Observing Dynamical Features of BosonSampling with Matrix Product States

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BosonSampling is a well-defined scheme for demonstrating quantum supremacy with photons in near term. Although relying only on multi-photon interference in nonadaptive linear-optical networks, it is hard to simulate classically. Here we study BosonSampling using matrix product states, a powerful method from quantum many-body physics. We show that this method is efficient to simulate the dynamics of a multi-particle optical quantum circuit, which allows us to reveal the dynamical features of BosonSampling, such as entanglement entropy growth, by employing correlation measurements. Furthermore, we provide numerical evidence that for large enough losses, BosonSampling could be easily simulated classically. Our work, in principle, demonstrates that matrix product states is a powerful platform to simulate optical quantum circuits. Furthermore, it is readily extended to study quantum dynamics in multi-particle quantum walks beyond BosonSampling.

I. INTRODUCTION

Multi-photon interference lies at the heart of optical quantum information processing [1, 2], including optical quantum computing [3], quantum cryptography [4], quantum simulation [5], and quantum metrology [6]. Based on some basic interference phenomena, such as the Hong-Ou-Mandel (HOM) effect [7], it is possible for us to make use of quantum advantages to realize some complex processing tasks beyond the current classical limit [8], by increasing the number of single photons and the complexity of the optical quantum circuit.

In particular, BosonSampling [9], an intermediate model of linear optical quantum computing, utilizes only passive multi-port optical interferometer for the evolution of input single-photon sources, and then samples the output events using single-photon detectors, which is a well-defined problem that can be naturally and efficiently solved on a specialized photonic quantum simulator. However, it has been shown to be classically intractable because the amplitude associated with each term in the output quantum state of BosonSampling is related to the calculation of a matrix permanent [9], which is known to be a #P-problem [10]. Thus, BosonSampling is considered as a promising candidate to experimentally demonstrate the quantum supremacy in the near future [11]. So far, a number of elegant BosonSampling experiments has been achieved with linear optics on a small scale [12–22]. In addition, BosonSampling can be regarded as a special multi-particle quantum walk, and thus investigating its nonclassical correlations during the quantum dynamics is also an interesting task [23–27].

It is important to directly simulate the working process of BosonSampling (or, more broadly, the behavior of multi-particle quantum walks) running on a linear optical quantum circuit. Firstly, since the quantum state is directly accessible, it is possible to measure intermediate observables such as correlations, entanglement entropy, to have a better understanding of the underlying dynamical process. Secondly, it provides a platform to benchmark and verify the output quantum state of a real quantum device. Last, it could be used as an alternative approach to simulate the sampling process, along-side with the existing approaches such as brute force sampling and the Metropolised independence sampling (MIS) [28, 29].

However, simulating the evolution of an optical quantum circuit classically is very difficult. For an optical quantum circuit with \( M \) photonic modes and \( N \) input photons, the number of parameters in the quantum state will grow as \( (M + N - 1) M^{-1} \). At the same time, trying to reconstruct the quantum state by computing all the amplitudes of the quantum state with a classical algorithm, such as Ryser’s algorithm [30], would also be difficult since the time complexity of computing a single amplitude is already \( O(2^M N^2) \). In this work, we use matrix product states (MPS) to study BosonSampling and show that MPS could allow us to go to much larger systems than the above approaches. MPS is a very successful numerical tool in solving one-dimensional quantum manybody problems [31], for both the unitary systems [32–34] and the dissipative systems [35–37]. Briefly speaking, MPS works by compactly rewriting a one-dimensional quantum manybody state as a product of many low dimensional tensors. For certain types of quantum systems which obey the so-called area law [38, 39], the sizes of the low dimensional tensors are bounded, which makes MPS to be a very memory efficient representation of the quantum state. The time complexity of MPS is also low in that the local unitary operations can be performed on local tensors only, without affecting other tensors. Moreover, measuring observables, especially local observables with MPS can be performed extremely efficiently. For a review of MPS one could refer to [40].

In particular, we highlight that we have developed a generic MPS platform to study optical quantum circuits. It can be used to simulate different particle types including both the bosons and the fermions. Simulating an open quantum system can be done almost in parallel with the unitary case. The changes of the entanglement entropy during each depth of the evolution can be measured efficiently with MPS. Furthermore, we estimate the numerical complexity of the classical simulation by showing the decaying of the singular values of the final state, for different input states, such as bosons, fermions, and bosons with losses, and provide numerical evidence that for BosonSampling with large enough losses, the complexity...
could be substantially reduced. The paper is organized as follows: In Sec. II, we briefly introduce the MPS algorithms. In Sec. III, we show the faster growth of the entanglement entropy of BosonSampling than FermionSampling, and how the numerical complexity of BosonSampling is affected by losses. Finally we summarize in Sec. IV.

II. METHOD

In this section, we first give a brief introduction to MPS, and then show that MPS can be used to simulate many-particle dynamics in various cases, such as bosons and fermions in an ideal environment, as well as in a lossy environment.

A quantum many-body state living on a bosonic or fermionic optical lattice of size $M$ can be written as

$$
|\psi\rangle = \sum_{n_1,n_2,\ldots,n_M} c_{n_1,n_2,\ldots,n_M} |n_1,n_2,\ldots,n_M\rangle,
$$

where $n_i$ labels the local Fock state on the $i$-th site of the lattice, $n_i$ is unbounded for bosons and $n_i = 0, 1$ for fermions. The coefficient $c_{n_1,n_2,\ldots,n_M}$ is an $M$ dimensional tensor. Assuming the size of the local Hilbert space is $l$, then the tensor $c$ would contain $M^l$ complex numbers in general. MPS rewrites $c$ as a product of $3$ dimensional tensors:

$$
c_{n_1,n_2,\ldots,n_M} = \sum_{a_1,\ldots,a_{M+1}} B_{a_1,a_2}^{n_1} B_{a_2,a_3}^{n_2} \cdots B_{a_{M+1},a_M}^{n_M}.
$$

Here we have used $a_i$ to denote the auxiliary degree of freedoms, with $a_1 = a_{M+1} = 1$ added for notational convenience. The largest size of $a_i$ is referred to as the bond dimension $D$, which essentially characterizes the complexity of MPS. In principle, any $M$ dimensional tensor $c$ can be systematically converted into an MPS as in Eq.(2) by successively reshaping and singular value decomposition (SVD) [40]. During this procedure singular values smaller than a given threshold are thrown away. For an arbitrary quantum state, the number of remaining singular values, which is the actual bond dimension $D$, could still grow exponentially with $M$. For the classes of quantum states which obey the area law, $D$ will be constant or only grow polynomially with system size [38, 39].

MPS keeps invariant when inserting a pair of matrices $U$, $U^{-1}$ between a pair of sites $i$ and $i+1$, which is also referred to as bond $i$. To fix this gauge degree of freedoms, one can prepare the MPS in canonical forms [40]. In our simulation we keep MPS in the right canonical form, which means that each tensor $B_{a_i,a_{i+1}}$ satisfies the condition

$$
\sum_{a_{i+1},n_i} B_{a_i,a_{i+1}}^{n_i} \text{conjugate}(B_{a_i',a_{i+1}}^{n_i'}) = \delta_{a_i,a_i'},
$$

where conjugate$(a)$ means taking the element-wise conjugate of the tensor $a$.

Local unitary transformations on the quantum state in Eq.(1) can be easily translated into operations on MPS. Here we exemplify this by showing how to apply one-body and nearest-neighbour two-body operations to MPS. The application of one-body operations $R_{n_i}$ on site $i$ is simply

$$
B_{a_i,a_{i+1}}^{n_i} = \sum_{n_i} B_{a_i,a_{i+1}}^{n_i} R_{n_i}.
$$

We can see that one-body operation will not break the right canonical condition in Eq.(3) as long as $R_{n_i}$ is unitary.

For a two-body operation $O_{n_i,n_{i+1}}^{n_i'}$ acting on sites $i$ and $i+1$ (bond $i$), we first multiply $B_{a_i,a_{i+1}}^{n_i}$ and $B_{a_i+1,a_{i+2}}^{n_{i+1}}$:

$$
\Phi_{a_i,a_{i+2}}^{n_i,n_{i+1}} = \sum_{a_{i+1}} B_{a_i,a_{i+1}}^{n_i} B_{a_{i+1},a_{i+2}}^{n_{i+1}},
$$

then we apply $O_{n_i,n_{i+1}}^{n_i'}$ to $\Phi$ and get

$$
\Phi_{a_i,a_{i+2}}^{n_i',n_{i+1}'} = \sum_{n_i,n_{i+1}} \Phi_{a_i,a_{i+2}}^{n_i,n_{i+1}} O_{n_i,n_{i+1}}^{n_i',n_{i+1}'},
$$

after that we do an SVD to $\Phi$:

$$
\sum_{a_{i+1}} U_{a_i,a_{i+1}}^{n_i} S_{a_i,a_{i+1}}^{n_i'} V_{a_{i+1},a_{i+2}}^{n_{i+1}} = \text{svd}(\Phi_{a_i,a_{i+2}}^{n_i,n_{i+1}}),
$$

FIG. 1. (a) Universal $M$-mode multiport interferometer (shown here for $M=6$) for BosonSampling [41]. Sequence of phase shifters and beam splitters acting on the optical quantum circuit. (b) Mapping from the optical quantum circuit to a quantum circuit consisting of one-body (yellow square, corresponding to the phase shifter) and two-body (blue rectangular, corresponding to the beam splitter) gate operations and acts on an MPS, in analogous to the t-MPS algorithm. A layer of two-body gate operations is counted as one depth.
where we have grouped the indexes \((a_{i+2}, n_{i+1})\) and \((a_i, n'_i)\) so that SVD is performed on a two-dimensional tensor. By definitions of SVD, the tensor \(V\) satisfies the right canonical condition in Eq.(3) and the tensor \(U\) satisfies the left canonical condition

\[
\sum_{a_i, n_i} U^a_i U^a_i = \delta_{a_i, a'_i+1}, \quad (8)
\]

With these results, we can update \(B_{a_{i+1}, a_{i+2}}^{n_{i+1}}\) and \(B_{a_{i}, a_{i+1}}^{n_{i}}\)

\[
B_{a_{i+1}, a_{i+2}}^{n_{i+1}} = V_{a_{i+1}, a_{i+2}}^{n_{i+1}}, \quad (9)
\]

\[
B_{a_{i}, a_{i+1}}^{n_{i}} = \sum_{a_i, a_{i+1}} U_{a_i, a_{i+1}}^{n_i} S_{a_{i+1}, a_{i+1}} / S_{a_{i}, a_{i}}, \quad (10)
\]

where \(S_{a_{i}, a_{i}}\) are the singular values on the \(i-1\) th bond. It is straightforward to verify that the new tensors \(B_{a_{i+1}, a_{i+2}}^{n_{i+1}}\) and \(B_{a_{i}, a_{i+1}}^{n_{i}}\) produced in Eqs.(9, 10) still satisfy the right canonical condition in Eq.(3). The division by very small singular values in Eq.(10) could make this algorithm numerically unstable, which could be overcome by the algorithm in [44] with very little additional effort.

In BosonSampling, only phase shifters and beam splitters are used. A phase shifter is a one-body operation, and a beam splitter is a two-body operation. Moreover, as in Fig. 1, the beam splitter acts only on nearest-neighbouring sites. Therefore the above operations would suffice for BosonSampling. We also note that the successive application of phase shifters and beam splitters to MPS would be analogous to the time-dependent matrix product states (t-MPS) algorithm [40, 45–47].

### A. Bosonic circuit

One important property of a optical bosonic circuit made of phaser shifters and beam splitters is that the total number of particles in the system is conserved. Namely if the input quantum state has a fixed total number of particles \(N\), then during the evolution, \(N\) is preserved. This means that we only need to consider the coefficients \(c_{n_1, n_2, \ldots, n_M}\) which satisfy

\[
\sum_{i=1}^{M} n_i = N. \quad (11)
\]

Without loss of generality, the initial state \(|\psi\rangle\) is chosen so that the first \(N\) modes have one photon as inputs, while for the rest there is no input photon. This state could be written as

\[
|\psi\rangle = |1\rangle^{N} \otimes |0\rangle^{M-N}. \quad (12)
\]

For this kind of circuit, we will make use of a specially designed MPS in presence of a global U(1) symmetry, which could often reduce the complexity of the numerical simulation drastically. We will not go into the details of the implementation of MPS in presence of a global U(1) symmetry. For a detailed technical description, one can refer to, for example, [48].

To this end, we note that in the literature the phase shifter and beam splitter are often written as linear mappings in the operator space, namely mapping from one quantum operator to another. To use them with MPS, one need to rewrite them as quantum operators which map one quantum state to another. A phase shifter with a rotation angle \(\phi\) can straightforwardly be written as

\[
U_{\text{ps}}^\theta(\phi)|n\rangle = e^{2\pi i n \phi}|n\rangle. \quad (13)
\]

For a beam splitter with an angle \(\theta\), it is usually written in the operator space as

\[
U_{\text{bs}}^\theta(\theta) \left( \begin{array}{c} \hat{a}^1 \hat{b}^1 \\ \hat{a}^2 \hat{b}^1 \end{array} \right) = \left( \begin{array}{cc} \cos(2\pi\theta) & -\sin(2\pi\theta) \\ \sin(2\pi\theta) & \cos(2\pi\theta) \end{array} \right) \left( \begin{array}{c} \hat{a}^1 \\ \hat{b}^1 \end{array} \right) \quad (14)
\]

where \(\hat{a}^1\) and \(\hat{b}^1\) are bosonic creation operators. Written as an operator on a quantum state \(|m, n\rangle\), it would be

\[
U_{\text{bs}}^\theta(m, n) = U_{\text{bs}}^\theta(\theta) \left( \begin{array}{c} \hat{a}^1 \\ \hat{b}^1 \end{array} \right) |0, 0\rangle = \left( \begin{array}{c} \cos(2\pi\theta) \hat{a}^1 - \sin(2\pi\theta) \hat{b}^1 \\ \sin(2\pi\theta) \hat{a}^1 + \cos(2\pi\theta) \hat{b}^1 \end{array} \right) |0, 0\rangle \quad (15)
\]

For example, for an input state \(|1, 1\rangle\), Eq.(15) will be

\[
U_{\text{bs}}^\theta(1, 1) = \sqrt{2} \cos(2\pi\theta) \sin(2\pi\theta) |2, 0\rangle - \sqrt{2} \cos(2\pi\theta) \sin(2\pi\theta) |0, 2\rangle + \cos^2(2\pi\theta) - \sin^2(2\pi\theta) |1, 1\rangle. \quad (16)
\]

### B. Fermionic circuit

In comparison with BosonSampling, FermionSampling is related to calculating determinants of matrices, for which there exists efficient classical algorithms. Nevertheless, it would still be insightful to see whether FermionSampling would be a difficult problem or not with MPS. The simulation of FermionSampling is done by mapping the fermionic circuit to a one-dimensional spin chain by the Jordan-Wigner transformation [49, 50]. As a result, the beam splitter for the fermionic operator \(U_{\text{bs}}^f\), in the zero- and one-particle sections, would remain the same as Eq.(15), while in the two-particle section, it is trivially

\[
U_{\text{bs}}^f(1, 1) = |1, 1\rangle, \quad (17)
\]

due to the fermionic anti-commutation relation.

### C. Lossy bosonic circuit

A lossy linear optical circuit could be modeled by a lossless circuit, but with input to be a mixed state instead of a pure state.
Such an input state can be written as
\[
\rho = \sigma^N \otimes |0\rangle \langle 0|^{M-N},
\]
where each \(\sigma\) is a local density operator. Here \(N\) means the largest possible total number of particles instead. To deal with this kind of input state with MPS, one could reshape \(\rho\) into a long vector which we denote as \(\|\rho\|\)
\[
|\rho\rangle = |\sigma\rangle^N \otimes |00\rangle^{M-N},
\]
the local Hilbert space would then be enlarged to \((N+1) \times (N+1)\). Correspondingly, any unitary gate \(U\) operating on the corresponding unitary system, will become
\[
U^o = \text{kron}(U, \text{conjugate}(U)).
\]
Here \(\text{kron}(a, b)\) means the kronecker product of two tensors \(a\) and \(b\).

We note that although the initial mixed state may not have a fixed total number of particles, the optical quantum circuit remains the same as the unitary case. Therefore, an MPS in presence of the \(U(1)\) symmetry could still benefit. In our simulations of the lossy cases, we have made use of this properties, which allows us to study an open system with \(D\) larger than 10000. For simplicity, in this work we focus on a special local mixed state \(\sigma\), which is
\[
\sigma = \bar{n}|1\rangle \langle 1| + (1-\bar{n})|0\rangle \langle 0|,
\]
\(\bar{n}\) is the average filling of bosons which satisfies \(0 \leq \bar{n} \leq 1\).

### III. RESULT

By simulating the multi-particle dynamics with MPS, we can visualize the evolution of physical quantities such as entanglement entropy through measurements. Entanglement is an elementary property of manybody quantum states and underlies the complexity of simulating quantum states on a classical computer. An important advantage of MPS is that one could explicitly monitor the growth of entanglement entropy \(S\) during the dynamics, which is defined as
\[
S = -\text{tr} [\rho_A \log(\rho_A)], \quad \rho_A = \text{tr}_B \rho.
\]

Here the subscripts \(A\) and \(B\) mean two subsystems resulting from a bipartition of the system, and the density operator \(\rho = |\phi\rangle \langle \phi|\) with \(|\phi\rangle\) being the wave function of the system.

In Fig. 2, we randomly simulate 100 samples for bosons and fermions with \(M = 20\) and \(N = 10\), to a maximum depth \(d_{\text{max}} = M = 20\). In Fig. 2(a) we plot the growth of entropy \(S\), which is averaged over those samples, with the evolution depth \(d\), for both the bosonic and the fermionic cases.

The entanglement entropy \(S\) of a quantum system has dramatical influence on our ability to simulate it on a classical computer. From the perspective of computational complexity, BosonSampling corresponds to calculating the matrix permanent, which is a hard problem, while FermionSampling corresponds to calculating the matrix determinant, which is an easy problem. Interestingly, this is also reflected in Fig. 2(a), we could see clearly that the entropy \(S\) of a bosonic circuit is much larger than that of a fermionic circuit as to both the absolute value and the increasing rate (For large \(d\) in the bosonic case the entropy already saturates, thus it increases slower), indicating that BosonSampling is much harder to classically simulate with MPS than FermionSampling.

In fact, it is very simple and natural to measure \(S\) during the dynamical process in the optical quantum circuit in Fig. 1. The singular values are stored alongside with the MPS whenever a two-body gate operation is performed, thus allowing to compute the entropy with almost no additional effort. We can simulate BosonSampling circuit with \(M = 26\), \(N = 13\) and \(d = 26\) in only about 5500s on a personal computer with 2 cores of 2.8 GHz frequency and 16 Gb memory, where we have measured the entropy \(S\) of each depth. We note that if we measure the entropy by first reconstructing the quantum state at each depth, we need to spend a huge amount of time to calculate all of the amplitudes of a quantum state. Moreover, it would require about 87 Gb memory on a classical computer if one stores all these amplitudes exactly. Concretely, a pure python program using the Ryser’s algorithm is able to compute the permanent of a matrix of size 13 in 0.09s. Taking into considerations the huge number of matrix permanents to be computed to reconstruct the quantum state, MPS will be \(10^9\) times faster than the Ryser’s algorithm. The acceleration effect is more obvious as the system size increases (see Fig. 3).

We also apply MPS to study BosonSampling in presence of losses, which is called lossy BosonSampling [51]. The hardness of MPS used to represent a density operator for an open quantum system can be evaluated by the operator space entan-
glement entropy (OSEE), which we denote as $S^o$ in comparison to the unitary case in Eq. (22). Mathematically, OSEE is defined as \[ S^o = -\text{tr}_A[R \log(R)], \quad R = \langle \rho \rangle^{-1} \text{tr}_B[\rho] \langle \rho \rangle. \] (23)

In Fig. 4, we plot the growth of $S^o$ with depth $d$ for different values of losses. We can see that the larger the loss is, the slower $S^o$ increases, that is, the corresponding quantum system is easier to be simulated with MPS. However, we note that $S^o$ is essentially a different concept than $S$ and does not represent the entanglement of a density operator [52]. It just characterizes the hardness of an density operator written as an MPS. Thus, we cannot study the difference between ideal BosonSampling and lossy BosonSampling by directly comparing the entanglement entropy $S$ and the OSEE $S^o$.

By analyzing the distribution of singular values in the final state, it is possible to make a rough estimation of the difficulty to simulate lossy BosonSampling with MPS. In Fig. 5, we plot the distribution of the singular values of the final state for the ideal BosonSampling, ideal FermionSampling, and lossy BosonSampling with $\bar{n} = 0.2, 0.6, 0.99$ respectively, where we have concatenated the singular values of 100 random samples. In general, for MPS related algorithms one would throw away singular values which are too small. Therefore the faster the singular values decay, the easier the quantum system is to be simulated with MPS. When the loss is small, such as $\bar{n} = 0.99$, the distribution of singular values of lossy BosonSampling is close to the ideal one. However, as the loss increases, the singular values decay faster. For BosonSampling with very large loss $\bar{n} = 0.2$, the singular values even decay faster than those of FermionSampling. These results indicate that when the loss is very low, simulating lossy BosonSampling is still hard for a classical computer, which is in correspondence with the theoretical results in Ref. [51]. On the contrary, if the loss is high enough, simulating lossy BosonSampling could even become easier than FermionSampling.

To this end, we note that MPS is an approximate representation of the quantum state, in that each time a two-body gate operation is performed, an SVD is done and the singular values under a threshold $\epsilon$ are thrown away. Therefore it is possible that such small errors during the evolution will accumulate after many steps of evolution. For the sampling problems, the number of two-body gate operations is approximately $M^2/2$. Thus in the worst case the error $\epsilon$ of our simulations would scale as

$$\epsilon \approx \frac{M^2 t}{2}. \quad \text{(24)}$$

For the case $M = 12$ and $N = 6$, the value of $\epsilon$ would be around $7.2 \times 10^{-7}$ at most. In Fig. 5(a), we plot the absolute error $\epsilon_{\text{abs}}^p$ and the relative error $\epsilon_{\text{rel}}^p$ between our MPS simulation and a classical program using the Ryser’s algorithm, which are defined as

$$\epsilon_{\text{abs}}^p = |\text{perm}^{\text{MPS}} - \text{perm}^{\text{Ryser}}| \quad \text{(25)}$$

$$\epsilon_{\text{rel}}^p = \frac{\epsilon_{\text{abs}}^p}{\text{perm}^{\text{Ryser}}}, \quad \text{(26)}$$

with $\text{perm}^{\text{MPS}}$ and $\text{perm}^{\text{Ryser}}$ to be the permanents computed with MPS and the Ryser’s algorithm. Similarly in Fig. 5(b), we plot the absolute error $\epsilon_{\text{abs}}^d$ and the relative error $\epsilon_{\text{rel}}^d$ between our MPS simulation and the det function from python to compute the determinant. The numerical difference between our results with the standard algorithm can
We could also increase this precision by a lower $t$, which would also mean that more resources would be required. The differences are sorted from large to small, and $j$ is the index of the sample. The system size for both cases are $M = 12$, $N = 6$.

![Graphs showing absolute and relative differences of determinants computed by MPS and a python function using the Ryser’s algorithm in the bosonic case.](image)

In summary, we have used MPS to study BosonSampling as a dynamical evolution of an optical quantum circuit. We monitor the entanglement entropy growth during the dynamical process, and find that the entropy of a bosonic circuit is much larger than that of a fermionic circuit as to both the absolute value and the increasing rate, which explains from a physical perspective why classically simulating BosonSampling is significantly more difficult than simulating FermionSampling. We have shown that MPS is more efficient than other algorithms to calculate the entanglement entropy at each depth of the optical quantum circuit. For example, for a system with $M = 26$, $N = 13$ and $d = 26$, MPS is about $10^6$ faster than a method which reconstructs the quantum state by computing all the matrix permanents. Moreover, we have also studied the BosonSampling showing that as the loss increases, the complexity of the classical simulation decreases. For large enough losses, BosonSampling could even be easier than FermionSampling. MPS provides a suitable platform to study universal multi-particle quantum walks. More investigations into interesting quantum phenomena in other types of multi-particle quantum walks could be carried out in future works. Other BosonSampling protocols that could significantly reduce the physical resource requirements, and validation methods based on high-order correlation measurements, such as the work in Ref. [27], could also be further investigated.

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