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Local entanglement entropy of fermions as a marker of quantum phase transition in the one-dimensional Hubbard model

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ABSTRACT

We study quantum phase transition of interacting fermions by measuring the local entanglement entropy in the one-dimensional Hubbard model. The reduced density matrices for blocks of a few sites are constructed from the ground state wave function in infinite systems by adopting the matrix product state representation where time-evolving block decimations are performed to obtain the lowest energy states. The local entanglement entropy, constructed from the reduced density matrices, as a function of the chemical potential shows clear signatures of the Mott transition. The value of the central charge, numerically determined from the universal properties of the local entanglement entropy, confirms that the transition is caused by the suppression of the charge degrees of freedom.

1. Introduction

Entanglement is a peculiar trait of quantum states [1], with no classical counterpart, which includes the inseparability between parts of the states. The unique features of entanglement have motivated intensive research on many-particle quantum systems as essential elements in establishing quantum phases. How entanglement [2,3] is connected with quantum phase transitions is also an important question for a deeper understanding of interacting quantum systems [4,5]. Especially, entanglement appears to be an adequate tool to treat transitions carrying no symmetry breaking. Recently, the entanglement entropy, a measure of entanglement, has drawn much attention as a marker of quantum phase transition in interacting spin [6–8], fermion [9–11], and boson [12] systems.

The one-dimensional Hubbard model has become a prototype playground [13] for theoretical studies of quantum correlations partly because the exact Bethe ansatz solution is known [14]. The entanglement entropy of a single site has been calculated analytically [9] as an indicator of the quantum phase transition. Numerical approaches are still needed, however, to extend the calculation of the entanglement entropy for bigger blocks.

In this paper, we focus on the quantum phase transition of the one-dimensional Hubbard model of interacting fermions by observing the local entanglement entropy for blocks of several sites. By using the matrix product state (MPS) representation of the ground state wave function [15,16], we construct the ground state wave functions and determine the matrices through the infinite time-evolving block decimation (iTEBD) method [17–19]. The reduced density matrices of the blocks are then obtained by tracing out the rest of the system. We find that the local entanglement entropy shows signature of the Mott transition and some universal properties associated with the transition. These results suggest that the local entanglement entropy is a quite convenient tool to investigate the role of entanglement in quantum phase transitions.

2. Model and method

The Hubbard model is a simplest quantum system of interacting itinerant fermions on a lattice. The Hamiltonian of the one-dimensional Hubbard model is given by

$$H = -t\sum_{\langle ij\rangle}\left(c_{i\uparrow}^{\dagger}c_{j\uparrow}+c_{j\uparrow}^{\dagger}c_{i\uparrow}+c_{i\downarrow}^{\dagger}c_{j\downarrow}+c_{j\downarrow}^{\dagger}c_{i\downarrow}\right) + U\sum_{i}\left(n_{i\uparrow}-\frac{1}{2}\right)\left(n_{i\downarrow}-\frac{1}{2}\right)-\mu\sum_{i}\left(n_{i\uparrow}+n_{i\downarrow}\right), \quad (1)$$

where $\langle ij\rangle$ represents nearest-neighbor pairs, $n_{i\uparrow}$ and $n_{i\downarrow}$ are the spin-up and the spin-down number operators, respectively, t is the hopping strength, U is the strength of on-site repulsion, and μ is the chemical potential. We set the hopping strength $t = 1$ and tune the chemical potential to drive the transition between the Mott insulating and metallic phases for various U.

When a Hamiltonian is written as a sum of local operators, a

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powerful method called iTEBD is introduced [17–19] for finding correlation functions in the MPS. Since our Hamiltonian is local and has the translational symmetry, we can apply the iTEBD method to find the ground state with a few matrices. In order to perform iTEBD, we divide the Hamiltonian into two parts, which are denoted by e(even) and o(odd), such as $H = \sum_{\langle ij\rangle} h_{ij} = H_e + H_o$. Note that H_e and H_o are decomposed in terms of elementary operators h_{ij}:

$$\begin{aligned} h_{ij} = & -t(c_{i\uparrow}^{\dagger}c_{j\uparrow} + c_{j\uparrow}^{\dagger}c_{i\uparrow} + c_{i\downarrow}^{\dagger}c_{j\downarrow} + c_{j\downarrow}^{\dagger}c_{i\downarrow}) \\ & + \frac{U}{2}(n_{i\uparrow} - \frac{1}{2})(n_{i\downarrow} - \frac{1}{2}) - \frac{\mu}{2}(n_{i\uparrow} + n_{i\downarrow}) \\ & + \frac{U}{2}(n_{j\uparrow} - \frac{1}{2})(n_{j\downarrow} - \frac{1}{2}) - \frac{\mu}{2}(n_{j\uparrow} + n_{j\downarrow}). \end{aligned} \tag{2}$$

Our strategy is to use iTEBD with these elementary operators in a small subset of the Hilbert space. This small subset is composed of the MPS characterized by two matrices, one for odd sites and the other for even sites.

The two matrices in our MPS, P_{ab}^{σ} and Q_{cd}^{ν}, has three indices, among which σ and ν are the physical indices. For the internal bond degrees of freedom, the indices a (left) and b (right) for P run from 1 to χ, where χ is the bond dimension. The Schmidt coefficients between P_{ab}^{σ} and Q_{bc}^{ν} are denoted by λ_b^{PQ}. A state in the space of the matrix product states is written as

$$|\Psi\rangle = \sum_{\cdots\sigma\nu\kappa\eta\cdots} \mathrm{Tr}(\cdots P_{ab}^{\sigma}\lambda_b^{PQ}Q_{bc}^{\nu}\lambda_c^{QP}P_{cd}^{\kappa}\lambda_d^{PQ}Q_{de}^{\eta}\cdots)|\cdots\sigma\nu\kappa\eta\cdots\rangle, \tag{3}$$

where Tr means that the internal bond indices a, b, c, d, $\cdots$ are summed up.

To define the entanglement entropy, we divide the system into two parts A and B in a quantum system. We introduce a density matrix $\rho = |\Psi\rangle\langle\Psi|$ with a pure quantum state $|\Psi\rangle$, and obtain the reduced density matrix $\rho_A = \mathrm{Tr}_B\rho$ by tracing out the subsystem B. The entanglement entropy is the von Neumann entropy, which is given by $S_A = -\mathrm{Tr}(\rho_A \log \rho_A)$.

3. Numerical results: Local entanglement entropy

For the one-dimensional Hubbard model, we calculate local entanglement entropy S_L for blocks of size L by representing the ground states in the form of the MPS with bond dimension $\chi = 24$. By diagonalizing the reduced density matrices ρ_L for $L = 1, 2, 3$, and 4, we determine S_L from the eigenvalues λ_i:

$$S_L = -\sum_i \lambda_i \log_2\lambda_i. \tag{4}$$

The numerical results of the local entanglement entropy S_1, S_2, S_3, and S_4 as a function of μ for various U, are presented in Fig. 1.

A symmetrical shape around $\mu = 0$ implies the particle-hole symmetry. The areas of a flat appearance in the range between $-\mu_c < \mu < \mu_c$ with a finite μ_c ($\mu_c = 0$ for $U = 0$) imply the existence of the Mott insulating phase for finite U. This feature is well consistent with the analytical calculation based on the Bethe ansatz solutions for S_1 [9]. Here, the numerical method using the MPS representation enables us to find S_L for blocks of size up to 4 sites.

The numerical value $\mu_c = 2.377(2)$ for $U = 8$, for example, is also fairly consistent with the analytical result $\mu_c = 2.3398$ [13]. In the numerical calculation, we use randomly-prepared initial states or sometimes load the ground states nearby in the parameter space as an initial state in the iTEBD process. We find that the energy levels for Mott insulating and metallic phases are crossing at a point and define it as the transition point. It seems that a larger value of χ will produce a more accurate value of μ_c.

It is instructive to present explicitly the eigenvalues of the reduced density matrices as shown in Fig. 2. Here we compare the eigenvalue spectra of the single-site reduced density ρ_1 and the double-site reduced density ρ_2. The characteristic feature commonly found is a singular

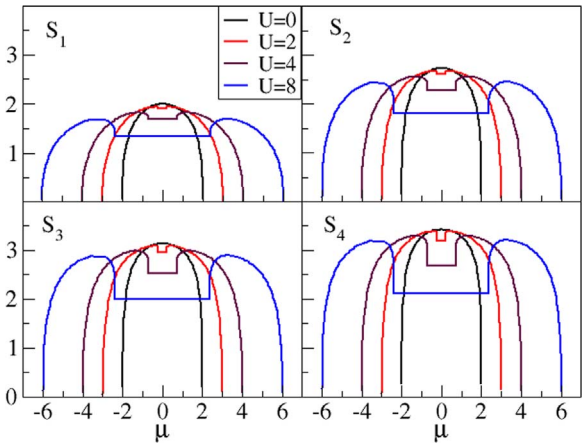

Fig. 1. Local entanglement entropy for blocks of size 1, 2, 3, and 4 sites in the one-dimensional Hubbard model as a function of the chemical potential for different interaction strengths. Features of the Mott insulating phase with constant entanglement entropy are clearly visible.

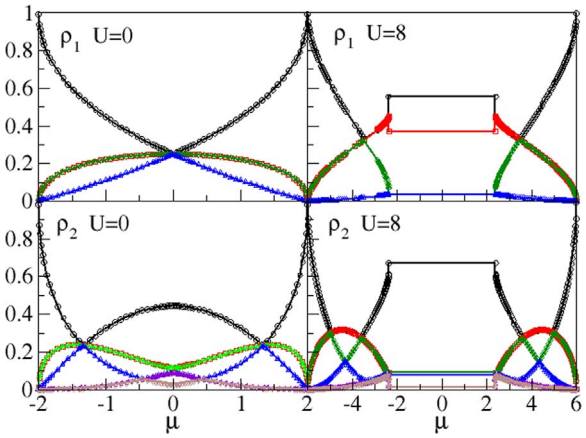

Fig. 2. A few largest eigenvalues of the reduced density matrices ρ_1 and ρ_2 for single- and double-site blocks, respectively, in non-interacting and interacting regions.

discontinuity at the transition and flat appearance in the Mott insulating phases due to the lift of the spin degeneracy at an odd (or even) site. Furthermore, the spectra of the eigenvalues for ρ_1 and ρ_2 show different structures although S_1 and S_2 in Fig. 1 present a similar shape. It is known [9] that the eigenvalues of ρ_1 are expressed in terms of one-site physical quantities that rather monotonically change as μ varies in the metallic region. Thus the complicated structure in the spectra of ρ_2 reflects the change of the entanglement between two sites as μ varies.

From the conformal field theory, S_L is expected to show the universal scaling behavior [20–22]

$$S_L = \frac{c}{3}\log_2 L + \tilde{s}, \tag{5}$$

when L is sufficiently large to have an asymptotic behavior, where c is the central charge, a universal property of a gapless state, and $\tilde{s}$ is a non-universal constant. In order to find this behavior, the block entanglement entropy S_L^0 at $\mu = 0$ is plotted in Fig. 3 as a function of $\log_2 L$ for $L = 1, 2, 3$, and 4 for various U. Surprisingly, the universal scaling behavior seems to be achieved in the blocks composed of a few sites in non-interacting ($U = 0$) regions and in strongly interacting ($U \to \infty$) regions.

Whether this behavior shows truly the universal properties, we calculate the central charge

$$c_L = \frac{3(S_L - S_{L-1})}{\log_2 L - \log_2(L-1)}. \tag{6}$$

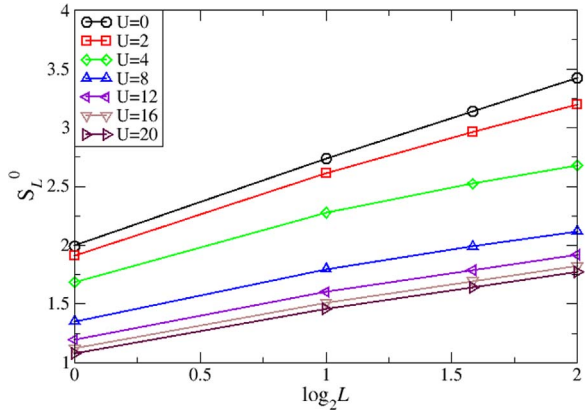

Fig. 3. The block entanglement entropy at $\mu = 0$ for different interaction strengths as a function of the block size L. They are expected to follow the universal scaling behavior $S_L^0 \sim (c/3)\log_2 L$ for sufficiently large sizes.

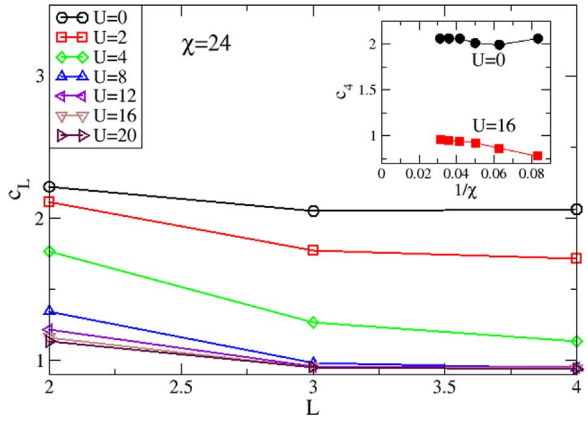

Fig. 4. The central charge determined numerically by fitting the block entanglement entropy to the universal scaling ansatz as a function of the block size in non-interacting ($U = 0$) and interacting ($U > 0$) systems. Inset: In the non-interacting limit, we find $c_4 = 2.03(5)$, roughly independent of the bond dimension χ, which is consistent with metallic behavior characterized by the presence of both charge and spin fluctuations. In the opposite limit with strong interaction ($U = 16$), however, c_4 approaches 1 as χ increases, confirming that the repulsive interaction suppresses the charge fluctuations in the Mott insulating phase.

Note that the low energy properties of the model are described by a spin and charge separated Luttinger liquid [13], in which each degree of freedom is associated with central charge $c = 1$. In metallic phase, therefore, we theoretically expect that the universal behavior is governed by $c = 2$, while, in the Mott insulating phase where the charge fluctuations are suppressed, it is governed by $c = 1$. As shown in Fig. 4, c_L appears to follow the expected behavior by showing $c_4 = 2.03(5)$ in non-interacting regions and $c_4 \to 1$ in strongly interacting regions as χ increases.

4. Conclusion

In summary, we investigate the quantum phase transition in the one-dimensional Hubbard model by observing the local entanglement entropy for blocks of size 1, 2, 3, and 4 sites while tuning the chemical potential. We construct the ground state wave functions in the form of the MPS and determine the matrices by approaching the lowest energy state through the iTEBD method. The ground state wave functions then enable us to calculate the reduced density matrices of the blocks whose amounts of entanglement with the rest of the system are characterized by the local entanglement entropy. We find that the local entanglement entropy shows clear signature of the Mott transition between metallic and insulating phases. By fitting the block entanglement entropy to a universal scaling ansatz, we find that the value of the central charge, determined numerically, is well consistent with theoretical expectation: $c = 2.03(5)$ for the metallic phase in the non-interacting limit, while c approaches 1 for the Mott insulating phase with finite repulsive interaction as the bond dimension of the MPS wave function increases. These results suggest that the local entanglement entropy is a quite convenient tool applicable to investigate not only distinct features of ground state wave functions in different phases but also universal properties associated with quantum phase transitions in various interacting quantum systems.

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References

[1] R. Horodecki, P. Horodecki, M. Horodecki, K. Horodecki, Rev. Mod. Phys. 81 (2009) 865.
[2] A. Osterloh, L. Amico, G. Falci, R. Fazio, Nature 416 (2002) 608.
[3] T.J. Osborne, M.A. Nielsen, Phys. Rev. A 66 (2002) 032110.
[4] L. Amico, R. Fazio, A. Osterloh, V. Vedral, Rev. Mod. Phys. 80 (2008) 517.
[5] J. Eisert, M. Cramer, M.B. Plenio, Rev. Mod. Phys. 82 (2010) 277.
[6] L. Tagliacozzo, T.R. de Oliveira, S. Iblisdir, J.I. Latorre, Phys. Rev. B 78 (2008) 024410.
[7] B. Pirvu, G. Vidal, F. Verstraete, L. Tagliacozzo, Phys. Rev. B 86 (2012) 075117.
[8] F. Pollmann, A.M. Turner, E. Berg, M. Oshikawa, Phys. Rev. B 81 (2010) 064439.
[9] D. Larsson, H. Johannesson, Phys. Rev. Lett. 95 (2005) 196406.
[10] Shi-Jian Gu, Shu-Sa Deng, You-Quan Li, Hai-Qing Lin, Phys. Rev. Lett. 93 (2004) 086402.
[11] F. Iemini, T.O. Maciel, R.O. Vianna, Phys. Rev. B 92 (2015) 075423.
[12] M. Pino, J. Prior, A.M. Somoza, D. Jaksch, S.R. Clark, Phys. Rev. A 86 (2012) 023631.
[13] F.H.L. Essler, H. Frahm, F. Göhmann, A. Klümper, V.E. Korepin, The One-dimensional Hubbard Model, Cambridge University Press, Cambridge, 2005.
[14] C. Yang, A.N. Kocharian, Y.L. Chiang, J. Phys.: Condens. Matter 12 (2000) 7433.
[15] U. Schollwöck, Ann. Phys. 326 (2011) 96.
[16] F. Verstraete, V. Murg, J. Cirac, Adv. Phys. 57 (2008) 143.
[17] G. Vidal, Phys. Rev. Lett. 93 (2004) 040502.
[18] G. Vidal, Phys. Rev. Lett. 98 (2007) 070201.
[19] R. Orus, G. Vidal, Phys. Rev. B 78 (2008) 155117.
[20] G. Vidal, J.I. Latorre, E. Rico, A. Kitaev, Phys. Rev. Lett. 90 (2003) 227902.
[21] J.I. Latorre, E. Rico, G. Vidal, Quant. Inf. Comput. 4 (2004) 048.
[22] P. Calabrese, J. Cardy, J. Stat. Mech. (2004) P06002.