Entanglement entropy of two-species hard-core bosons in one dimension

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Abstract
We study the bipartite entanglement entropy of a model for two-species hard-core bosons in one dimension. In this model, the same-species bosons satisfy hard-core conditions while the different-species bosons are allowed to occupy the same site with a local interaction strength $U$. We measure the bipartite entanglement entropy of the ground states of an infinite-size system as a function of $U$ in the half-filled and the off-half-filled cases. To achieve this goal, we use a time-evolution-block-decimation method with large bond dimensions up to 300.

Keywords Two-species bosons · Entanglement entropy · Tensor network states

1 Introduction

Entropy is one of the most important quantities in physics. The second law of thermodynamics states that the entropy of an isolated system never decreases. For pure quantum states with definite energy, the number of degeneracy defines entropy in the quantum statistical ensemble theory [1]. Also, in quantum physics and quantum information science, a quantity called “entanglement entropy” (EE) of some part of the whole quantum system has attracted much attention recently [2].

Entanglement entropy is a measure of entanglement between a given part of a system and the rest of the system. Researchers have found that the EE satisfies scaling laws. If one takes a many-body quantum state randomly, the entanglement entropy of a part of the system scales with the volume. This scaling law is known as the “volume law”. Meanwhile, the ground state of a quantum system has a peculiar property that EE scales with area [2]. Some of the integrable models, such as the models for boson harmonic chains, fermion chains, and XY chains, have been studied to understand this “area law”.

The recent development of representing quantum many-body states with tensor network states [3] has allowed direct measurement of the entanglement entropy by using singular value decompositions [4]. The exponential growth of Hilbert space with the number of sites limits the exact diagonalization. Also, the density matrix of a part of a system is hard to construct. The evolution of tensor network states by using density matrix renormalization group (DMRG) transformation with matrix product operators [5] and time-evolution-block-decimation [6] (TEBD) has opened an effective way of obtaining the EE.

In this paper, we study the bipartite entanglement entropy of ground states of a model of two-species hard-core bosons in one dimension. The hard-core condition implies that the same-species bosons cannot occupy the same site, but different-species bosons may. For the two species, we denote them as $a$ and $b$ boson. Therefore, the possible quantum states for a single site are $|0\rangle$, $|a\rangle$, $|b\rangle$, and $|ab\rangle$, where $|0\rangle$ denotes the vacuum state. Here, the $|ab\rangle$ state will have a local interaction $U$. The local interaction $U$ between different species bosons at the same site can be either attractive or repulsive. By using the inverse Jordan–Wigner transformation, one can map the model to the Hubbard model in one dimension. However, we stick to the terminology of bosons because we do not consider fermionic statistics for other physical quantities such as correlation functions [7]. At half-filling, the model has three quantum phases at zero temperature: a superfluid (SF) ($U = 0$), a Mott insulator (MI) ($U > 0$), and a paired charge density wave (CDW) ($U < 0$). An MI transforms into a CDW with a particle-hole transformation. Because a phase transition occurs at $U = 0$, studying the
ground states near $U = 0$ is very important. We also investigate the bipartite EE of ground states in the off-half-filling cases. A related model with both intra-species and inter-species interactions without the hard-core condition has been studied [8, 9], where the interest was the competition between intra- and inter-species interactions.

Our work focuses on the behavior of the EE in a basic model of a two-species hard-core boson system. To obtain the bipartite EE, we use an infinite-size time-evolution-block-decimation (iTEBD) with infinite-size matrix product states (iMPS). We also used an infinite-size matrix renormalization group (iDMRG) with the matrix product operators (MPO) [5, 6] to check whether our iTEBD results are consistent with iDMRG. Both methods give reliable ground-state energies.

We found that the bipartite EE has a peculiar behavior as a function of $U$ for finite bond dimensions and $U_{on}$, which yields local maximum EE, decreases very slowly to zero as we increase bond dimension.

This paper is organized as follows. In Sect. 2, we present our model of interacting two-species hard-core bosons with local interaction $U$ for different species. Section 3 describes the methods used in this work: iTEBD and iDMRG with MPO. We discuss the accuracy of both methods. Section 4 is the main result of our work. We measure the bipartite entanglement entropy in the half-filled and the off-half-filled cases. In Sect. 6, we discuss our results and future research topics.

## 3 Methods and accuracy

The infinite-size matrix product state is constructed with two-site tensors:

$$|\text{iMPS}\rangle = \sum_{\{p\}} \sum_{\{a\}} \Gamma_{a_{1}a_{2}}^{p_{1}|p_{2}} |a_{1}|^{p_{1}} |a_{2}|^{p_{2}}, \quad (2)$$

where $\Gamma$'s are tensors with a physical variable $p$ and indices of $a$, and $\lambda$'s are the singular values connecting two neighboring sites. In a infinite-size time-evolution-block-decimation scheme (iTEBD) [6], |iMPS⟩ evolves with the repeating operation of a time evolution operator $e^{-\epsilon H}$. In the application of this time-evolution operator, we decompose the operator as

$$e^{-e^{-\epsilon H/2}} \times e^{-e^{-\epsilon H/2}}. \quad (3)$$

Here, the operator $e^{-e^{-\epsilon H/2}}$ acts on

$$e^{-e^{-\epsilon H/2}} \lambda_{a_{1}a_{2}}^{[2]} |p_{1}|^{p_{2}} |\lambda_{a_{1}a_{2}}^{[2]} |p_{2}|^{p_{2}}.$$ \quad (4)

This procedure updates $\Gamma^{p_{1}}$, $\Gamma^{p_{2}}$, and $\lambda^{[1]}$ by using singular value decomposition. Similarly, applying $e^{-e^{-\epsilon H/2}}$ updates $\Gamma^{p_{2}}$, $\lambda^{[2]}$, and completes a single iteration. When iterations are repeated, |iMPS⟩ will converges to a tensor product state representing a ground state of $H$. This is similar to a power method.

The infinite-size density matrix renormalization group (iDMRG) method transforms a matrix product state to another matrix product state by using the singular value decomposition of the lowest eigenvalue state for the block Hamiltonian. We adopt a matrix product operator (MPO) scheme [5] in making the block Hamiltonian. Here, we just show the MPO we use in our work:

$$W = \begin{pmatrix}
I & 0 & 0 & 0 & 0 & 0 & b \times V_{\text{loc}}
\end{pmatrix}, \quad (5)
$$

where $V_{\text{loc}} = -\mu(n_{b} + n_{a}) + U(n_{a} - \frac{1}{2} I)(n_{b} - \frac{1}{2} I), I$ stands for the identity operator, and all the operators have a dimension of $4 \times 4$ because the size of a possible quantum state at a local site is 4, i.e., vacuum, $a$ boson only, $b$ boson only, and $a$ and $b$ bosons. A detailed algorithm can be found in Ref. [5].
The iDMRG method has the advantages of (1) not using the parameter $\epsilon$ in iTEBD and (2) no need to construct a density matrix as in the old DMRG algorithm [10].

Many previous articles have shown that the energy will converge in relatively low number of iterations of iTEBD [11, 12]. We found that the convergence of other physical quantities should be checked before concluding that we had reached reasonable values for them. Especially, we found that even though the energy converged to the exact value, the half-chain entanglement entropy reached different values for different $\epsilon$. One should note that we need $\epsilon \to 0$ and $\chi \to \infty$ for a thermodynamic value in iTEBD. To overcome this difficulty, we used a well-known adaptive $\epsilon$ method for fast convergence of the entropy. The idea is similar to the temperature annealing method in classical Monte Carlo simulations. We started from $\epsilon = 1/4$, and we change $\epsilon \to 1/4 \times \epsilon$ when EE reached a stable value. $\epsilon$ is reduced until the EE does not change as we continue to $1/4 \times \epsilon$.

Figure 1 shows the difference in the energy per site for iTEBD and iDMRG and the exact value of the energy from Bethe Ansatz as a function of $U$. The exact value of the ground-state energy in the thermodynamic limit has been studied by using Bethe Ansatz [7, 13]. The ground-state energy per site for an infinite lattice is given by an integral form as

$$E/N = -\frac{U}{4} - 4 \int_0^\infty \frac{dx}{x} \frac{J_0(x)J_1(x)}{\exp\left(\frac{Ux}{2}\right) + 1}. \quad (6)$$

Here, we found the energy per site to an error of less than $10^{-4}$.

4 Bipartite entanglement entropy

The bipartite entanglement entropy can be obtained from the entanglement weights between two half chains. If a infinite-chain quantum state $|\Psi\rangle$ is decomposed with two half chains, $A$ and $B$, by using a singular value decomposition, $|\Psi\rangle$ can be written as

$$|\Psi\rangle_{\text{SVD}} = \sum_i \lambda_i |\phi_A\rangle_i |\phi_B\rangle_i. \quad (7)$$

where $|\phi_{A(B)}\rangle_i$ is the partial wavefunction for $A(B)$ and $\lambda_i$'s are singular values. A normalization condition forces { $\lambda_i$ } to satisfy

$$I = \text{svd}(\langle\Psi|\Psi\rangle_{\text{SVD}}) = \sum_i \lambda_i^2, \quad (8)$$

so that the normalized $|\Psi\rangle_{\text{SVD},n}$ is

$$|\Psi\rangle_{\text{SVD},n} = \sum_i \frac{\lambda_i}{\sqrt{\sum_j \lambda_j^2}} |\phi_A\rangle_i |\phi_B\rangle_i. \quad (9)$$

The reduced density matrix for the chain $A$ is obtained by tracing out $B$ from the full density matrix:

$$\rho_A = \text{Tr}_B|\Psi\rangle\langle\Psi|. \quad (10)$$

Because $\rho_A$ is diagonal in the space of $|\phi_A\rangle$'s, the entropy is

$$S_h = -\sum_i \frac{\lambda_i^2}{\sum_j \lambda_j^2} \log \frac{\lambda_i^2}{\sum_j \lambda_j^2}. \quad (11)$$

With the Bethe Ansatz, obtaining the half-chain entropy in closed form is very hard, but with iMPS, we can easily measure $S_h$ numerically because we calculate { $\lambda_i$ } with time evolution. Figure 2 shows the half-chain entanglement entropy obtained from iTEBD as a function of $U$ for the half-filled case. Because the phase transition occurs at $U = 0$, we should focus on the behavior of $S_h$ near $U = 0$. The EE has a local minimum at $U = 0$, and it increases up to a finite value and then decreases as $U$ becomes large. Although the maximum EE occurs for finite $U_m$, we observed that $U_m$ decreases as we increase $\chi$. Because a finite bond dimension changes the quantum phase transition like the mean field, we believe that $U_m$ eventually goes to $U_c = 0$ when $\chi \to \infty$. However, determining the peculiar behavior of EE for finite $\chi$ would be interesting.

Also, $S_h$ increases as $\chi$ increases for a fixed $U$. For $U = 0$, if $\xi \sim \chi^c$, then the fitting form becomes $\frac{c}{\xi} \log(\chi)$ [14, 15]. Our fitting result is $c\xi/6 = 0.2763(5)$, which is consistent with the previous numerical results [16] (0.294) for the fermionic Hubbard model when the maximum of $\chi$ was 108. We also found that $S_h$ did not scale as a logarithmic function for $U = 5.0$, which might be a
Entanglement entropy of two-species hard-core bosons in one dimension

We do not present \( S_h \) from iDMRG because intrinsic oscillation of the EE for odd and even number of half-chain sites exists for finite \( U \) [17]. We also used the original DMRG algorithm of White [10] and obtained the entanglement entropy with density matrices. For finite \( U \), we found that the EE oscillates with iterations as iDMRG, but we observed that our EE results as a function of \( U \) are overall the same as iDMRG results.

\section{5 Off-Half-filling case}

We are also interested in obtaining the entanglement entropy in the off-half-filling case, which has not been covered in the previous work [17]. The bipartite entanglement entropy \( (S_h) \) as a function of \( U \) is shown in Fig. 3 for \( \mu = 0.0 \sim 0.5 \). The symmetry of positive \( U \) and negative \( U \) is broken [7] naturally because the density of bosons changes as a function of \( U \). This can be seen in Fig 4, where the density of bosons as a function of \( U \) for each \( \mu \) is presented. For positive \( U \), as \( U \) increases, the density reduces to 1 at a critical \( U \), which means the system becomes again a half-filled Mott insulator. After \( U \) reaches this critical value, EE follows the same curve because the density of bosons is locked to 1.

For negative \( U \), as \( |U| \) becomes large, the EE first decreases and then increases. We believe that the entanglement between two half chains becomes strong for a high density of bosons with large \( |U| \) because paired bosons make a

more strong superfluid. As one can see, the concavity changing point in Fig. 4 is related to the EE minimum, where the density of bosons starts to grow rapidly.
6 Discussion

In this paper, we obtained the infinite-size ground-state properties of two-species hard-core bosons in one dimension. In our model, the bosons have a hard core for the same species, but they interact locally if they are different species. With infinite-size matrix product states, we used a time-evolution-block-decimation method and infinite-size density matrix renormalization group procedure. For the half-filling, where the quantum critical point is a well-known point of $U_c = 0$, we find that the maximum bipartite entanglement entropy point is finite but decreases very slowly as we increase $\chi$. We believe that this is the effect of the finite bond dimension and that this point will eventually go to zero when $\chi \to \infty$. Also, we obtained the bipartite EE in the off-half-filling case. The symmetry of the entanglement entropy with respect to $U$ is broken because the density of bosons changes as a function of $U$. We find that positive strong $U$ leads to a Mott insulator system and that negative strong $U$ leads to a strong superfluid system and increases the bipartite EE.

We are working on the soft-core boson models, which will demonstrate more interesting features of bosons in optical lattices. We expect that the bipartite entanglement entropy will be a good property for understanding quantum phase transitions.

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