Phase transitions in the one-dimensional ionic Hubbard model

Myung-Hoon Chung

Received: 7 January 2021 / Revised: 12 January 2021 / Accepted: 13 January 2021 / Published online: 10 February 2021
© The Korean Physical Society 2021

Abstract
We study quantum phase transitions by measuring the bond energy, the number density, and the half-chain entanglement entropy in the one-dimensional ionic Hubbard model. By using the matrix product operator to perform the infinite density matrix renormalization group, we obtain the ground states in the canonical form of matrix product states. Depending on the chemical potential and the staggered potential, the number density and the half-chain entanglement entropy shows clear signatures of a Mott transition. Our results confirm the success of using the matrix product operator method to investigate itinerant fermion systems.

Keywords Infinite density matrix renormalization group · Matrix product operator · Hubbard model · Entanglement entropy

1 Introduction

The intrinsic characteristics of quantum entanglements [1, 2] are essential elements in the study of quantum phase transitions [3]. In recent years, there has been a great deal of interest in entanglement entropy [4], which is a quantum phase transition marker [5] in the interacting spin [6–8], boson [9], and fermion [10–13] systems.

When the von Neumann entropy of two neighboring central sites in a long chain for fermionic models is studied [14], the two-site entropy is a better indicator of a quantum phase transition than the calculated gaps, order parameters, or the single-site entropy are. Thus, because the half-chain is even larger than two-site, the half-chain entanglement entropy is a good marker for detecting quantum phase transitions.

Some cold atoms can obey the same statistical rules as electrons if atoms with an odd number of neutrons are fermions [15]. Thus, some cold atoms [16] in an optical lattice can mimic the behavior of electrons in a real solid material. Because cold fermion systems are produced in quasi one-dimensional optical lattices [17], the one-dimensional fermion Hubbard model can be realized physically. The one-dimensional fermion Hubbard model [18] was analytically studied and became a prototype playground, where theoretical results could be compared to physical reality.

In this paper, motivated by cold atoms, we study the one-dimensional Hubbard model with an energy offset between even and odd lattice sites. The main process in this study aims to discover the role of different potential energies that are produced by using a second laser disturbance in one-dimensional cold atom systems. In fact, we impose the potential energy as

\[ V(x) = V_1 \sin(kx) + V_2 \sin\left(\frac{k}{2}x\right), \]  

(1)

using a second laser with a twice as long wavelength. For example, we present the staggered potential with typical values in Fig. 1.

The ionic Hubbard model [19] stems from this staggered potential. Many investigations into the ionic Hubbard model have been done at half filling by using dynamical mean field theory [20, 21], determinant quantum Monte Carlo simulations [22], the exact diagonalization, and finite density matrix renormalization group (DMRG) [23].

The original one-dimensional Hubbard model is recovered if we use no staggered potential here. In the Hubbard model, the quantum phase transition between the Mott insulating and the metallic phase is well known to take place when the chemical potential exceeds some value. The essential feature of the Hubbard model can be described by using a Luttinger liquid. Remarkably, spin-charge separation [24] can be observed as

\[ \text{Myung-Hoon Chung} \\
mhchung@hongik.ac.kr \\
1 College of Science and Technology, Hongik University, Sejong 339-701, Korea \]
Phase transitions in the one-dimensional ionic Hubbard model

where \( \langle ij \rangle \) represents the nearest-neighbor hopping in a one-dimensional lattice, and \( n_i^\uparrow \) and \( n_i^\downarrow \) are the spin-up and the spin-down number operators, respectively. We let the hopping strength \( t \) be 1 and vary the strengths of the parameters: the on-site Coulomb repulsion \( U \), the chemical potential \( \mu \), and the staggered potential \( \Delta \). The role of the chemical potential is to control the number of fermions in the system. For the case of \( \Delta = 0 \), the exact solution of the original Hubbard model is obtained [27].

In order to handle \( \mu \) and \( \Delta \), we introduce two linear combinations \( \mu_e \) and \( \mu_o \) for even and odd sites: denoting

\[
\mu_e \equiv \mu - \frac{\Delta}{2}, \quad \mu_o \equiv \mu + \frac{\Delta}{2}. \tag{3}
\]

Because the Hamiltonian has two-site translational symmetry as shown in Fig. 1, we apply the iDMRG with a unit cell of two sites to determine the ground state. Our strategy is to use the MPO acting on the MPS.

In relation to the basis, we set the physical index \( \sigma_i \) in the MPS. The state on the \( i \)-th site is represented by \( \sigma_i = (\alpha_i, \beta_i) \), such as \( 0 = (0, 0) \) for empty, \( 1 = (0, 1) \) for spin-down, \( 2 = (1, 0) \) for spin-up, and \( 3 = (1, 1) \) for both spin-up and spin-down. Thus, the physical index runs from 0 to 3. The basis of the Fock space can be written in terms of the creation operators \( c_i^\dagger \) and \( c_i \) as follows:

\[
|\sigma_0^L \cdots \sigma_{L-1}^L\rangle = (c_{0_L}^\dagger)^{\sigma_0}(c_{1_L}^\dagger)^{\sigma_1}(c_{1_L}^\dagger)^{\sigma_1}(c_{2_L}^\dagger)^{\sigma_2}(c_{2_L}^\dagger)^{\sigma_2}(c_{3_L}^\dagger)^{\sigma_3}(c_{3_L}^\dagger)^{\sigma_3}|0\rangle, \tag{4}
\]

where \( \sigma_i(\beta_i) = 0 \) or 1 means that a spin-up (down) fermion vacancy or occupancy exists at the \( i \)-th site, respectively. Maintaining the order of fermions in the state of the Fock space to deal with the negative sign caused by fermion exchange is important. We adopt the order of spin-up, then spin-down as described above.

In the iDMRG process, we have to find the MPO for the Hamiltonian in Eq. (2). We are convinced that the MPO of the \( i \)-th site is, indeed, given by the following form:
where

\[
M_i = \begin{pmatrix}
1 & c_{i1}^\dagger & c_{i1}^\dagger & b_i \\
0 & 0 & 0 & 0 & -t_{ci} \\
0 & 0 & 0 & 0 & -t_{ci} \\
0 & 0 & 0 & 0 & t_{ci} \\
0 & 0 & 0 & 0 & 0 & 1 \\
\end{pmatrix},
\]

(5)

Here, we have not presented the boundary operators. We note that the MPO for even sites is slightly different from the MPO for odd sites, where \(\mu_e \) must be replaced with \(\mu_o\). Because \(c \) and \(c^\dagger \) are fermion operators, the commutation relations between \(M \) and \(c^\dagger_\sigma (i \neq j, \sigma = \uparrow, \downarrow) \) are given by

\[
M_i c^\dagger_\sigma = c^\dagger_\sigma M_i^*,
\]

where

\[
M_i^* = \begin{pmatrix}
1 - c_{i1}^\dagger & -c_{i1}^\dagger & c_{i1} & -c_{i1} & b_i \\
0 & 0 & 0 & 0 & 0 & t_{ci} \\
0 & 0 & 0 & 0 & 0 & -t_{ci} \\
0 & 0 & 0 & 0 & 0 & -t_{ci} \\
0 & 0 & 0 & 0 & 0 & 0 & 1 \\
\end{pmatrix}
\]

(8)

When the Hamiltonian acts on the basis, the sign caused by fermion exchange must be taken care of

\[
M_0 \cdots M_{L-1} (c_{01}^\dagger)^{\nu_0} (c_{01}^\dagger)^{\nu_0} (c_{11}^\dagger)^{\nu_1} (c_{11}^\dagger)^{\nu_1} \\
\cdots (c_{L-1}^\dagger)^{\nu_{L-1}} (c_{L-1}^\dagger)^{\nu_{L-1}} |0 \rangle \\
= M_0 (c_{01}^\dagger)^{\nu_0} (c_{01}^\dagger)^{\nu_0} \tilde{M}_i (c_{11}^\dagger)^{\nu_1} (c_{11}^\dagger)^{\nu_1} \\
\cdots \tilde{M}_{L-1} (c_{L-1}^\dagger)^{\nu_{L-1}} (c_{L-1}^\dagger)^{\nu_{L-1}} |0 \rangle,
\]

(9)

where the total number of fermions to the left of the \(i\)-th site, \(N_i = \sum_{k=0}^{i-1} (\alpha_k + \beta_k)\), determines the \(6 \times 6\) matrix:

\[
\tilde{M}_i = \begin{cases} 
M_i & \text{for } N_i = \text{even,} \\
M_i^* & \text{for } N_i = \text{odd.}
\end{cases}
\]

(10)

In order to manage the sequence in Eq. (9), we note that the even and the odd structures of the fermion numbers \((E, O)\) are kept recursively by \(e \equiv \{ |0 \rangle, c_{i1}^\dagger c_{i1}^\dagger |0 \rangle \}\) and \(o \equiv \{ c_{i1}^\dagger |0 \rangle, c_{i1}^\dagger |0 \rangle \}\) such that

\[
\begin{pmatrix}
e O \end{pmatrix} = \begin{pmatrix}
e O \end{pmatrix} = \begin{pmatrix}
e O \end{pmatrix} = \begin{pmatrix}
e O \end{pmatrix}.
\]

Using the relation in Eq. (11), we double the MPO for the \(i\)-th site, \(M_i\), which is modified into a \(12 \times 12\) matrix, \(D_i\), such that

\[
D_i e = \begin{pmatrix} M_{ie} & 0 \\ 0 & M_{ie}^* \end{pmatrix}, \quad D_i o = \begin{pmatrix} 0 & M_{io} \\ M_{io}^* & 0 \end{pmatrix},
\]

(12)

where \(M_{ie}^*\) is used in the second row because an odd number of fermions are to the left of the \(i\)-th site. By including the 4-dimensional physical index, we present the effective MPO as a graphical diagram with a four-leg tensor \(D\) having \(4 \times 12 \times 12 \times 4\) elements, for which the number of non-zero elements is small:

\[
\cdots - D - D - D - \cdots
\]

(13)

The so-called fermionic matrix product states \([28]\) are introduced in a similar fashion of doubling the MPO. We have already tested this MPO approach \([29]\). The numerical results obtained by doubling the MPO were compared with those obtained using the Jordan-Wigner transformation and were found to be in good agreement.

By adopting the two-site iDMRG algorithm, we optimize two tensors in our MPS, \(A_{ab}^\sigma\) and \(B_{bc}^\sigma\). The physical index \(\sigma\) takes a value from 0 to 3, and the indices \(a\) (left) and \(b\) (right) run from 0 to \(\chi - 1\), where \(\chi\) is the internal bond dimension. The Schmidt coefficients are denoted by \(\lambda_{ab}\) between \(A_{ab}^\sigma\) and \(B_{bc}^\sigma\), and by \(\lambda_{ba}\) between \(B_{ab}^\sigma\) and \(A_{bc}^\sigma\). A state in the MPS space can be represented in graphic notation as

\[
\cdots - A - \lambda_{ab}^\sigma - B - \lambda_{ba}^\sigma - A - \cdots
\]

(14)

By evaluating the \(4 \times 12 \times 12 \times 4\) elements of \(D\), we use the iDMRG by acting the MPO of Eq. (13) on the MPS of Eq. (14). Regardless of the values of \(t\), \(U\), \(\mu_e\), and \(\mu_o\) used in our calculations, we observe a smooth convergence. Our numerical iDMRG results show that the ground-state solutions are divided into two classes: the MPS with a unit cell of two sites is either of the form \(\cdots \text{ABABAB} \cdots\) or uniform \(\cdots \text{AAAAAA} \cdots\). We will identify the state of \(\cdots \text{ABABAB} \cdots\) as a Mott phase near half filling, while we will identify the uniform state as a metallic phase further away from half filling.
3 Numerical results

By setting $t = 1$ and $U = 4$ for a given $\mu_e$ and $\mu_o$, we calculate the ground state using the two-site iDMRG. With the ground state, we extract three physical quantities corresponding to even and odd sites: the bond energies $\langle h_e \rangle$ and $\langle h_o \rangle$, the number densities $\langle n_e \rangle$ and $\langle n_o \rangle$, and the half-chain entanglement entropies $S_e$ and $S_o$. Here, the bond Hamiltonian $h_e$ ($i = \text{even}$) can be written as

$$
\begin{align*}
    h_e &= -t(c_i^\dagger c_j^\dagger + c_i^\dagger c_j + c_i^\dagger c_j^\dagger + c_j^\dagger c_j) \\
    &+ \frac{U}{2} (n_i^\dagger - \frac{1}{2})(n_j^\dagger - \frac{1}{2}) - \frac{\mu_e}{2} (n_i + n_i^\dagger) \\
    &+ \frac{U}{2} (n_j^\dagger - \frac{1}{2})(n_j - \frac{1}{2}) - \frac{\mu_o}{2} (n_j + n_j^\dagger).
\end{align*}
$$

(15)

In addition, the occupation number density operator $n_e$ ($i = \text{even}$) can be written as

$$
n_e = n_i^\dagger + n_i = c_i^\dagger c_i^\dagger + c_i^\dagger c_i. 
$$

(16)

Using the Schmidt coefficients $\lambda_\alpha$ between $A$ and $B$ in the MPS, we determine $S_e$. Keeping the normalization with $\sum_{\alpha=0}^{\chi-1} \lambda_\alpha^2 = 1$, we calculate the half-chain entanglement entropy $S_e$, which is given by

$$
S_e = -\sum_{\alpha=0}^{\chi-1} \lambda_\alpha^2 \log_2 \lambda_\alpha^2. 
$$

(17)

Obviously, we choose $i = \text{odd}$ for $h_o$ and $n_o$. We use the Schmidt coefficients $\lambda^BA$ between $B$ and $A$ in the MPS for $S_o$.

To verify the correctness of the calculation, we use an important analytic result [18] from the critical point of $\mu_e$ at which the Mott insulator–metallic phase transition takes place in the restricted parameter space of $\mu_e = \mu_o$ or $\Delta = 0$

In fact, the transition point $\mu_e$ is given by

$$
\mu_e = 2 + \frac{U}{2} + 2 \int_0^\infty d\omega \frac{J_1(\omega) \exp(-\omega U/4)}{\cosh(\omega U/4)}.
$$

(18)

For $U = 4$, we obtain the exact critical point, $\mu_e = \mu_o = 0.643364$. We present the average bond energy $\langle (h_e + h_o)/2 \rangle$ in Fig. 2, where level-crossing takes place at $\mu_e = \mu_o \sim 0.65$.

In Fig. 2, to determine the level-crossing of the average bond energy, we compute the ground state starting from $\mu_o = 0$. On the other hand, we can also calculate the ground state of the uniform solution by decreasing $\mu_o$ from large values. In each iDMRG calculation, the tensors of the initial environment are given by the previous solution for different $\mu_o$.

To determine the Mott transition in the parameter space of $\mu_e$ and $\mu_o$, we compute the average number density $\langle n_e \rangle$ and $\langle n_o \rangle$ and the average entanglement entropy $S_e$ and $S_o$. Fixing $\mu_o$, we present $\langle n_e \rangle$ and $\langle n_o \rangle$ and $\langle S_e \rangle$ and $\langle S_o \rangle$ by varying $\mu_e$, we show the results in Figs. 3.
and 4, respectively. We note that the abrupt behavior corresponds to a Mott transition.

As the main numerical result, we present the phase diagram in Fig. 5. One notices the robustness of the Mott state. In fact, we find that a small difference in the energy offsets, which is the staggered potential $\Delta = \mu_o - \mu_e$, cannot destroy the Mott phase.

**4 Conclusions**

In summary, we have used the iDMRG with the MPO to obtain the ground state in the one-dimensional ionic Hubbard model. We calculate the occupation number density and the half-chain entanglement entropy to determine the Mott transition. We draw the phase diagram in the two-dimensional parameter space of the chemical potential and the staggered potential.

Extending our method to manage the number of fermions in two-dimensional systems would be interesting. A typical topic of interest would be the two-dimensional fermion Hubbard model, for which our first task would be to build a local tensor product operator like the MPO. Although we do not encounter the notorious sign problem here, we should be able to overcome the sign problem in the two-dimensional Hubbard model by using the tensor product operator. As we double the MPO as explained above, we can double the tensor product operator in order to support the number of fermions. We anticipate progress in the two-dimensional case.

**Acknowledgements** This work was partially supported by the Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education, Science and Technology (Grant No. NRF-2017R1D1A1A0201845). The author would like to thank M. C. Cha for helpful discussions.

**References**

1. A. Osterloh, L. Amico, G. Falci, R. Fazio, Nature 416, 608 (2002)
2. T.J. Osborne, M.A. Nielsen, Phys. Rev. A 66, 032110 (2002)
3. S. Sachdev, Quantum phase transitions (Cambridge University Press, New York, 2011)
4. J. Eisert, M. Cramer, M.B. Plenio, Rev. Mod. Phys. 82, 277 (2010)
5. M.C. Cha, M.H. Chung, Phys. B 536, 701 (2018)
6. L. Tagliacozzo, T.R. de Oliveira, S. Iblisdir, J.I. Latorre, Phys. Rev. B 78, 024410 (2008)
7. F. Pollmann, A.M. Turner, E. Berg, M. Oshikawa, Phys. Rev. B 81, 064439 (2010)
8. B. Pirvu, G. Vidal, F. Verstraete, L. Tagliacozzo, Phys. Rev. B 86, 075117 (2012)
9. M. Pino, J. Prior, A.M. Somoza, D. Jaksch, S.R. Clark, Phys. Rev. A 86, 023631 (2012)
10. Gu Shi-Jian, Shu-Sa Deng, You-Quan Li, Hai-Qing Lin, Phys. Rev. Lett. 93, 086402 (2004)
11. D. Larsson, H. Johannesson, Phys. Rev. Lett. 95, 196406 (2005)
12. F. Jemini, T.O. Maciel, R.O. Vianna, Phys. Rev. B 92, 075423 (2015)
13. M.C. Cha, Phys. Rev. B 98, 235161 (2018)
14. Ö. Legeza, J. Sólyom, Phys. Rev. Lett. 96, 116401 (2006)
15. M.F. Parsons, F. Huber, A. Mazurenko, C.S. Chiu, W. Setiawan, K. Wooley-Brown, S. Blatt, M. Greiner, Phys. Rev. Lett. 114, 213002 (2015)
16. L.W. Cheuk, M.A. Nichols, M. Okan, T. Gersdorf, V.V. Ramasesh, W.S. Bakr, T. Lompe, M.W. Zwierlein, Phys. Rev. Lett. 114, 193001 (2015)
Phase transitions in the one-dimensional ionic Hubbard model

17. M. Schreiber, S.S. Hodgman, P. Bordia, H.P. Lüschen, M.H. Fischer, R. Vosk, E. Altman, U. Schneider, I. Bloch, Science 21, 842 (2015)
18. F.H.L. Essler, H. Frahm, F. Göhmann, A. Klümper, V.E. Korepin, The one-dimensional Hubbard model (Cambridge University Press, New York, 2005)
19. M. Hafez-Torbati, N.A. Drescher, G.S. Uhrig, Phys. Rev. B 89, 245126 (2014)
20. S. Bag, A. Garg, H.R. Krishnamurthy, Phys. Rev. B 91, 235108 (2015)
21. H.F. Lin, H.D. Liu, H.S. Tao, W.M. Liu, Sci. Rep. 5, 9810 (2015)
22. K. Bouadim, N. Paris, F. Hebert, G.G. Batrouni, R.T. Scalettar, Phys. Rev. B 76, 085112 (2007)
23. A.P. Kampf, M. Sekania, G.I. Japaridze, P. Brune, J. Phys.: Cond. Matt. 15, 5895 (2003)
24. D.G. Angelakis, M. Huo, E. Kyoseva, L.C. Kwek, Phys. Rev. Lett. 106, 153601 (2011)
25. U. Schollwöck, Annals Phys. 326, 96 (2011)
26. I.P. McCulloch, arXiv:0804.2509 (2008)
27. C. Yang, A.N. Kocharian, Y.L. Chiang, J. Phys.: Cond. Matt. 12, 7433 (2000)
28. N. Bultinck, D.J. Williamson, J. Haegeman, F. Verstraete, Phys. Rev. B 95, 075108 (2017)
29. M.H. Chung, E. Orignac, D. Poilblanc, S. Capponi, Phys. B 604, 412665 (2021)

Publisher's Note Springer Nature remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.