Efficient classical simulation of matchgate circuits with generalized inputs and measurements

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Matchgates are a restricted set of two-qubit gates known to be classically simulable under particular conditions. Specifically, if a circuit consists only of nearest-neighbor matchgates, an efficient classical simulation is possible if either (i) the input is a computational-basis state and the simulation requires computing probabilities of multiqubit outcomes (including also adaptive measurements) or (ii) if the input is an arbitrary product state, but the output of the circuit consists of a single qubit. In this paper we extend these results to show that matchgates are classically simulable even in the most general combination of these settings, namely, if the inputs are arbitrary product states, if the measurements are over arbitrarily many output qubits, and if adaptive measurements are allowed. This remains true even for arbitrary single-qubit measurements, albeit only in a weaker notion of classical simulation. These results make for an interesting contrast with other restricted models of computation, such as Clifford circuits or (bosonic) linear optics, where the complexity of simulation varies greatly under similar modifications.

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I. INTRODUCTION

Matchgates are a class of restricted two-qubit gates with intriguing computational capabilities. Circuits composed of matchgates acting on nearest-neighboring qubits (on a linear array) were shown to be classically simulable by Valiant [\[1\]](#page-8-0) and soon after shown to correspond to free fermions by Terhal and DiVincenzo [\[2\]](#page-8-0). Several other papers investigated the classical simulation of matchgates through different formalisms [\[3–7\]](#page-8-0). However, matchgates also can become universal for quantum computation by the addition of seemingly simple resources. They were shown to be universal when supplemented by the SWAP gate $[6,8]$, by some two-qubit nondemolition measurements [\[9\]](#page-8-0), by specific multiqubit magic states [\[10\]](#page-8-0), by almost any parity-preserving two-qubit gate [\[11\]](#page-8-0), and on any connectivity graph that is not a path or a cycle [\[12,13\]](#page-8-0).

In this paper, we are interested in how the complexity of simulating matchgates depends on restrictions on the inputs and outputs of the circuit. More concretely, we restrict our attention to circuits composed only of nearest-neighbor matchgates and modify the computational model by allowing different types of input states and different restrictions on the size of the output. This is motivated by apparent differences between two previous results: that of Valiant [\[1\]](#page-8-0) and Terhal and DiVincenzo [\[2\]](#page-8-0), where the matchgate circuits act only on computational-basis inputs but any number of qubits can be measured at the end, and that of Jozsa and Miyake [\[6\]](#page-8-0), where the circuit can act on arbitrary product inputs but the output consists of the measurement of a single qubit. Each of these settings was chosen with a specific application in mind, and it is not *a priori* clear whether there is a common cause for the simulability of the different resulting computational models. Here we argue that it is indeed possible to unify these results; we show that matchgates can be simulated classically even if the input is in an arbitrary product state and the output consists of measurements of arbitrary subsets of the qubits, and this remains true even if one is allowed to adapt subsequent gates depending on intermediate measurement outcomes. By considering a weaker, sampling-based, classical simulation,

Besides refining our understanding of the computational power of matchgates, our results have other consequences that may be of more general interest. The first is that they provide a no-go result for some types of magic-state injection protocols, namely if the magic states are singlequbit states. More specifically, universal quantum computation with nearest-neighbor matchgates is possible when certain auxiliary multiqubit states are available [\[10\]](#page-8-0). However, since we show that matchgates are simulable for arbitrary product inputs and adaptive measurements, this rules out a scheme similar to that of $[10]$ that only uses single-qubit ancillae. Noticeably, since the previous simulations were restricted to either computational-basis inputs or single-qubit outputs, they could not be used to make this argument.

Our results can also be used to sharpen comparisons between matchgates and other restricted models of quantum computation. We are especially interested in two examples: Clifford circuits and (bosonic) linear optics.

Clifford circuits are a particular class of quantum circuits widely known to be classically simulable under certain conditions [\[14\]](#page-8-0), with some similarities to matchgates [\[7\]](#page-8-0). However, several results have made it clear that the complexity of Clifford circuits is heavily dependent on the combined choices of inputs and outputs that the circuit has access to. The "complexity landscape" of Clifford circuits has recently been mapped out in $[15]$, where the authors consider all combinations of (i) computational basis versus arbitrary product inputs; (ii) single-qubit versus multiqubit measurements; (iii) adaptive versus nonadaptive measurements; and (iv) weak versus strong simulation. The authors find that, by varying these conditions, the complexity of simulating Clifford circuits can go from (sub-)classical, to BQP-hard (i.e., as hard as the hardest problems solvable by a universal quantum computer), to #*P*-hard (cf. Fig. 1 in [\[15\]](#page-8-0)). This has also been extended to include arbitrary single-qubit measurements and different notions of strong simulation [\[16\]](#page-8-0). Our results consist, in a fashion, of a similar mapping of the complexity landscape of matchgate circuits, but with strikingly less diverse results; matchgates are classically simulable in all possible combinations of the choices of [\[15\]](#page-8-0) and almost all of those in [\[16\]](#page-8-0).

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we are also able to extend these results to the case where measurements can be performed in arbitrary single-qubit bases.

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Matchgates are also often compared to linear optics, due to a common underlying physical connection. While linear optics is identified with noninteracting bosons, matchgates are often identified with noninteracting fermions (indeed, sometimes referred to as "fermionic linear optics"). The mathematics behind linear optical circuits and matchgate circuits are surprisingly similar in some aspects (a point we return to often throughout the paper; see also discussions in $[2,3]$) but, while matchgate circuits are classically simulable, linear optics is not (see, e.g., [\[17\]](#page-8-0) for the KLM scheme for universal quantum computing with adaptive linear optics or [\[18\]](#page-8-0) for a model based on nonadaptive linear optics known as BosonSampling). However, these statements can be misleading if made without care; the separation in computational power between bosons and fermions is clear in the multiqubit output setting, but if one is restricted to a single-output measurement, then bosonic linear optics can be simulated [\[19\]](#page-8-0) in almost the same way as matchgates [\[7\]](#page-8-0). With the investigation we undertake here, we aim to shed further light on this comparison.

Finally, we believe that our results could also be used to inform the search for classical models of matchgates. More specifically, recent results have shown that both Clifford circuits [\[20\]](#page-8-0) and linear-optical systems [\[21\]](#page-8-0), if constrained enough, can admit a classical probabilistic description. In other words, it is possible to construct hidden variable models for these systems which would preclude not only a computational speedup, but also other signature quantum features such as contextuality [\[22\]](#page-8-0). The classical simulability of matchgates raises the natural question of whether a similar classical model can be constructed for these circuits, and the results obtained here could guide this search by suggesting sets of states and measurements that are more likely to introduce nonclassical behaviors.

This paper is organized as follows. In Sec. II we give some preliminary definitions and background discussions. More specifically, in Sec. II A we describe the Jordan-Wigner transformation and the mapping between matchgates and fermions, and in Sec. [II B](#page-2-0) we define a few different notions of classical simulation that we need. In Sec. ΠC we give a brief outline of the simulation obtained by Valiant [\[1\]](#page-8-0) and Terhal and DiVincenzo [\[2\]](#page-8-0), and in Sec. [II D](#page-3-0) we do the same for the simulation of Jozsa and Miyake [\[6\]](#page-8-0). In Sec. [III](#page-4-0) we prove our main result, which generalizes the two results discussed in the preceding sections, and discuss some possible extensions. We finish with some concluding remarks in Sec. [IV,](#page-6-0) as well as several open questions. The paper also contains an appendix with some further technical details omitted from the main text.

Notation. We denote X_i , Y_i , and Z_i the usual Pauli matrices acting on qubit *i*, and we omit tensor product signs throughout. We denote the anticommutator by ${A, B} = AB + BA$. We denote the all-zeroes state on *n* qubits by $|\bar{0}_n\rangle = |00 \cdots 0\rangle$.

Throughout this paper, we interchangeably refer to (unitary) quantum gates and their generating Hamiltonian. Since we always consider quantum computations in the circuit model (i.e., in a discrete-time description), whenever we refer to a gate by its generating Hamiltonian, we in fact mean any unitary in the family generated by that Hamiltonian.

Finally, throughout the paper we use the following three acronyms to describe three types of circuit: CI-MO (computational input and multiqubit output), PI-SO (product input and single-qubit output), and PI-MO (product input and multiqubit output). The precise corresponding definitions can be found in Sec. [II B.](#page-2-0)

II. BACKGROUND

A. Preliminary definitions: The Jordan-Wigner transformation

Let us begin with the following definition.

Definition 1: Matchgates. Let *G*(*A,B*) be the two-qubit gate given by

$$
G(A,B) = \begin{pmatrix} A_{11} & 0 & 0 & A_{12} \\ 0 & B_{11} & B_{12} & 0 \\ 0 & B_{21} & B_{22} & 0 \\ A_{21} & 0 & 0 & A_{22} \end{pmatrix}.
$$
 (1)

Then $G(A, B)$ is a *matchgate* if det $A = \det B$.

The set of all two-qubit gates $G(A, B)$ acting on qubits $\{i, j\}$ corresponds to those generated by

$$
\mathcal{A}_{i,j} = \{X_i X_j, X_i Y_j, Y_i X_j, Y_i Y_j, Z_i, Z_j\}.
$$
 (2)

It is well known that the operators in $A_{i,i+1}$ are closely connected to the physics of noninteracting fermions. To see that, let us define the following Jordan-Wigner operators [\[23\]](#page-8-0) acting on *n* qubits,

$$
a_j^{\dagger} := \left(\prod_{k=1}^{j-1} Z_k\right) \left(\frac{X_j - iY_j}{2}\right),\tag{3a}
$$

$$
a_j := \left(\prod_{k=1}^{j-1} Z_k\right) \left(\frac{X_j + iY_j}{2}\right),\tag{3b}
$$

for $j \in \{1, \ldots, n\}$. These operators satisfy the anticommutation relations one would expect for fermionic operators,

$$
\{a_i^\dagger, a_j^\dagger\} = 0,\tag{4a}
$$

$$
\{a_i, a_j\} = 0,\t\t(4b)
$$

$$
\{a_i, a_j^{\dagger}\} = \delta_{i,j},\tag{4c}
$$

for all $i, j \in \{1, ..., n\}$. If we identify states $|0\rangle$ and $|1\rangle$ of qubit *i* with the empty and occupied states of fermionic mode *i*, respectively, then a_i^{\dagger} (a_i) behaves precisely as a fermionic creation (annihilation) operator. From Eqs. (3) we also obtain

$$
Z_k = (a_k^{\dagger} - a_k)(a_k + a_k^{\dagger})
$$
 (5)

for $k \in \{1, \ldots, n\}$ and

$$
X_k X_{k+1} = -(a_k - a_k^{\dagger})(a_{k+1} + a_{k+1}^{\dagger}), \tag{6a}
$$

$$
Y_k Y_{k+1} = (a_k + a_k^{\dagger})(a_{k+1} - a_{k+1}^{\dagger}), \tag{6b}
$$

$$
Y_k X_{k+1} = i(a_k + a_k^{\dagger})(a_{k+1} + a_{k+1}^{\dagger}), \tag{6c}
$$

$$
X_k Y_{k+1} = i(a_k - a_k^{\dagger})(a_{k+1} - a_{k+1}^{\dagger}), \tag{6d}
$$

for $k \in \{1, \ldots, n-1\}$. Equations (5) and (6) connect the generators of *nearest-neighbor* matchgates, $A_{i,i+1}$, precisely to quadratic fermionic Hamiltonians.

To avoid ambiguity, we should point out that the notion of locality is not preserved by the Jordan-Wigner transformation. In particular, a quadratic operator acting between distant

fermionic modes, e.g., $(a_1 - a_1^{\dagger})(a_3 + a_3^{\dagger})$, maps to the multiqubit operator $X_1Z_2X_3$, not to the two-qubit matchgate X_1X_3 . In fact, the most general multiqubit operators obtained from quadratic fermionic operators are $A_i Z_{i+1} Z_{i+2} \cdots Z_{j-1} B_j$, for $i < j$, where *A* and *B* are either *X* or *Y*. Since any such Hamiltonian can be implemented by a poly-sized circuit of nearest-neighbor matchgates, $\frac{1}{1}$ as shown in [\[6\]](#page-8-0), they are (computationally) equivalent to nearest-neighbor matchgates. In contrast, almost any gate generated by $A_{i,j}$, where *i* and *j* are non-neighboring qubits, leads to universal quantum computation [\[13\]](#page-8-0). In light of these considerations, unless stated otherwise, throughout this paper we restrict our attention to circuits of *nearest-neighbor* matchgates in the qubit picture or quadratic fermionic operators between *arbitrary pairs of modes* in the fermionic picture, keeping in mind that these are computationally equivalent.

A consequence of this observation, which will be useful later on, is that the overall ordering of the qubits is irrelevant. More specifically, given any circuit of nearest-neighbor matchgates *M*, we can find the corresponding transformation in the fermionic picture, apply some permutation *P* on the labels of the fermionic modes, then map everything back to the qubit picture to obtain a different circuit *M* . However, by the considerations of the previous paragraph, the new circuit *M'* can be decomposed as a circuit of matchgates with only polynomial overhead, and furthermore these matchgates now act between nearest neighbors according to the relabeling of the qubits induced by the permutation *P*.

An important property of quadratic gates, which is crucial to the classical simulation schemes that follow, is that they act *linearly* on creation and annihilation operators (hence, matchgates are often called fermionic linear optics). More specifically, if *M* is a unitary operator corresponding to a circuit of nearest-neighbor matchgates, then we can write (for a simple proof, see [\[6\]](#page-8-0))

$$
Ma_i^{\dagger} M^{\dagger} = \sum_{j=1}^n R_{ij} a_j^{\dagger} + \sum_{j=1}^n R'_{ij} a_j.
$$
 (7)

If *M* further only consists of "number-preserving" matchgates, i.e., those $G(A, B)$ for which *A* is diagonal,² then $R' = 0$. Curiously, an analogous version of Eq. (7) also holds for *bosonic* linear optics; thus, we expect that, even if Eq. (7) is behind the classical simulability of matchgates, it cannot be the whole story. We return to this point several times as we discuss the different types of simulation results throughout this section.

B. Preliminary definitions: Classical simulation

Before moving to our main result, let us define precisely what is meant by classical simulation. In particular, suppose

our model of computation consists of a uniform family of quantum circuits, $\{C_n\}$, which act on yet-unspecified *n*-qubit input states $|\psi_n\rangle$. Suppose also that the circuits are followed by measurements of some subset of *k* of the *n* qubits in the computational basis. Then, for any *k*-bit string \tilde{y} corresponding to some assignment of the *k* measured qubits, we write the probability of observing measurement outcome $|\tilde{y}\rangle$ as

$$
Pr(\tilde{y}|\psi_n) = \text{tr}\,\langle \tilde{y}|C_n|\psi_n\rangle \langle \psi_n|C_n^{\dagger}|\tilde{y}\rangle,\tag{8}
$$

where the partial trace is taken over the unmeasured qubits. We can now divide our notions of classical simulation into a few convenient types (this is not an exhaustive list; see [\[25,26\]](#page-8-0) for more detailed discussions).

Definition 2: Strong simulation. The uniform family of quantum circuits $\{C_n\}$, acting on the *n*-qubit input state $|\psi_n\rangle$, is *strongly simulable* if, for every assignment of *k* output qubits \tilde{y} , and for every *k*, it is possible to compute $Pr(\tilde{y}|\psi_n)$ to *m* digits of precision in $poly(n,m)$ time on a classical computer.

Definition 3: Weak simulation. The uniform family of quantum circuits $\{C_n\}$, acting on the *n*-qubit input state $|\psi_n\rangle$, is *weakly simulable* if, for every choice of *k* out of *n* qubits to be measured, for every *k*, it is possible to produce a sample from the probability distribution defined by $Pr(\tilde{y}|\psi_n)$ in poly(*n*) time on a classical computer.

Note that, as defined, strong simulation implies weak simulation. 3 Weak simulation is often considered to be more physically motivated, since any quantum device only outputs samples from a probability distribution, and requiring a classical device to compute the probabilities to high precision does not make for a fair comparison of their respective computational powers. On the other hand, for part of the cases considered in this paper, it will be simple enough to prove that strong simulation is possible. We also define two variants of the above.

Definition 4: Single-output strong simulation. The uniform family of quantum circuits $\{C_n\}$, acting on the *n*-qubit input state $|\psi_n\rangle$, is *strongly simulable with a single output* if the quantity $\langle \psi_n | C_n^{\dagger} Z_i C_n | \psi_n \rangle$, for any $1 \leq i \leq n$, can be computed to m digits of precision in $poly(n,m)$ time on a classical computer. Note that $\langle \psi_n | Z_i | \psi_n \rangle = p_i(0) - p_i(1)$, where $p_i(j)$ is the probability that qubit *i* will be measured in state $|j\rangle$.

This definition is useful if one wants to characterize some restricted computational model in terms of the *decision problems* it can solve (i.e., problems with a single "yes" or "no" answer), where the answer to the problem is encoded in a single output qubit.

Definition 5: Adaptive simulation. Let $\{C_n\}$ be a uniform family of *adaptive* quantum circuits, that is, quantum circuits where one is allowed to make intermediate measurements and condition subsequent operations on their outcomes. Then ${C_n}$, acting on the *n*-qubit input state $|\psi_n\rangle$, is *adaptively simulable* if (i) all intermediate measurements can be weakly simulated (in the sense of Definition 3) and (ii) the final measurements on the circuit determined by the outcomes of (i) can be strongly simulated.

¹This is the fermionic analogue of the well-known fact that any photonic interferometer can be decomposed in terms of $O(n^2)$ nearestneighbor beam splitters [\[24\]](#page-8-0).

²Equivalently, those corresponding to quadratic operators restricted to the combinations $a_j a_k^{\dagger}$ and $a_k a_j^{\dagger}$, or matchgates generated by $X_k X_{k+1} + Y_k Y_{k+1}, X_k Y_{k+1} - Y_k X_{k+1}$, and Z_k .

³However, the reverse is not true, since there are examples for which weak simulation is easy, but strong simulation is #*P*-hard [\[25\]](#page-8-0).

We presented this hybrid definition of classical simulation to capture more closely the workings of an adaptive protocol: The complete circuit is not known at the beginning of the computation, as it depends on intermediate measurement outcomes. Then Definition 5 requires the classical computer to randomly choose the outcomes of intermediate measurements according to the correct distribution and, after the complete circuit is determined, to calculate the probabilities of the computational outcomes. 4 This would be unnecessary if we had a universal set of quantum gates at hand; we could simply replace measurement adaptations by coherently controlled gates, defer all intermediate measurements to the end of the circuit, and perform a strong simulation of the resulting circuit [\[27\]](#page-8-0). However, these controlled gates might not be available in a given restricted model, and in fact measurement adaption plays an important role in several models of quantum computation, most notably bosonic linear optics [\[17\]](#page-8-0), Clifford circuits with magic-state injection [\[28\]](#page-9-0), and measurementbased quantum computation [\[29\]](#page-9-0).

Since the main focus of this work is the interplay between restrictions in the inputs and measurements of the circuits, we also define the following nomenclature. A computational input/multiqubit output, or CI-MO, simulation is a restriction of Definitions 2, 3, or 5 to the case where the input state, $|\psi_n\rangle$, is just a computational-basis state $|x\rangle$ for some bit string *x*. A product input/single-qubit output, or PI-SO, simulation is a restriction of Definition 4 to the case where the input $|\psi_n\rangle$ is an arbitrary product state. Finally, a product input/multiqubit output simulation, or PI-MO, is the natural extension where the input can be an arbitrary product state and the measurements are over any subset of the qubits.

C. CI-MO simulation of matchgates

Let us now describe the CI-MO simulation of matchgates due to Valiant [\[1\]](#page-8-0) and Terhal and DiVincenzo [\[2\]](#page-8-0) (for convenience we follow more closely the latter). We begin by stating the following.

Theorem 1 [\[1,2\]](#page-8-0). Let $\{M_n\}$ be a uniform family of (possibly adaptive) quantum circuits composed of poly(*n*) nearestneighbor matchgates acting on *n* qubits, and let the input to the circuit be a state $|x\rangle$ for any *n*-bit string *x*. Then, there are polynomial-time classical algorithms to simulate the outcomes of measurements over arbitrary subsets of the output qubits in the weak, strong, and adaptive senses.

In the Appendix we outline the proof of Theorem 1 for the particular case of "number-preserving" matchgates [i.e., when $R' = 0$ in Eq. [\(7\)](#page-2-0). The crucial property of matchgates that makes Theorem 1 true is the fact that all outcome probabilities [cf. Eq. [\(8\)](#page-2-0)] can be written in terms of *matrix determinants*. For example, if *y* and \tilde{y} are arbitrary *n*-bit and *k*-bit strings, respectively, corresponding to a total or partial assignment of the output qubits, we can write

$$
Pr(y|x) = |\langle y|M_n|x\rangle|^2 = |\det(R_{x,y})|^2, \tag{9}
$$

$$
\Pr(\tilde{y}|x) = \text{tr}\,\langle \tilde{y}|M_n|x\rangle \langle x|M_n^{\dagger}|\tilde{y}\rangle = \text{Pf}(\tilde{M}),\tag{10}
$$

where $R_{x,y}$ is a specific submatrix of the matrix R from Eq. [\(7\)](#page-2-0) and \tilde{M} is a poly-sized antisymmetric matrix constructed out of the matrix elements of *R* in a specific manner. We direct the interested reader to the Appendix for a description of the intuition behind these expressions or to the original paper [\[2\]](#page-8-0) for lookup tables that explain how to construct $R_{x,y}$ and M. The Pfaffian $Pf(A)$ that appears in Eq. (10) is a matrix polynomial that, for an $n \times n$ antisymmetric matrix A, is 0 if n is odd and satisfies the relation

$$
Pf(A)^2 = \det(A)
$$

if *n* is even. In the Appendix we give a small generalization of Theorem 1, showing that it holds also for periodic boundary conditions (i.e., if matchgates can also act between the first and last qubits).

As discussed in Sec. [II A,](#page-1-0) although the linearity of Eq. (7) seems important for the simulation of matchgates, it is indeed not the whole story: For a CI-MO simulation, the probabilities in Eqs. (9) and (10) involve, *a priori*, the sum of an exponentially large number of terms, and yet the final expressions coalesce into easy-to-compute determinants. In fact, it is interesting to contrast this CI-MO simulation of matchgates to their bosonic counterpart. Bosonic linear optics includes Boson-Sampling [\[18\]](#page-8-0), a model for which there is strong evidence that an efficient classical simulation is impossible, and when imbued with adaptive measurements it is capable of universal quantum computation [\[17\]](#page-8-0). Thus, bosons apparently display a great computational advantage over fermions, and this seems to be a consequence of the fact that, rather than determinants (or Pfaffians), bosonic evolution is described by permanents, which are dramatically harder to compute (in fact, they are among the hardest problems in the complexity class #*P* [\[30\]](#page-9-0)).

D. PI-SO simulation of matchgates

For completeness, we now provide a brief outline of the simulation scheme used, e.g., by Jozsa and Miyake in [\[6\]](#page-8-0), although our main result in following sections is based on Theorem 1. We begin by stating the following.

Theorem 2 [\[6\]](#page-8-0). Let $\{M_n\}$ be a uniform family of quantum circuits composed of poly(*n*) nearest-neighbor matchgates acting on *n* qubits, and let the input be an arbitrary *n*-qubit product state $|\psi\rangle = |\psi_1\rangle |\psi_2\rangle \dots |\psi_n\rangle$. Then we can efficiently compute the expectation value $\langle Z_k \rangle = \langle \psi | M_n^\dagger Z_k M_n | \psi \rangle$; i.e., there is an efficient strong simulation in the single-output sense of Definition 4.

Theorem 2 is a consequence of the linearity of Eq. [\(7\)](#page-2-0). First note that, by Eq. [\(5\)](#page-1-0), we can write $Z_k = a_k^{\dagger} a_k - a_k a_k^{\dagger}$. However, then, by Eq. [\(7\)](#page-2-0) there are R and R' such that

$$
\langle \psi | M_n^{\dagger} a_k^{\dagger} a_k M_n | \psi \rangle
$$

=
$$
\langle \psi | \sum_{j,l}^{n} (R_{kj} a_j^{\dagger} + R'_{kj} a_j) (R_{kl}^{*} a_l + R'_{kl}^{*} a_l^{\dagger}) | \psi \rangle, \quad (11)
$$

⁴Note that Definition 5 does *not* require the classical computer to strongly simulate the final measurement outcomes of C_n , which would correspond to computing the average probabilities of the final measurements weighed by the probabilities of all possible intermediate outcomes.

and similarly for $\langle \psi | M_n^{\dagger} a_k a_k^{\dagger} M_n | \psi \rangle$. Equation [\(11\)](#page-3-0) consists of a sum of a polynomial number of terms of the type $\langle \psi | a_j^\dagger a_k | \psi \rangle$ for all quadratic combinations of creation and annihilation operators. However, from Eqs. (5) and (6) and subsequent discussion, all such quadratic terms are tensor products of Pauli matrices. Since $|\psi\rangle$ is a product state, all expectation values that appear in Eq. (11) factor into products of single-qubit expectation values of Pauli matrices. Thus, it is clear that $\langle Z_k \rangle$ can be computed with only poly(*n*) computational effort, which essentially proves Theorem 2. This result was further extended in [\[6\]](#page-8-0) to allow for measurement of a logarithmicsized subset of the output qubits and in [\[13\]](#page-8-0) to allow for periodic boundary conditions.

In contrast to Theorem 1, the proof of Theorem 2 seems to rely on the fact that Eq. [\(7\)](#page-2-0) is a linear transformation between creation and annihilation operators rather than on any intrinsically fermionic property. This is further supported by the fact that, for bosonic linear optics, a similar quantity to $\langle Z_k \rangle$ can also be computed efficiently [\[31\]](#page-9-0), and it is easy to sample classically from a BosonSampling distribution if we are restricted to a single output mode [\[19\]](#page-8-0). The proof of both facts also seem to stem from the linearity of Eq. [\(7\)](#page-2-0).

The interpretation of the single-output setting of Theorem 2 in terms of decision problems has also led to interesting mappings between matchgate circuits and (classical) circuits of linear threshold gates [\[32\]](#page-9-0), or between matchgate circuits and arbitrary logspace quantum computers [i.e., universal circuits acting on $O(\log n)$ qubits] [\[33\]](#page-9-0). The latter result also led to novel proposals for compressed simulation of spin systems on small-scale quantum computers [\[34,35\]](#page-9-0). Since there seems to be less difference between bosons and fermions in the single-output setting, an interesting question arises as to whether the results of $[32-35]$ could have some nontrivial bosonic analogue.

III. MAIN RESULT: EFFICIENT PI-MO SIMULATION OF MATCHGATE CIRCUITS

The comparisons between fermionic and bosonic linear optics at the ends of Sec. [II C](#page-3-0) and Sec. [II D](#page-3-0) seem to suggest that efficient CI-MO and PI-SO simulations of matchgates are possible for fundamentally different reasons; the former is a consequence of fermionic probabilities being described by determinants, whereas the latter seems to be a consequence of the linear relation satisfied by free particles [i.e., Eq. [\(7\)](#page-2-0)], and in fact only the latter seems possible for free bosons.

In this section, we argue that this apparent difference is not fundamental. More specifically, we show how to extend the result of [\[2\]](#page-8-0) to allow efficient classical simulation of matchgate circuits with arbitrary product inputs and measurements of arbitrary subsets of the output in the computational basis (that is, a PI-MO simulation).

We begin by stating the following theorem.

Theorem 3. Let $\{M_n\}$ be a uniform family of (possibly adaptive) quantum circuits composed of poly(*n*) nearestneighbor matchgates acting on *n* qubits, and let the input be an arbitrary *n*-qubit product state $|\psi\rangle = |\psi_1\rangle |\psi_2\rangle \cdots |\psi_n\rangle$. Then there are polynomial-time classical algorithms to simulate the corresponding outcomes in the weak, strong, and adaptive senses.

FIG. 1. By adding a $|+\rangle$ ancilla at the end of the circuit to act as a catalyst, it is possible to sequentially prepare the qubits in an arbitrary product state.

The first step to prove Theorem 3 is to replace the arbitrary product state $|\psi\rangle = |\psi_1\rangle |\psi_2\rangle \cdots |\psi_n\rangle$ with a circuit of matchgates acting on a fiducial state. To that end, we use the identities (see, e.g., $[12,13]$)

$$
G(H, H)|\phi\rangle|+\rangle = (H|\phi\rangle)|+\rangle,\tag{12a}
$$

$$
G(Z, X)|\phi\rangle|0\rangle = |0\rangle|\phi\rangle, \tag{12b}
$$

$$
G(Z, X)|0\rangle |\phi\rangle = |\phi\rangle |0\rangle, \qquad (12c)
$$

where $|\phi\rangle$ is an arbitrary single-qubit state and *H* is the usual single-qubit Hadamard matrix. Equation (12a) means that $G(H, H)$ can induce an *H* gate on a qubit state $|\phi\rangle$ when it has access to an ancilla in the $|+\rangle$ state, and Eqs. (12b) and $(12c)$ mean that the fermionic SWAP gate, defined as f-SWAP := $G(Z, X)$, behaves exactly as the SWAP gate when one of the qubits is in the $|0\rangle$ state. These identities are useful because neither *H* nor SWAP are matchgates on their own. In fact, either gate, when added to the set of matchgates, leads to universal quantum computation [\[2,6\]](#page-8-0), and so we clearly do not expect to be able to replace them by matchgates in general. Nevertheless, Eqs. (12) show how to do this in some particular cases by a suitable use of ancilla states.⁵

Consider now the circuit of Fig. 1. By repeated application of Eqs. (12), it starts from the $(n + 1)$ -qubit state $|\bar{0}_n\rangle|$ + \rangle and prepares the desired state $|\psi_1\rangle |\psi_2\rangle \cdots |\psi_n\rangle |+\rangle$ via the following procedure:

(i) Use the $|+\rangle$ ancilla to apply *H* gates to qubit *n* via Eq. (12a), which, together with single-qubit *Z* rotations (matchgates themselves), can be used to prepare qubit *n* in state $|\psi_1\rangle$.

(ii) Since all qubits from 1 to $n - 1$ are initially in the $|0\rangle$ state, use Eq. (12c) to effectively f-SWAP the state of qubit *n* all the way up to qubit 1.

(iii) At this point, we have the state $|\psi_1\rangle |\overline{0}_{n-1}\rangle |+\rangle$.

(iv) Repeat steps (i)–(iii) to sequentially prepare each state $|\psi_i\rangle$ and f-SWAP it to the qubit at position *i*.

After following steps (i) – (iv) we are left with the state $|\psi_1\rangle |\psi_2\rangle \cdots |\psi_n\rangle |+\rangle$. From this point on we can ignore qubit

⁵These simple identities provide quite a lot of leverage and were crucial to show that matchgates are universal when acting on almost all connectivity graphs in [\[12,13\]](#page-8-0).

 $n + 1$ and perform the original matchgate circuit M_n from Theorem 3.

The procedure above allows us to replace the initialization of any input product state by the initialization of a standard input state, $|\overline{0}_n\rangle|$ + \rangle , followed by the matchgate circuit of Fig. [1,](#page-4-0) which we denote by *U*. Our claim is that it is possible to compute, with only twice the computational effort, the same quantities as in the CI-MO simulation of Sec. HC . We can do this by applying the same methods to the circuit *MnU*, although this is not immediately apparent since the input in Fig. [1](#page-4-0) is not in the computational basis. To show how this can be circumvented, let *y*˜ be some assignment of a subset of *k* out of the *n* qubits, for any $k \le n$, and write

$$
Pr(\tilde{y}|\psi) = \langle \psi | M_n^{\dagger} P_{\tilde{y}} M_n | \psi \rangle
$$

= $\frac{1}{2} \langle \bar{0}_{n+1} | (1 + a_{n+1}) U^{\dagger} M_n^{\dagger} P_{\tilde{y}} M_n U (1 + a_{n+1}^{\dagger}) | \bar{0}_{n+1} \rangle,$
(13)

where we rewrote state $|+\rangle$ as fermionic operators acting on $|0\rangle$. Here $P_{\tilde{y}} := |\tilde{y}\rangle\langle\tilde{y}|$ is a projector that can be written as a string of creation and annihilation operators as follows. First, label the *k* qubits assigned by \tilde{y} as $\{l_1, l_2, \ldots, l_k\}$. Then, for each bit \tilde{y}_i assigned to qubit l_i , choose either $(a_{l_i}^\dagger a_{l_i})$ if it is 1 or $(a_{l_i} a_{l_i}^\dagger)$ if it is 0. Finally, define $P_{\tilde{y}}$ as the product of these operators. For example, one could obtain $P_{\tilde{y}} = (a_{l_1}^{\dagger} a_{l_1})(a_{l_2}^{\dagger} a_{l_2}) \cdots (a_{l_k} a_{l_k}^{\dagger}),$ for some bit string $\tilde{y} = 11 \dots 0$.

Following the same steps that lead to Eq. (10) (which we omit, but are outlined in the Appendix and worked out in full detail in [\[2\]](#page-8-0)), we can obtain

$$
Pr(\tilde{y}|\psi) = \frac{1}{2} \langle \bar{0}_{n+1} | U^{\dagger} M_n^{\dagger} P_{\tilde{y}} M_n U | \bar{0}_{n+1} \rangle + \frac{1}{2} \langle \bar{0}_{n+1} | a_{n+1} U^{\dagger} M_n^{\dagger} P_{\tilde{y}} M_n U a_{n+1}^{\dagger} | \bar{0}_{n+1} \rangle = \frac{1}{2} [Pf(\tilde{M}_1) + Pf(\tilde{M}_2)],
$$
(14)

where \tilde{M}_1 and \tilde{M}_2 are defined as in Eq. [\(10\)](#page-3-0) and can be easily constructed using the lookup tables found in [\[2\]](#page-8-0). Intuitively, this simplification is possible because matchgates preserve parity, and so the combined circuit M_nU acts independently on $|\vec{0}_n\rangle|0\rangle$ and $|\vec{0}_n\rangle|1\rangle$; thus, these two parity branches never interfere.

From Eq. (14) and Fig. [1,](#page-4-0) it is clear that the strong simulation of Theorem 3 is possible, since tracking the parallel evolution of the two parity branches of the state reduces to simulating two independent CI-MO instances, as per Theorem 1.

The circuit of Fig. [1](#page-4-0) is closely related to another trick, used in [\[3,](#page-8-0)[36\]](#page-9-0), where one maps *linear* fermionic operators [i.e., those in Eqs. [\(3\)](#page-1-0)] on *n* fermionic modes to quadratic operators [i.e., those in Eqs. [\(5\)](#page-1-0) and [\(6\)](#page-1-0)] on $n + 1$ fermionic modes, by adding one ancilla mode. Even so, the authors of [\[3,](#page-8-0)[36\]](#page-9-0) only considered either PI-SO or CI-MO settings.

Another surprising aspect of this construction is the fact that the two parity branches of state $|\psi\rangle$ can be obtained using nearest-neighbor matchgates from a superposition of the simplest bit strings of different parities. Since matchgates preserve parity, we should of course have expected that the two parity branches of $|\psi\rangle$ would evolve independently. Nonetheless, if we start from an arbitrary product state |*ψ* and look at its projection onto the even-parity subspace, say, we are left with a complicated entangled state, and it is not obvious that it would have an efficient description that would preserve the classical simulability of matchgates. The circuit of Fig. [1](#page-4-0) shows that this is in fact the case.

Finally, let us show why the adaptive simulation of Theorem 3 is possible, using a similar argument as for the CI-MO case [cf. the discussion surrounding Eq. $(A7)$]. For simplicity, suppose the whole adaptive circuit M_n we wish to simulate consists of (i) an *n*-qubit matchgate circuit *M*, (ii) measurement of a single qubit *y*1, and (iii) either of two matchgate circuits, which we represent by M_{y_1} depending on the outcome of y_1 . As before, this circuit acts on some input product state $|\psi\rangle = |\psi_1\rangle |\psi_2\rangle \cdots |\psi_n\rangle |+\rangle$, and at the end we wish to compute the probability of the *k*-bit string \tilde{y}_2 on some assignment of k out of the $n - 1$ remaining qubits.

To do this, we first replace the state $|\psi\rangle$ with the circuit of Fig. [1](#page-4-0) acting on $|\bar{0}_n\rangle|$ + \rangle , as before. Then we perform the simulation as follows:

(i) Compute $Pr(y_1|\psi)$ by applying Eq. (14).

(ii) Classically sample according to the probabilities computed in (i), and fix the corresponding outcome for *y*1.

(iii) Compute $Pr(\tilde{y}_2, y_1 | \psi)$, given by

$$
\begin{split} &\tfrac{1}{2}\langle\bar{0}_{n+1}|U^{\dagger}M^{\dagger}P_{y_1}M_{y_1}^{\dagger}P_{\tilde{y}_2}M_{y_1}P_{y_1}MU|\bar{0}_{n+1}\rangle \\ &+ \tfrac{1}{2}\langle\bar{0}_{n+1}|a_{n+1}U^{\dagger}M^{\dagger}P_{y_1}M_{y_1}^{\dagger}P_{\tilde{y}_2}M_{y_1}P_{y_1}MUa_{n+1}^{\dagger}|\bar{0}_{n+1}\rangle, \end{split} \tag{15}
$$

where, again, both P_{y_1} and $P_{\tilde{y}_2}$ are strings of creation and annihilation operators determined by the assignments *y*¹ and \tilde{y}_2 , respectively, as done for Eq. (13) . Clearly, the main difference between Eq. (15) and Eq. (14) is the introduction of the projector P_{y_1} between the two parts of the circuit. However, this operator is also even in the fermionic operators, so the same argument as before applies, and the probability factors as the sum of the probabilities of two independent (adaptive) CI-MO simulations.

Another way to state this result is that a projective measurement of a single qubit on the computational basis is itself a parity-preserving operation, so the adaptive measurement preserves the structure of two parallel simulations of matchgate circuits acting on well-defined parity states. Clearly, one can extend this simulation to allow for a polynomial number of rounds of measurements on different subsets of qubits, such as done for the CI-MO case in [\[2\]](#page-8-0).

Measurement on noncomputational bases

After extending the results of classical simulability of matchgates to include arbitrary input product states, the next natural question that arises is whether we can also change the *measurements* to allow for arbitrary non-computational-basis measurements. Conceptually, this could be framed as an even stronger simulation than that of Definition 2, since we would be able to compute the probabilities of a *tomographically complete* set of measurements. (For comparison, note that this is possible for Clifford circuits in all cases where they are strongly simulable, since they include the gates that map the computational basis to the *X* and *Y* bases.)

Currently, it is not clear how to perform this simulation for the most general single-qubit measurements, or even only in a tomographically complete set of measurement bases.

FIG. 2. This circuit rotates the measurement basis of the last qubit using $a |+ \rangle$ ancilla and a sequence of matchgates. The outcome controls classically control which variant of the f-SWAP gate, *G*(*Z,X*) or *G*(−*Z,X*), is used to swap the postmeasurement states of qubits *n* and $n + 1$. The notation is identical to Fig. [1.](#page-4-0)

Short of that, we show how to perform a *weak* simulation of the circuits (cf. Definition 3). Although this provides a much less precise description of the output state, it already suffices to rule out the possibility that matchgates could leverage arbitrary single-qubit measurements to perform universal quantum computation.

The main idea behind this simulation is to use the circuit of Fig. [1](#page-4-0) in reverse, such as indicated in Fig. 2. The main issue is that, in Fig. [1,](#page-4-0) we could use Eqs. $(12b)$ and $(12c)$ to swap the states of the qubits only because we knew upfront that one of the qubits being acted on was in the $|0\rangle$ state. Now, in Fig. 2, we once again use these identities, but in the postmeasurement states.

The simulation is very similar to the one described previously for matchgate circuits with adaptive measurements. We begin by using the $|+\rangle$ ancilla to implement an arbitrary single-qubit gate on the final qubit, which effectively rotates the measurement basis; then we compute the probability of the corresponding measurement outcomes, $Pr(y_1|\psi)$, using the method from the previous section. We sample classically according to the computed probabilities, fix the outcome of *y*1, and replace the measurement in the circuit by the projector P_{y_1} . Since the state of that qubit after the measurement is either $|0\rangle$ or $|1\rangle$, we then use either *G*(*Z*,*X*), as in Eq. [\(12b\)](#page-4-0), or *G*(−*Z*,*X*) [which satisfies an equation analogous to Eq. $(12b)$, but when one of the inputs is in state $|1\rangle$] to swap the states of the final two qubits. We can now iterate this process to simulate the measurement of the last k qubits, fixing the outcomes one by one, which consists of a weak simulation.

Although this procedure seems to only allow for the simulation of measurements on the last *k* qubits, it is in fact completely general. Recall, from the discussion after Eq. [\(6\)](#page-1-0), that the overall ordering of the qubits is irrelevant. So, if the circuit we wish to simulate is not restricted to measurements of the last *k* qubits, we can just map it into the fermionic picture, apply a permutation of the fermionic modes, and map it back, resulting in an equivalent circuit in which the measured qubits are the last *k* ones.

This concludes the proof that matchgate circuits remain (weakly) simulable even after replacing measurements in the computational basis by arbitrary single-qubit measurements.

IV. SUMMARY AND OPEN QUESTIONS

We have shown that matchgates are classically simulable, in a strong sense, when the circuit acts on arbitrary product input states, includes an arbitrary number of intermediate measurements that condition the subsequent circuits, and is followed by measurement of an arbitrary subset of the output qubits, thereby generalizing previous known simulation results [\[1,2,6\]](#page-8-0). We have also shown how to include measurements of the qubits in rotated bases, but only by switching to a weaker notion of simulation.

These results present an interesting parallel with other restricted models of computation. It is well known that complexity of simulation cannot be attributed only to the allowed operations, but also to the allowed inputs and measurements, as well as the strength of the required simulation. Clifford circuits, for example, range from classically simulable, to universal for quantum computation, to #*P*-hard to simulate (strongly) [\[15,16\]](#page-8-0). Another example is linear optics, which can be classically simulated if the quasiprobability distributions of the input states and of the measurements satisfy certain conditions [\[21](#page-8-0)[,37,38\]](#page-9-0), is hard to simulate classically if Fock state inputs and number-resolving measurements are available [\[18\]](#page-8-0), and becomes universal for quantum computing if adaptive measurements are allowed [\[17\]](#page-8-0). In contrast to these examples, matchgates do not seem to gain any type of computational advantage from the addition of arbitrary product input states, even when adaptive measurements are allowed, and there is evidence that they do not gain any advantage from (singlequbit) non-computational-basis measurements either.

With these remarks in mind, we pose a few open questions, both as continuations of the present work and as interesting investigations on the parallels between the different models:

(i) Is it possible to extend the result of Sec. [III](#page-4-0) to allow for *strong* simulation of measurements in arbitrary bases?

(ii) Although matchgates do not seem to benefit from arbitrary single-qubit inputs and measurements, we know that they become universal when certain multiqubit input states or measurements are allowed. Is it possible to repeat the work done here, but to fully characterize the behavior of matchgate circuits when supplemented with arbitrary twoqubit resources?

(iii) The matchgate simulation was extended to include periodic boundary conditions (i.e., extra matchgates between the first and last qubit) in the PI-SO setting in [\[13\]](#page-8-0) and in the CI-MO setting in the Appendix. Can we also extend the result of Sec. [III](#page-4-0) to this geometry? Curiously, the circuit that is equivalent to Fig. [1](#page-4-0) for periodic boundary conditions corresponds to a geometry where matchgates are universal, as seen, e.g., in Fig. 4(b) of [\[12\]](#page-8-0), although it might just use this geometry in a very restricted manner that does not break the simulability.

(iv) We have argued that, in the PI-SO setting, linear optics are classically simulable for the same reasons as matchgates, i.e., the linearity of Eq. [\(7\)](#page-2-0). Can this parallel be extended further, to allow simulation of linear optics with inputs that are superpositions of photon numbers? What about to obtain bosonic versions of other matchgate results such as the mapping to logspace quantum computation [\[33\]](#page-9-0) or the compressed simulations of [\[34,35\]](#page-9-0)?

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APPENDIX: FERMIONIC TRANSITION AMPLITUDES AND PFAFFIANS

In this appendix, we give a few additional details on how determinants and Pfaffians arise in the fermionic transition amplitudes of Sec. [II C,](#page-3-0) following mostly along the steps of $[2]$. Throughout this appendix we consider only a CI-MO scenario, where an input bit string $|x\rangle$ is acted on by some matchgate circuit *M*, and we wish to compute the corresponding outcome probabilities. We restrict ourselves to the case where the circuit of matchgates preserves the number of "fermions," i.e., the Hamming weight of the bit strings. This corresponds to taking $R' = 0$ in Eq. [\(7\)](#page-2-0), but the argument is very similar in the more general case.

As an illustration, suppose initially we want to compute the transition amplitude between two *n*-bit strings *x* and *y* (i.e., all qubits are measured), given by $\langle y|M|x\rangle$. Clearly, this is nonzero only if *x* and *y* have the same Hamming weight, which we denote by *h*. Also, let indices $\{i_1, i_2, \ldots, i_h\}$ label the positions of the *h* ones in *x*. Then, by recalling that a_i^{\dagger} act as fermionic creation operators, we write

$$
\langle y|M|x\rangle = \langle y|M a_{i_1}^{\dagger}a_{i_2}^{\dagger} \cdots a_{i_h}^{\dagger}|\bar{0}_n\rangle
$$

=
$$
\sum_{p_1\cdots p_h} R_{i_1,p_1}R_{i_2,p_2} \cdots R_{i_h,p_h} \langle y|a_{p_1}^{\dagger}a_{p_2}^{\dagger} \cdots a_{p_h}^{\dagger}|\bar{0}_n\rangle.
$$

If similarly we use indices $\{l_1, l_2, \ldots, l_h\}$ to label the positions of the ones in *y*, it is easy to see that the only terms that survive in this sum are those for which the p_j 's are some permutation of the *lj* 's. Furthermore, the anticommutation relations induce a minus sign on all odd permutations. This leads to the simple expression

$$
\langle y|M|x\rangle = \det(R_{x,y}),\tag{A1}
$$

where $R_{x,y}$ is an $h \times h$ submatrix of *R* constructed as follows. First, make an $h \times n$ matrix R_x by choosing the rows of R that correspond to ones in *x*, and then construct $R_{x,y}$ by choosing the columns of R_x that correspond to ones in *y*. Since the determinant of an $h \times h$ matrix, for $h \leq n$, can be computed in $poly(n)$ time, this gives a method for efficiently computing $\langle y|M|x\rangle$.

Let us now consider the probabilities when only a subset of *k* out of *n* qubits is measured after the circuit *M*, which is what we actually need for the strong simulation of Theorem 1. Note first that, for any given qubit j , we can write

$$
a_j a_j^{\dagger} = |0\rangle\langle 0|_j,\tag{A2a}
$$

$$
a_j^{\dagger} a_j = |1\rangle\langle 1|_j. \tag{A2b}
$$

Remarkably, the measurement projectors themselves are quadratic in the fermionic operators, which has previously been identified as a crucial difference between quantum computing with fermionic and bosonic linear optics [\[3\]](#page-8-0). Let us proceed by again indexing the *h* ones of *x* by $\{i_1, i_2, \ldots, i_h\}$, and let l_i indicate the position of the qubit assigned by the *i*th bit of \tilde{y} . We can then write

$$
Pr(\tilde{y}|x) = \text{tr}\,\langle \tilde{y}|M|x\rangle \langle x|M^{\dagger}|\tilde{y}\rangle = \langle x|M^{\dagger}P_{\tilde{y}}M|x\rangle. \tag{A3}
$$

Here $P_{\tilde{y}}$ is the projector $|\tilde{y}\rangle\langle\tilde{y}|$, which can be replaced by a string of creation and annihilation operators where, for each index l_i , we chose $a_{l_i} a_{l_i}^{\dagger}$ or $a_{l_i}^{\dagger} a_{l_i}$ depending on whether \tilde{y}_i is 0 or 1 [cf. the discussion just after Eq. [\(13\)](#page-5-0)]. For example, for $\tilde{y} = 01 \dots 0$ we would have

$$
P_{\tilde{y}} = (a_{l_1} a_{l_1}^{\dagger}) (a_{l_2}^{\dagger} a_{l_2}) \cdots (a_{l_k} a_{l_k}^{\dagger}). \tag{A4}
$$

Using Eq. [\(7\)](#page-2-0) (with $R' = 0$) we can write

$$
Pr(\tilde{y}|x) = \sum_{n' \text{ and } m' \text{ s}} R^*_{l_1, m_1} R_{n_1, l_1} \cdots R_{l_k, m_k} R^*_{n_k, l_k}
$$

$$
\times \langle \bar{0}_n | a_{i_n} \cdots a_{i_1} (a_{n_1}^\dagger a_{m_1} \cdots a_{m_k}^\dagger a_{n_k}) a_{i_1}^\dagger \cdots a_{i_h}^\dagger | \bar{0}_n \rangle.
$$

(A5)

In order to simplify the above equation, usually one resorts to Wick's theorem, which provides a systematic way of rearranging creation and annihilation operators so as to reduce the expectation values in Eq. $(A5)$ to complex numbers. We do not enter into the more arid details of Wick's theorem here, as the full procedure has already been carried out in [\[2\]](#page-8-0); we just cite the final result:

$$
Pr(\tilde{y}|x) = Pf(\tilde{M}).
$$
 (A6)

Here \tilde{M} is a $2(h + k) \times 2(h + k)$ antisymmetric matrix constructed in a specific manner from the matrix elements of *R*. The interested reader can find lookup tables with the rules for obtaining the matrix elements of \tilde{M} in [\[2\]](#page-8-0) (for a more direct relation between Wick's theorem and Pfaffians, although in a somewhat different formalism, we direct the reader to [\[4\]](#page-8-0)). The Pfaffian Pf (A) , which appears in Eq. $(A6)$, is a matrix polynomial related to the determinant. More specifically, if *A* is an $N \times N$ antisymmetric matrix (as in our case), Pf(*A*) is 0 if *N* is odd, and for even *N* it satisfies the relation

$$
Pf(A)^2 = \det(A).
$$

Thus, once more the desired probabilities are given in terms of determinants of matrices constructed out of elements of *R* and thus can be computed efficiently. In fact, the original matchgate simulation of Valiant [\[1\]](#page-8-0) exploited the fact that probabilities of matchgate circuits are given by Pfaffians, with no relation to fermions or Wick's theorem. Only later was this connection made explicit by Terhal and DiVincenzo in [\[2\]](#page-8-0).

One aspect of Theorem 1 introduced in [\[2\]](#page-8-0) that was not found in [\[1\]](#page-8-0) is simulation in the *adaptive* setting. Let us give an idea why the simulation remains possible in this case. Suppose the circuit we wish to simulate consists of some initial matchgate circuit *M* acting on an *n*-qubit state $|x\rangle$, followed by a measurement of the first qubit, *y*1, and then one of two circuits M_1 or M_0 corresponding to the two outcomes of y_1 . We then wish to compute the probabilities of some *k*-qubit outcome \tilde{y}_2 on a subset of the $n-1$ remaining qubits. We can do this as follows:

(i) Compute $Pr(y_1|x)$ using Eq. (A6) with $k = 1$.

(ii) Classically sample according to the probabilities computed in (i), and fix *y*¹ accordingly.

(iii) We now wish to compute $Pr(\tilde{y}_2|x,y_1)$. To that end it suffices to compute

$$
Pr(\tilde{y}_2, y_1 | x) = \langle x | M^{\dagger} P_{y_1} M_{y_1}^{\dagger} P_{\tilde{y}_2} M_{y_1} P_{y_1} M | x \rangle, \tag{A7}
$$

where P_{y_1} is $a_1a_1^{\dagger}$ or $a_1^{\dagger}a_1$ if y_1 is 0 or 1, respectively. It is clear that this expression is amenable to exactly the same treatment in terms of Wick's theorem as Eq. $(A3)$. In [2] it is also shown how to rewrite this expression as the Pfaffian of some efficiently computable antisymmetric square matrix.

Clearly, steps (i)–(iii) can be generalized to allow for any number of rounds of intermediate measurements, with any number of qubits being measured in each round.

One small extension of these arguments follows directly from the work of [2], although it does not seem to be pointed out anywhere: Efficient classical simulation remains possible even if we allow for "periodic boundary conditions," that is, if we also allow matchgates to act between the first and the last qubits. To see that, note that we can write, for

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example,

$$
X_1X_n=-\left(\prod_{i=1}^n Z_i\right)Y_1Z_2Z_3\cdots Z_{n-1}Y_n,
$$

with equivalent equations for the other matchgate generators of Eqs. [\(6\)](#page-1-0). However, $\prod_{i=1}^{n} Z_i$ is just the operator that measures the overall parity of the whole *n*-qubit state. Since a circuit of matchgates preserves the parity of the initial state, whenever the input is in the computational basis this operator can just be replaced by $+1$ or -1 depending on the parity of the input. Also recall that any gate generated by a Hamiltonian of the type $Y_1 Z_2 Z_3 \cdots Z_{n-1} Y_n$ can be decomposed into a circuit of $O(n^2)$ nearest-neighbor matchgates [6]. Thus, any matchgate circuit with periodic boundary conditions can be replaced by a circuit of nearest-neighbor matchgates that has the same action on that input state, with only polynomial overhead, and thus Theorem 1 still holds. Remarkably, this is the only type of non-nearest-neighbor matchgate we can add to the set without leading to universal quantum computation [13].

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