Classical Simulation of Boson Sampling Based on Graph Structure

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Classical simulation of boson sampling based on graph structure

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Boson sampling is a fundamentally and practically important task that can be used to demonstrate quantum supremacy using noisy intermediate-scale quantum devices. In this work, we present classical sampling algorithms for single-photon and Gaussian input states that take advantage of a graph structure of a linear-optical circuit. The algorithms' complexity grows as so-called treewidth, which is closely related to the connectivity of a given linear-optical circuit. Using the algorithms, we study approximated simulations for local Haar-random linear-optical circuits. For equally spaced initial sources, we show that when the circuit depth is less than the quadratic in the lattice spacing, the efficient simulation is possible with an exponentially small error. Notably, right after this depth, photons start to interfere each other and the algorithms' complexity becomes sub-exponential in the number of sources, implying that there is a sharp transition of its complexity. Finally, when a circuit is sufficiently deep enough for photons to typically propagate to all modes, the complexity becomes exponential as generic sampling algorithms. We numerically implement a likelihood test with a recent Gaussian boson sampling experiment and show that the treewidth-based algorithm with a limited treewidth renders a larger likelihood than the experimental data.

Sampling from the probability distributions of random quantum circuits is one of the problems to demonstrate quantum supremacy using noisy intermediate-scale quantum devices [1–5]. Boson sampling (BS) is one such sampling problem using linear-optical devices believed to be hard to classically simulate under some plausible assumptions [6, 7]. While a scale of experimental BS grows rapidly due to its importance [8–10], classical simulation algorithms taking advantage of current BS experiments' limitations are still restricted. Photon loss and distinguishability of photons are representative limitations, which have been extensively studied recently and shown to be detrimental to quantum advantages [11–17]. Another limitation of current experiments is that the number of modes is not sufficiently large to reach a collision-free BS, which may also reduce the complexity of classical simulation [18, 19].

In this Letter, we focus on limited connectivity of a linear-optical circuit. In general, typical global Haar-random linear-optical circuits' input and output modes are fully connected, which makes it hard to classically simulate. One possible implementation of global Haar-random circuits is to prepare local beam-splitter arrays [20], which corresponds to the current BS experiments' setup. However, a deviation from a global Haar-random unitary is apparent in the recent experiments [8, 9] because either the circuit depth is small or appropriate ensemble of beam splitters are not employed [21]. Hence, there is a chance that the connectivity of the circuit is limited and that sampling from the underlying system may not be as difficult as from a global Haar-random circuit.

We propose classical algorithms using dynamical programming [22, 23] taking advantage of a given circuit's limited connectivity for single-photon BS (SPBS) and Gaussian BS (GBS) [6, 7]. Particularly, our algorithms' complexity depends on connectivity of a relevant matrix's graph structure, characterized by the so-called treewidth [24]. Since the algorithms' complexity grows as the treewidth instead of the system size, we may be able to sample from some linear-optical circuits of a limited treewidth faster than generic classical algorithms. By applying our algorithm to local beam-splitter circuits, we analyze how the algorithms' complexity grows as a circuit depth and reveal a hierarchy of the complexity depending on the depth, namely, polynomial, sub-exponential, and exponential regimes.

Boson sampling.— Consider an M-mode bosonic system consisting of beam-splitter arrays characterized by a unitary matrix U with N identical sources. Specifically, the unitary matrix U represents the transformation of mode operators $\{\hat{a}_j\}_{j=1}^M$ as $\hat{a}_j^\dagger \to \hat{U}^\dagger \hat{a}_j^\dagger \hat{U} = \sum_{k=1}^M U_{jk}\hat{a}_k^\dagger$ for a given beam splitter circuit $\hat{U}$. Let $\mathcal{S} \equiv \{s_i\}_{i=1}^N \subset [M]$ be the set of input modes for identical sources. If we measure an output state $\hat{\rho}$ after beam splitters with the photon number basis $\hat{\boldsymbol{m}} = \otimes_{j=1}^M |m_j\rangle\langle m_j|$, the probability of an outcome $\boldsymbol{m} = (m_1, ..., m_M)$ is given by $P(\boldsymbol{m}) = \mathrm{Tr}(\hat{\rho}\hat{\boldsymbol{m}})$. For simplicity, we define an equivalent description of the output as $\boldsymbol{r} = (r_1, \ldots, r_N)$, where r_i's represent modes that click. For single-photon state input, the probability is written as [6]

$$P(\boldsymbol{m}) = \frac{|\mathrm{Per}(U_{\boldsymbol{r}}^{\mathcal{S}})|^2}{\boldsymbol{m}!} = \frac{1}{\boldsymbol{m}!}\left|\sum_{\sigma}\prod_{i=1}^{N} U_{r_i, s_{\sigma(i)}}\right|^2, \qquad (1)$$

where the sum is over all permutations σ. Here, $U_{\boldsymbol{r}}^{\mathcal{S}}$ is an $N \times N$ matrix obtained by choosing $\mathcal{S}$ columns and $\boldsymbol{r}$ rows, and $\mathrm{Per}(U)$ is the permanent of matrix U, which is related to counting bipartite perfect matchings in the

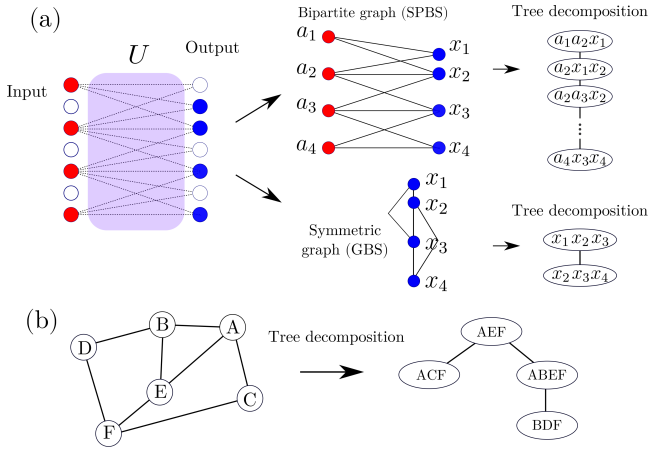

FIG. 1. (a) Input (red dots) and output (blue dots) photon configuration, corresponding bipartite and symmetric graphs and their tree decompositions of width $w = 2$. (b) Graph and its possible tree decomposition of width $w = 3$.

corresponding graph [25]. Meanwhile, for a squeezed vacuum state input, the probability of an outcome $\boldsymbol{m}$ is given by [7]

$$P(\boldsymbol{m}) = \frac{|\mathrm{Haf}(B_{\boldsymbol{m}})|^2}{\boldsymbol{m}!\sqrt{\det(V + \mathbb{1}/2)}}, \tag{2}$$

where $B_{\boldsymbol{m}}$ is a matrix obtained by repeating ith column and row of $B \equiv UDU^{\mathrm{T}}$ for m_i times, and $\mathrm{Haf}(B_{\boldsymbol{m}})$ is the hafnian of matrix $B_{\boldsymbol{m}}$, which is related to counting perfect matchings in the corresponding graph [26]. Here, $D \equiv \oplus_{j=1}^{M} \tanh r_j$, and V is the output state's the covariance matrix. Squeezing parameters are given by $r_j = r$ for $j \in \mathcal{S}$, and $r_j = 0$ otherwise.

Let us clarify the relation between graphs and BS (see Fig. 1 (a)). To compute the (marginal) probability for an outcome, we consider all possible paths from input photons to the output configuration, which essentially corresponds to interference. They can be described by all perfect matchings of a bipartite graph of $U_{\boldsymbol{r}}^{\mathcal{S}}$ with the input modes $\mathcal{S}$ and output modes $\boldsymbol{r}$ being bipartite vertex sets and the paths between them being edges for SPBS. For GBS, vertices of a symmetric graph of $B_{\boldsymbol{m}}$ consist of an output-photon configuration, and two vertices have an edge if the two photons can come from the same source. To compute a probability in this case, we consider all possible perfect matchings of output photons, which corresponds to finding sources from which each pair of photons come. From this observation, when a given unitary matrix's connectivity is limited, we can expect that the number of possible perfect matchings for each outcome is small so that the induced graphs' structure allows to reduce the complexity.

Computing permanent and loop hafnian using dynamical programming.— Before presenting sampling algorithms, we first introduce classical algorithms computing the permanent and loop hafnian of a matrix. Here, loop hafnian is generalized hafnian, related to counting perfect matchings including loops [27, 28], which is necessary for the sampling algorithm below. The complexity of the best-known algorithms computing the permanent and loop hafnian of a general $N \times N$ matrix scales as 2^N and $2^{N/2}$, respectively [29, 30]. Meanwhile, there are also various algorithms exploiting a matrix's structures [27, 31, 32]. A particularly interesting algorithm is dynamical programming that computes permanent [23]. A high-level idea of the algorithm is to construct tree decomposition of bipartite graph for a given matrix, which reveals the matrix's structure (see Fig. 1). The algorithm's complexity grows as so-called treewidth, which measures connectivity by exploiting the treelike structure of the graph [22]. We generalize the treewidth-based algorithm to loop hafnian by using tree decompositions for a given symmetric matrix and present the following lemma, including the result in Ref. [23] as:

Lemma 1. If the treewidth of a graph representation of an $N \times N$ matrix is w, then dynamical programming can compute its permanent and loop hafnian in $O(Nw^2 2^w)$.

We provide the proofs of Lemmas and Theorems in Ref. [33]. Notably, Lemma 1 shows that the complexity's exponent does not scale as the matrix size N but the treewidth w. Therefore, for some structured matrices, the complexity of computing their permanent or loop hafnian can be highly reduced. For example, a forest, i.e., disjoint union of trees, has treewidth 1 [34], so the complexity does not grow exponentially as matrix size. On the other hand, a complete graph, whose vertices are all connected, has the treewidth $N - 1$ (N for bipartite complete graph) [34]. Note that we recover the same exponent of the algorithm for a general matrix, i.e., 2^N, for permanent whereas it has a gap for loop hafnian ($2^{N/2}$ for general loop hafnian) [27, 30].

Classical sampling algorithms based on treewidth.— We now introduce classical sampling algorithms of SPBS and GBS using limited connectivity. Although we have algorithms computing permanent or loop hafnian using a given graph's structure, how to use such algorithms for sampling is not clear. Remarkably, we show that if we employ as a main routine chain rule of marginal probabilities, such as the Clifford-Clifford algorithm [35] for SPBS, and a recently proposed GBS algorithm [36], and use our dynamical programming to compute permanent or loop hafnian as a subroutine, we can fully utilize the graph structure of a given circuit including computing marginal probabilities [33]. For simplicity, we focus on collision-free events, i.e., $m_i = \{0, 1\}$, while we provide algorithms for collisions in Ref. [33].

Theorem 1. (Classical sampling algorithm) If the treewidths of bipartite graphs of $U_{\boldsymbol{r}}^{\mathcal{S}}$ are at most w for all possible outcome $\boldsymbol{r}$, we can classically simulate SPBS in $O(MN^2w^2 2^w)$. Similarly, if symmetric graphs of $B_{\boldsymbol{m}}$

have the treewidths at most w for all outcomes $\boldsymbol{m}$, we can classically simulate GBS in $O(MNw^2 2^w)$.

Theorem 1 enables us to recover and generalize some previously known results. One such example is efficient simulability of shallow 1D GBS, i.e., depth $D = O(\log M)$ by using limited bandwidth of the circuit's unitary matrix [37, 38]. Since bandwidth is a special case of treewidth, we recover the result and also find that the result holds for 1D SPBS. For 2D cases, however, even for a constant depth, we encounter with an output described by a graph including $\sqrt{N} \times \sqrt{N}$ grid, whose treewidth is $w = \sqrt{N}$ [33, 39]. This is consistent with the recent hardness result of high-dimensional GBS [40].

Approximate sampling.— When an approximation of a given circuit has limited connectivity, we can expect that an approximate sampling is possible using this structure. However, it is not straightforward to apply the same method if we approximate the circuit matrix by a nonunitary matrix because the corresponding process or the output state may no longer be physical. Also, the chain-rule-based algorithms implicitly assume unitarity of the process or a legitimate quantum state. We present a method to overcome this by introducing additional virtual M modes to make the process physical again and investigate its approximation error in Ref. [33]:

Theorem 2. (Approximate sampling) If a circuit unitary matrix U is approximated by $U - dU$, one can implement sampling with the same complexity up to constant as Theorem 1 with an error of $\mathrm{poly}(N, \|dU\|_F^{1/4})$.

We assess a simulation's error by total variation distance $\sum_{\boldsymbol{m}} |P(\boldsymbol{m}) - P_a(\boldsymbol{m})|/2$ between an ideal probability distribution $P(\boldsymbol{m})$ and a classical algorithm's output probability distribution $P_a(\boldsymbol{m})$ and desire an approximation error to be $O(1/\mathrm{poly}(N))$. In the following section, we study an experimentally relevant physical model, which is local Haar-random circuits. Since a current GBS experiment does not employ a specialized ensemble to implement a global Haar-random circuit [9], its setup can be considered as a typical instance of the model. Also, it can be interpreted as an extreme case where beam splitters' reflectivities have a large uncertainty. We emphasize that our approximation method in Theorem 2 is straightforwardly applicable to similar dynamics (e.g. Ref. [41]).

Approximate sampling for local Haar-random circuits.— Consider N identical sources equally distributed in $M = kN^\gamma$ modes of a d-dimensional lattice [42] and local Haar-random beam-splitter arrays, as illustrated in Fig. 2. The lattice consists of d-cube sublattices of edge length $L = (M/N)^{1/d}$, containing a single source. For simplicity, let L be a positive integer.

As recently studied, random beam-splitter arrays can be characterized by a classical random walk [43]. Therefore, photons propagate diffusively on average. Using this property, we find an upper-bound on the leakage

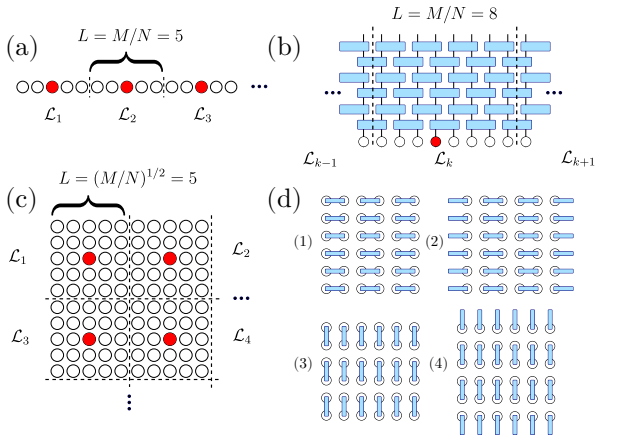

FIG. 2. Initial state in (a) 1D and (c) 2D architectures. Red dots represent sources. $\mathcal{L}_\alpha$ represents a sublattice having a single source s_α. Beam-splitter arrays in (b) 1D and (d) 2D architecture. A single round consists of four steps (1)-(4). The structure can be generalized for d-dimensional architecture, where a single round consists of $2d$ steps.

rate from a source at s_α up to κL denoted as $\eta_\alpha(\kappa) \equiv \sum_j |U_{j,s_\alpha}|^2$, where j is the sum over modes away from α more than κL:

Lemma 2. For depth $D \leq dk^{2/d}\kappa^2 N^{2(\gamma-1)/d-\epsilon}/2$ with $\epsilon > 0$, the leakage rate η_α to distance κL is bounded from above as

$$\eta_\alpha(\kappa) \leq \exp(-N^\epsilon) \tag{3}$$

with a probability $1 - \delta$ over Haar-random beam-splitter arrays, where δ is exponentially small in N.

For later usage for $d = 1$, we note that the same inequality holds for $D \leq k^2\kappa^2 N^{2(\gamma-1)-\epsilon}(\log N)^2/2$ for leakage rate to distance $\kappa L \log N$. Motivated by Lemma 2, our approximate sampling strategy is to discard the elements of a unitary matrix that are geometrically farther from sources than κL, i.e., $U \to \tilde{U} \equiv U - dU$ and implement Theorem 2. Since $\|dU\|_F^2 = \sum_{\alpha\in\mathcal{S}} \eta_\alpha(\kappa)$ is exponentially small, the sampling error is too. From now on, we focus on typical circuits, emphasizing that the portion of atypical circuits is exponentially small.

Consider a special case ($\kappa = 1/2$) where interference between photons from different sources is negligible typically. In this case, for SPBS, possible outputs can be described by a disconnected graph, in which at most two vertices are connected; thus, the treewidth is 1. For GBS, assuming that a single source emits constant number of photons at most, graphs describing possible outcomes are again disconnected with constant number of vertices and have bounded treewidth. One may also show that sampling for this regime is easy by noting that the hafnian of a low-rank matrix can be efficiently computed without the assumption [27]. Thus,

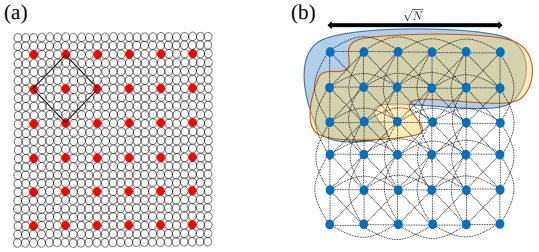

FIG. 3. GBS on 2D lattice with $N = 36$, $M = N^2$, and $\gamma = 2$. (a) Red dots represent initial sources. Black solid line describes the region at which a particular input photon can typically propagate for $D = \Theta(L^{2(1-\epsilon)}) = \Theta(N^{1-\epsilon})$. (b) Possible tree decomposition of the symmetric graph $B_{\boldsymbol{m}}$ when outputs are at the same position with input sources. An upper bound on the treewidth is $\Theta(\sqrt{N})$ as shown: the first bag (blue) and the second one (yellow).

Theorem 3. (Efficient-sampling regime) Approximate BS can be efficiently performed for typical circuits of depth $D \leq D_{\text{easy}} \equiv dk^{2/d}N^{2(\gamma-1)/d-\epsilon}/8 = \Theta(N^{2(\gamma-1)/d-\epsilon})$. Especially for $d = 1$, the upper bound becomes $D \leq k^2\kappa^2 N^{2(\gamma-1)-\epsilon}(\log N)^2/2$.

We note that the distinct upper-bound for 1D arises because the treewidth $O(\log N)$ can be efficiently simulated.

After $D > D_{\text{easy}}$ (or $\kappa > 1/2$), photons from a sublattice can now propagate to other lattices so that photons from different sources start to interfere (see Fig. 3 (a)). Thus, induced graphs have edges between sources and photons from different sublattices (SPBS) or photons from different sources (GBS) as shown in Fig. 3 (b). In this case for 2D architecture, there exists an outcome corresponding to a graph containing a grid whose treewidth is unbounded, i.e., $w = \sqrt{N}$. Therefore, the sampling complexity starts to scale exponentially in $\sqrt{N}$ [33], which reveals a sharp transition of the complexity at $D = D_{\text{easy}}$ from polynomial to sub-exponential. Similarly, when photons propagate further and for arbitrary dimension, i.e., $D = \Theta(N^{2\alpha/d}D_{\text{easy}})$ with $0 \leq \alpha \leq 1$ (equivalently $\kappa = \Theta(N^{\alpha/d})$), we can find a tree decomposition whose width is $\Theta(N^{\frac{\alpha}{d}+\frac{d-1}{d}})$ for any outcomes. Therefore, we have the following theorem:

Theorem 4. ((sub-)exponential regime) One can sample from typical linear-optical circuits of $D = \Theta(N^{2\alpha/d}D_{\text{easy}})$ with $0 \leq \alpha \leq 1$ by complexity $O(\text{poly}(N)2^{\Theta(N^{\frac{\alpha}{d}+\frac{d-1}{d}})})$.

Especially when $\alpha = 1$, any photons can propagate to all modes, i.e., photons fully interfere each other, which forms the complete graph for all outcomes, so that treewidth becomes $\Theta(N)$. Since generic global Haar-random circuits are fully connected, at least $\Theta(N^{2\gamma/d}) = \Theta(M^{2/d})$ order of depth is required to implement a global Haar-random circuit using a local Haar-random circuit and such an input configuration. Fig. 4 summarizes the result.

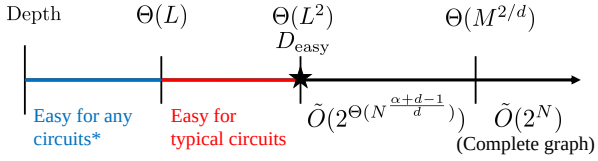

FIG. 4. The complexity diagram for local Haar-random BS. As the star-marked, a sharp transition occurs for the complexity of our algorithm. Easiness for any circuits (*) is proved in Ref. [41]. Note that for 1D, the depth that is easy for typical circuits is larger (see Theorem 3).

Interestingly, the recent GBS experiments' circuit depth scales as $\sqrt{M}$ [9, 10], which implies that their circuit is not sufficient to form a global Haar-random circuit. Nevertheless, aside from the deviation from global Haar-random matrices, locality in their circuit is not apparent because the scale is intermediate while our analysis focuses on an asymptotic regime. Therefore, our approximate algorithm might result in a large simulation error for this intermediate-scale GBS because of a large constant factor of the error.

One may also consider other initial configurations under local Haar-random circuits, for example sources are concentrated on a certain region. We show that for those cases, one already needs a depth $D = \Theta(ND_{\text{easy}})$ to reach collision-free regime, and thus collision occurs with a high probability, while equally spaced sources reach the collision-free regime when $D = \Theta(D_{\text{easy}})$ [33].

GBS validation test.— Finally, we implement the likelihood test to experimental samples [10] against samples generated by our treewidth-based approximate algorithm:

$$\text{ratio} \equiv \log \frac{\Pr_{\text{ideal}}(\text{Samples from experiment})}{\Pr_{\text{ideal}}(\text{Samples from treewidth algorithm})}, \tag{4}$$

which is equivalent to the test implemented in Refs. [9, 10]. Thus, we compare the likelihood of each sample set with respect to the (lossy) ideal probability distribution.

For the treewidth algorithm, we have approximated local Haar-random with limited propagation (see Fig. 5 (a)) and sampled from the approximated circuit using Theorem 2. Specifically, we have rearranged the 144 modes one-dimensionally and set a propagation length K for approximation. Note that setting a propagation length K implies that the corresponding GBS's treewidth is $w = 2K+1$ and that a complete graph has a treewidth $w = M$. To compensate the lost photons from the approximation, we have increased the squeezing parameters and thermal photons to have the same average total photon numbers.

In Fig. 5 (b), we present the likelihood ratio as the

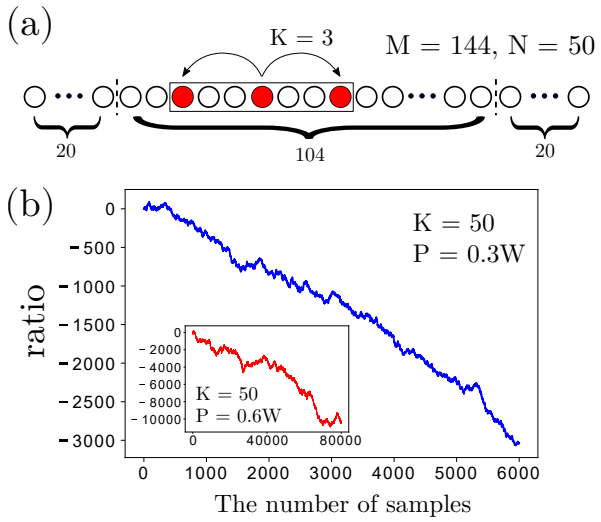

FIG. 5. Likelihood test for the recent GBS experiment [10]. (a) Rearranged mode-configuration with squeezed states sources (red dots). For approximated sampling, we discard elements of a circuit matrix U that is farther than K for the sources. (b) Log-likelihood ratio of experimental samples against those from the treewidth algorithm.

number of samples increases for two classically verifiable instances of the experiments in Ref. [10]. It clearly shows that the treewidth-based approximate algorithm renders larger likelihood than the experiment. We also provide evidence in Ref. [33] for GBS experiments in the quantum supremacy regime by investigating the likelihood ratio for marginals that the treewidth-based algorithm might give a larger likelihood with a limited treewidth. Therefore, the numerical results imply that a fully connected circuit is crucial for more rigorous quantum-advantage demonstration.

Discussion.— We have presented classical samplers taking advantage of limited connectivity of a circuit. It is an interesting open question to find more efficient sampling algorithms than the one based on the treewidth. Another open problem is to close the gap of complexity for computing loop hafnian between the treewidth-based algorithm (2^N) and the best-known algorithm ($2^{N/2}$) [36].

Finally, Theorem 3 shows that typical linear-optical circuits up to depth $D \leq D_{\text{easy}} = \Theta(N^{\frac{2}{d}(\gamma-1)-\epsilon})$ allow an efficient classical simulation except for an exponentially small fraction of random circuits. Meanwhile, there exists a circuit hard to classically simulate for $D = \Omega(N^{\frac{\gamma-1}{d}+\epsilon})$ under reasonable complexity-theoretic conjectures [6, 41, 44]. Theorem 3 can be compatible with the hardness results since together the implication is that the worst-case instances occupy only at most an exponentially small faction of the space of all linear optical circuits.

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