

Entanglement and Quantum Phase Transition in the Extended Hubbard Model

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We study quantum entanglement in a one-dimensional correlated fermionic system. Our results show, for the first time, that entanglement can be used to identify quantum phase transitions in fermionic systems.

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Quantum entanglement, as one of the most intriguing features of quantum theory, has been a subject of many studies in recent years, mostly because its nonlocal connotation [1] is regarded as a valuable resource in quantum communication and information processing [2,3]. One important issue is whether there exists any relation between entanglement and quantum phase transitions [4]. Several groups investigated this problem by studying quantum spin systems [5–14]. For example, the work of Osterloh *et al.* [8] and Osborne and Nielsen [9] on the spin model showed that the entanglement of two neighboring sites displays a sharp peak either near or at the critical point where quantum phase transition undergoes.

On the other hand, real systems consist of moving electrons with spin so to explore the relation between quantum entanglement and quantum phase transition in the fermionic system is necessary. Previously, there have been a couple of works which studied entanglement in fermionic lattices [15,16], but they did not discuss its relation to quantum phase transition. In this Letter, in the framework of the one-dimensional extended Hubbard model (EHM), we study the change of symmetry in the ground state on passing the phase boundary from the point of view of quantum entanglement, and demonstrate that entanglement is a unique quantity in describing quantum phase transitions in this system. The EHM is defined by the Hamiltonian

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

In Eq. (1), $\sigma = \uparrow, \downarrow$; $j = 1, \dots, L$; $\delta = \pm 1$, $c_{j\sigma}^\dagger$, and $c_{j\sigma}$ are creation and annihilation operators. U and V define the on-site and nearest-neighbor Coulomb interactions. The EHM is a prototype model in condensed matter theory, for it exhibits a rich phase diagram [17–19] where various quantum phase transitions occur between symmetry broken states. These states include the charge-density wave (CDW), the spin-density wave (SDW), and phase separation (PS). By calculating the entanglement as functions of electron-electron interaction U and V as well as fermion concentration N/L , we show that quantum phase transitions can be identified at places where local entanglement

is extremum or its derivative is singular. Our results, part of which are based on the exact solution of the one-dimensional Hubbard model (HM), are useful for people to explore quantum entanglement and quantum phase transition for interacting many-fermion systems.

For the spin-1/2 fermion system, there are four possible local states at each site, $|\nu\rangle_j = |0\rangle_j, |\uparrow\rangle_j, |\downarrow\rangle_j, |\uparrow\downarrow\rangle_j$. The dimension of the Hilbert space for a L -site system is then 4^L , and $|\nu_1, \nu_2 \cdots \nu_L\rangle = \prod_{j=1}^L |\nu_j\rangle_j$ are its natural basis vectors. We consider local density matrix of the ground state, $|\Psi\rangle$, which is a reduced density matrix $\rho_j = \text{Tr}_j |\Psi\rangle\langle\Psi|$, where Tr_j stands for tracing over all sites except the j th site. Accordingly, the von Neumann entropy E_v calculated from the reduced density matrix ρ_j measures the entanglement of states on the j th site with that on the remaining $L - 1$ sites. It is called the local entanglement [16] for it exhibits the correlations between a local state and the other part of the system. Since Hamiltonian (1) is invariant under translation, the local density matrix ρ_j is site independent,

$$\rho_j = z |0\rangle\langle 0| + u^+ |\uparrow\rangle\langle\uparrow| + u^- |\downarrow\rangle\langle\downarrow| + w |\uparrow\downarrow\rangle\langle\uparrow\downarrow|, \quad (2)$$

with

$$\begin{aligned} w &= \langle n_{j\uparrow} n_{j\downarrow} \rangle = \text{Tr}(n_{j\uparrow} n_{j\downarrow} \rho_j), & u^+ &= \langle n_{\uparrow} \rangle - w, \\ u^- &= \langle n_{\downarrow} \rangle - w, & & \\ z &= 1 - u^+ - u^- - w = 1 - \langle n_{\uparrow} \rangle - \langle n_{\downarrow} \rangle + w. \end{aligned} \quad (3)$$

Consequently, the corresponding von Neumann entropy (or the local entanglement as we will call it hereafter) is

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

Clearly, the local entanglement combines four quantities which are all important to determining the physical properties of the system. We discover, to be shown below, that this simple expression plays a more general and important role for the understanding of the system than any other single parameter.

We start with general behavior of the local entanglement for the half filling ($N = L$) case. In Fig. 1, we plot E_v on the U - V plane with its contour map. It is remarkable to see that the skeleton of the EHM's phase diagram [19]

can be directly obtained from the contour map. This is by no means trivial. In the conventional approach to obtain the phase diagram of the EHM, one has to study behaviors of different order parameters (say, CDW) in different regions, either by comparing ground state energy or critical exponents of correlation functions associated with broken symmetry. Whereas here, using a single quantity, E_v , the global picture of the system could be observed. One may be tempted to think that double occupancy could play the same role as E_v , but our detailed calculations show that is not the case. In fact, for the EHM, ordering parameters corresponding to CDW, SDW, and PS are all functions of single and double occupancies. None of them exhibit a unique property as E_v does. Obviously, this is not a coincidence. Rather, it reflects the underlying correlation between entanglement and quantum phase transition behind the superposition principle of quantum mechanics.

In order to clarify physical pictures further, we present our studies in details at some special transects. First, we study the HM, i.e., $V = 0$ in the EHM. Since the HM can be solved analytically for both finite and infinite lattices by the Bethe ansatz method [20], we can study the analyticity of the phase transition as well as checking the validity of the numerical exact diagonalization technique used for the EHM on finite lattices.

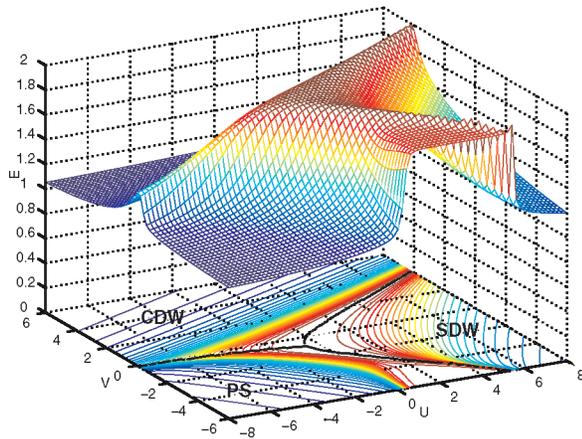


FIG. 1 (color online). The changes of symmetry in the ground state wave function is analyzed by considering the quantum correlation between local site and other parts of the system. The curved surface denotes E_v 's dependence on U and V , and colored curves on the $E_v = 0$ plane constitutes a contour map. Three solid lines on the plane denote the local extremum of a transect of "mountain" surface. Clearly, three main symmetry broken phases (CDW, SDW, and PS) can be sketched out from the contour map. Superconducting phase could not be identified, due to the fact that the broken symmetry is associated with off-diagonal long-range order. Finite size scaling analysis should be carried out.

For the HM at half filling, $\langle n_\uparrow \rangle = \langle n_\downarrow \rangle = 1/2$, $u^+ = u^- = 1/2 - w$ and the local entanglement is

$$E_v = -2w \log_2 w - 2(1/2 - w) \log_2 (1/2 - w). \quad (4)$$

By making use of particle-hole symmetry of the model, one easily finds that $w(-U) = 1/2 - w(U)$, so the local entanglement is an even function of U , i.e., $E_v(-U) = E_v(U)$. In the large U limit, $|U| \rightarrow \infty$, either all sites are singly occupied ($U > 0$) so $w = 0$, or half of the total sites are doubly occupied while the other half are empty so $w = 1/2$, one gets $E_v(|U| = \infty) = 1$. For finite $|U|$, hopping process enhances E_v , which reaches its maximum value two at $U = 0$ from both sides. We plot the local entanglement E_v as functions of U in Fig. 2, obtained from the Bethe ansatz method (for $L = \infty$ and $L = 70$) and exact diagonalization technique ($L = 10$). The excellent agreement justifies the validity of using small clusters for other calculations. The ground state of the HM at half filling is metallic for $U \leq 0$, and insulating for $U > 0$, so $U = 0$ is a critical point which separates metallic and insulating phases. Our result shows that the local entanglement reaches its extremum at the critical point where the system possesses maximum SO(4) symmetry and undergoes quantum phase transition.

Moreover, based on the Bethe ansatz solution, we can also study the asymptotic behavior of the entanglement analytically. Near the critical point $U = 0$, we have [21,22] $w = 1/4 - 7\zeta(3)U/8\pi^3 - 93\zeta(5)U^3/2^9\pi^5$, where ζ stands for the Riemann zeta function, which leads to $E_v = 2 - (1/\ln 2)[7\zeta(3)U/2\pi^3]^2 + \dots$. Clearly, E_v is analytic in the neighborhood of the critical point $U = 0$. This behavior is different from other models [8–10].

Second, we study the EHM at some fixed values of on-site Coulomb interaction U by varying nearest-neighbor interaction V . Results were obtained by the exact diagonalization of the EHM on finite chains up to

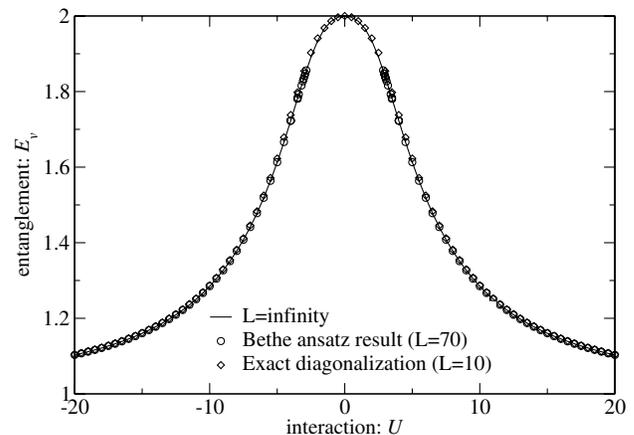


FIG. 2. Local entanglement E_v of the HM at half filling versus the on-site coupling U for a different size lattice.

ten sites. The ground state is always in the subspace of total $S_z = 0$, as can be shown rigorously. We did not perform finite size scaling since qualitative behavior as shown in Fig. 1 should be the same for an infinite system. For negative U , each site tends to be doubly occupied. When $V \gg |t|$, the CDW state is favored, while for $V \ll -|t|$, phase separation occurs. Both the CDW state and PS state lead to $E_v = 1$. Only in the region where $|V| \sim 0$ does electron itinerant motion dominate, tending to uniform density distribution so a local maximum of E_v occurs around $V = 0$, as shown in Fig. 3.

For positive U , the model is more relevant to the real materials. When $V > 0$, the competition between CDW and SDW leads E_v to an extremum where the phase transition undergoes, due to the fact that the local entanglement itself combines CDW order parameter and SDW order parameter at the same time. As shown in Figs. 2 and 3, the transition happens along a line $U \approx 2V$, consistent with other studies of the EHM [17–19]. When $V < 0$, the formation of electron clustering, i.e., the phase separated configuration, challenges the SDW state. In the large U and $|V|$ limit, it can be easily shown that phase transition happens at $U = -2V$ [17–19]. From Fig. 3, we also observe that the local entanglement exhibits singular behavior at the transition points. Moreover, for $U > 0$, we find that the local entanglement at two boundary lines is very close to 2, indicating that each of the four local modes has nearly equal population at the critical point.

Third, we study the variation of local entanglement as a function of chemical potential by adding the term $-\mu \sum_i n_i$ to the HM. Consequently, the total particle number of the ground state, hence the filling factor, could be tuned. We show the relations between local entanglement and the filling factor n for various on-site coupling U in Fig. 4. We only plot the part of $n = N/L < 1$ because the other part, $n > 1$, could simply be obtained by the mirror image relation

$$E_v(n) = E_v(2 - n). \quad (5)$$

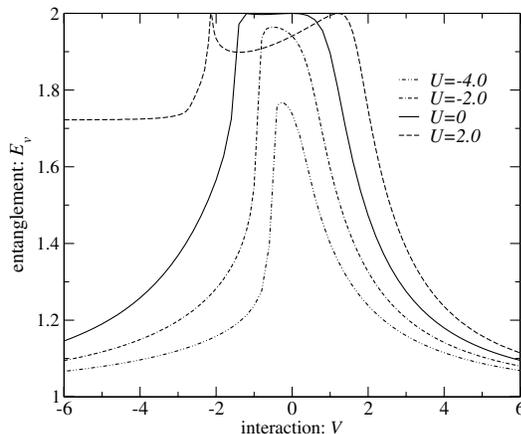


FIG. 3. Local entanglement E_v versus V for various U .

Figure 4 manifests that the ground state of the half-filled band is not maximally entangled as long as $U > 0$, whereas, the maximum of E_v lies in between $n = 2/3$ and $n = 1$. Let us take $U = \infty$, for example. When $U = \infty$, there is no double occupied site, which implies that $w = 0$ and $u^+ = u^- = N/2L$. Hence we have an analytical expression of the local entanglement $E_v = -(1-n)\log_2(1-n) - n\log_2(n/2)$ which has a maximum at $n = 2/3$. It is worthwhile to point out that at $1/3$ filling (i.e., $n = 2/3$) when $U = \infty$, the ground state is a singlet of $SU(2|1)$ Lie supersymmetry algebra which possesses the maximal symmetry allowed, while at $1/2$ filling, it is a $SU(2)$ singlet. For $U = 0$ the ground state is invariant under $SO(4)$ rotation at $1/2$ filling. This demonstrates that the local entanglement reaches a maximum value at the state with maximal symmetry. Accordingly, the maximum position for $0 < U < \infty$ is expected to lie between $n = 2/3$ and $n = 1$, which is numerically confirmed in Fig. 4.

Except at half filling where it becomes a Mott insulator, the system is an ideal conductor [20]. Consequently, the local entanglement E_v is not smoothly continuous at $n = 1$ for $U \neq 0$. It is then instructive to observe the derivative of E_v with respect to U ,

$$\left. \frac{dE_v}{dn} \right|_{n=1^-} = -(\log_2 u^+ - \log_2 z) \left[\frac{1}{2} + 2 \frac{d\Delta E}{dU} \right] \Big|_{n=1^-}, \quad (6)$$

where ΔE is the gap of charge excitation. Equation (5) gives rise to $dE_v/dn|_{n=1^+} = -dE_v/dn|_{n=1^-}$. Obviously, there exists a jump in the derivative of E_v across the point of insulating phase (see Fig. 4, right) unless $U = 0$.

From the above investigations, we find that the local entanglement manifests distinct features at the point where quantum phase transition undergoes. Since the local entanglement represents the symmetry of the sys-

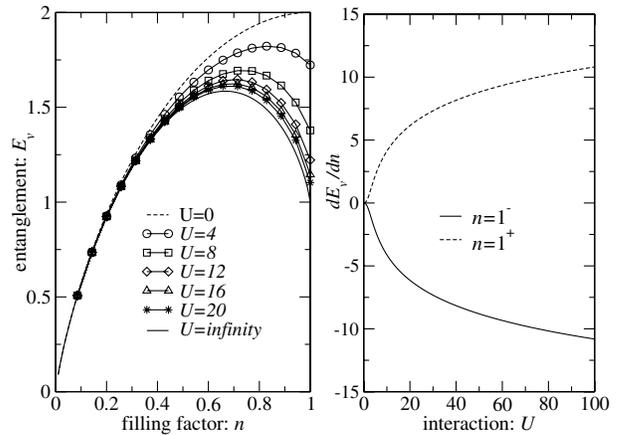


FIG. 4. Local entanglement E_v as a function of fermion concentration for the HM with different on-site U (left), and dE_v/dn at $n = 1^\pm$ as a function of U .

tem to a certain extent, naturally one expects that the maximum point of the local entanglement corresponds to the quantum phase transition point. In light of this conclusion, we speculate that the maximum point in Fig. 4 not only denotes the maximum symmetry, but could also be a critical point separating two different phases. On the other hand, the discontinuity properties of the local entanglement obviously indicate a phase transition. For example, the derivative of E_v in the region of $U > 0$ and $V < 0$ at half filling of the EHM, and of the HM caused by chemical potential shift, both are not smoothly continuous at the quantum phase transition points. This is similar to other studies, e.g., the one-dimensional XY model in a transverse magnetic field [8–10], where the derivative of the pairwise concurrence C with respect to the dimensionless coupling constant develops a cusp at the quantum phase transition point. However, such discontinuity is not universal, as shown by our results.

It was indicated [23] recently that two mechanisms may bring about quantum phase transitions in one-dimensional correlated fermionic systems. One is caused by the level crossing of the ground state and the other arises from the level crossing of the low-lying excited states when no level crossing occurs at the ground state. In the latter case, if the ground state wave function is smoothly continuous with respect to the variation of parameters that drive the quantum phase transition, the entanglement should also be smoothly continuous at the quantum phase transition point. On the other hand, the singularity of wave function may lead to the singularity of the local entanglement. For the former case, the level crossing of the ground state will clearly cause the entanglement not to be smoothly continuous at the transition point. Therefore the continuity property of the local entanglement might be an ancillary tool to judge the mechanism of quantum phase transition proposed in [23].

In summary, we have extensively studied the local entanglement in the EHM, characterized by the on-site Coulomb interaction U , the nearest-neighbor Coulomb interaction V , and band filling N/L . At half filling, we calculated local entanglement as functions of U and V . Our results indicated that the local entanglement either reaches the maximum value or shows singularity (or both) at the critical point where quantum phase transition undergoes. For the traditional Hubbard model ($V = 0$), the scaling behavior close to the critical point $U = 0$ manifests that the local entanglement is an analytical function of U . Furthermore, we analyzed the local entanglement by varying V while keep U fixed, and found that the local entanglement is not smoothly continuous in some critical regions. Finally, we studied the dependence of the local entanglement on the filling factor for the HM. The induced variation of the local entanglement showed that the local entanglement reaches maximum at a filling

factor n between $2/3$ and 1 . For any finite U , the local entanglement develops a cusp at $n = 1$. In the strong coupling limit, the $1/3$ filled band has the maximum local entanglement, suggesting that the ground state with maximal symmetry possesses the maximum magnitude of the local entanglement.

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