may suggest a change of phase from SS to CDW. Surprisingly, this result is consistent with the result of the first derivative of the phase from SS to CDW. Surprisingly, this result is consistent with the result of the first derivative of the block-block entanglement when the block size increases. By studying the dependence of the entanglement on system length, we also clarified its unusual behavior in the crossover from one PS to another and attribute it to the finite size effect. On the other hand, the derivatives of the block-block entanglement and the block-block entanglement in momentum space also gave us some interesting results.

However, it seems that the block-block entanglement still can not witness all phases of the system, such as the BOW and the TS. There are two possible reasons. One is that the system size we considered is not large enough, and the other is the limitation of the block-block entanglement itself. For the former, it is useful to apply other numerical method, such as density-matrix-renormalization-group, to this problem in the future studies. While for the later, it is necessary to search other kinds of proper way to quantify the entanglement in order to have a comprehensive understanding on the critical behavior in the ground state of a many-body systems, just as we did in this work. Possible choices include sub-lattice entanglement suggested by Chen et al. and the fermion concurrence proposed by Deng and Gu. Obviously, each choice has its own merits and limitations.

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VII. SUMMARY AND ACKNOWLEDGEMENT

In summary, we have studied the block-block entanglement in the ground state of half-filled one dimensional extended Hubbard model. We found that it can identify the main phases of EHM on the $U - V$ plane, SDW, CDW, PS and even SS. Obviously, since the block-block entanglement with block size larger than one comprises nonlocal correlation, it provides more information than the local entanglement. Then a richer structure has been obtained from its contour map on the $U - V$ plane. Moreover, the scaling analysis based on the block size implied that the $\log_2(l)$ behavior of the block-block entanglement may also exist in the noncritical region, such as PS. This result is quite different from the previous studies of spin systems. We interpret it due to the high density-of-state closing to the ground state in this region. The number of different configurations taken part in the ground state is proportional to the system length. While in other non-critical regions, such as CDW, the ground state is nearly doubly degenerate and comprises two configurations, this fact restrict the increase of the block-block entanglement when the block size increases. By studying the dependence of the entanglement on system length, we also clarified its unusual behavior in the crossover from one PS to another and attribute it to the finite size effect. On the other hand, the derivatives of the block-block entanglement and the block-block entanglement in momentum space also gave us some interesting results.

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