

Classical simulation of noninteracting-fermion quantum circuits

Barbara M. Terhal and David P. DiVincenzo

IBM, T. J. Watson Research Center, P.O. Box 218, Yorktown Heights, New York 10598

(Received 10 August 2001; published 1 March 2002)

We show that a class of quantum computations that was recently shown to be efficiently simulatable on a classical computer by Valiant [in Proceedings of the 33rd ACM Symposium on the Theory of Computing (2001), p. 114] corresponds to a physical model of noninteracting fermions in one dimension. We give an alternative proof of his result using the language of fermions and extend the result to noninteracting fermions with arbitrary pairwise interactions, where gates can be conditioned on outcomes of complete von Neumann measurements in the computational basis on other fermionic modes in the circuit. This last result is in remarkable contrast with the case of noninteracting bosons where universal quantum computation can be achieved by allowing gates to be conditioned on classical bits [E. Knill, R. Laflamme, and G. Milburn, *Nature (London)* **409**, 46 (2001)].

DOI: 10.1103/PhysRevA.65.032325

PACS number(s): 03.67.Lx, 05.30.-d

I. INTRODUCTION

To understand the power of a quantum computer, it is worthwhile to explore under what restrictions that power is weakened so as to make the computation efficiently simulatable with the use of a classical device. A nontrivial example is the Knill-Gottesman class of quantum computations [3]. These have been shown, by the analysis of operator equations of motion (the strategy we adopt below) to be efficiently simulatable on a classical computer. The Knill-Gottesman quantum circuit only allows 1-qubit Hadamard transformations, one-qubit $\pi/2$ phase shifts, one-qubit Pauli rotations, two-qubit controlled-NOT (CNOT) gates, and (as in the circuits we study below), measurements during the course of the circuit operation, provided that these measurements are projections in the two eigenspaces of any sequence of Pauli-matrix observables.

This question about restricted classes of quantum computation is also related to the question of universality of a quantum computation. What set of gates, or in more physical terms, what physical system can be used to implement universal quantum computation? Surprises have been found in this direction; for example it was shown that the two-qubit exchange interaction is sufficient for universal computation and, for example, that universal computation can be achieved with a network of phase shifters, beam splitters, and photon counters, i.e., noninteracting bosons, where logical gates can be conditioned on previous measurement outcomes [2].

In Ref. [1] a new class of quantum computations is introduced that is shown to be efficiently simulatable on a classical device. The class includes a special set of unitary 2-qubit gates on nearest-neighbor qubits. In this paper we will analyze this class of gates and show that it maps onto a system of noninteracting fermions (i.e., associated with Hamiltonian interactions that are quadratic in fermion creation and annihilation operators) in one dimension. The equivalence will enable us to give a straightforward derivation of the classical simulation, as well as extend the class of quantum computations to include (1) noninteracting fermions without nearest-neighbor restrictions and (2) gates that are applied conditionally on measurement outcomes. In particular, the second

result, when compared with the universal computation by linear optics in Ref. [2], shows a fundamental difference between bosons and fermions. One possible cause for the difference is that the bosonic modes, unlike fermionic modes, can contain more than one particle, a feature that is employed in the universality construction in Ref. [2].

The class of gates that Valiant shows to be classically simulatable is larger than the class that we start from in Theorem 1 (see below); his class includes nonunitary gates and also some special sets of two-qubit (possibly nonunitary) gates on the first two qubits. Knill has now shown [4] that this entire class is (indeed) weaker than full quantum computation. Furthermore, Knill shows that the extensions that we treat in this paper to non-nearest-neighbor interactions and conditionally applied gates are in fact included in Valiant's class of gates, albeit in a nonconstructive manner.

In Sec. II we establish the mapping from Valiant's gate set to a system of fermions. In Sec. III we show how the classical simulation comes about when we restrict ourselves to quadratic interactions that preserve the fermion number and in Sec. IV we handle the general case of noninteracting fermions. Finally, in Sec. V we show how classically conditioned gate operations can likewise be simulated with our methods.

II. NONINTERACTING FERMIONS

Let us first state the main theorem of Ref. [1]; we will give a slightly restricted version of the theorem that does not include the extra freedom of gate choice on the first two qubits nor the possibility to do nonunitary gates:

Theorem 1 (Valiant [1]). Let M be the unitary transformation representing a quantum circuit on n qubits that consists of two-qubit gates U on qubits x_i and x_{i+1} , $i=0, \dots, n-1$, where $e^{i\phi}U$ is of the form

$$e^{i\phi}U = \begin{pmatrix} U_{11}^1 & 0 & 0 & U_{12}^1 \\ 0 & U_{11}^2 & U_{12}^2 & 0 \\ 0 & U_{21}^2 & U_{22}^2 & 0 \\ U_{21}^1 & 0 & 0 & U_{22}^1 \end{pmatrix}, \quad (1)$$

where U^1 and U^2 are arbitrary elements of $SU(2)$ and ϕ is an arbitrary phase. There exist polynomial-time classical algorithms that evaluate (1) $\langle y|M|x\rangle^2$ for arbitrary bitstrings x and y , (2) $\text{Tr}(y^*|M|x\rangle\langle x|M^\dagger|y^*\rangle)$ where y^* corresponds to an assignment of an arbitrary k -bit subset for any k , and (3) sample, given an arbitrary input string $|x\rangle$, the probability distribution over outcomes y^* of a measurement (in the computational basis) on an arbitrary k -bit subset of the qubits.

Note that (3), which corresponds to the final simulation of a quantum computation, follows from (2) in a fairly straightforward manner (see Ref. [1]), whereas (2) could be strictly stronger than (1).

A first observation about the class of allowed gates is that they preserve the parity of an input bitstring $|x\rangle$, which is expressed by the fact that the $\{|00\rangle, |11\rangle\}$ sector is decoupled from the $\{|01\rangle, |10\rangle\}$ sector. Note that the overall phase factor $e^{i\phi}$ is irrelevant in the computation.

To make contact with physical models, we write a gate U acting on nearest-neighbor qubits i and $i+1$ as e^{iH} . This Hamiltonian H can be written as a sum of three types of interactions:

$$H_1 = \alpha_1 Z_i \otimes \mathbf{I}_{i+1} + \beta_1 \mathbf{I}_i \otimes Z_{i+1}, \quad (2)$$

$$H_2 = \alpha_2 X_i \otimes X_{i+1} + \beta_2 Y_i \otimes Y_{i+1}, \quad (3)$$

and

$$H_3 = \alpha_3 X_i \otimes Y_{i+1} + \beta_3 Y_i \otimes X_{i+1}, \quad (4)$$

where α_j, β_j are real, and X, Y, Z are the three Pauli matrices:

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (5)$$

At this point we note that the gate set in Theorem 1 seems extremely close to a universal set of gates. It has been proved [5] that universal quantum computation can be achieved by employing *only* the XY interaction, i.e., $H \propto X \otimes X + Y \otimes Y$, *if these gates can be applied on any pair of qubits*.¹ Since this form of interaction is certainly allowed in Theorem 1, we conclude that the nearest-neighbor constraint is crucial in the construction. Another observation is that adding arbitrary one-qubit gates to this gate-set would also result in universality; it has been proved that universal quantum computation can be obtained with a circuit with arbitrary one-qubit gates and only nearest-neighbor (one-dimensional) XY interactions [6].

Let us now consider the mapping onto a system of fermions. We can identify the n -bit computational basis states $|x\rangle$ with a state of n fermionic modes, each of which can be

occupied, corresponding to 1, or unoccupied, corresponding to 0. We have a set of operators, creation operators a_i^\dagger and (Hermitian conjugate) annihilation operators a_i associated with each mode i , which obey the anticommutation rules

$$\{a_i, a_j\} \equiv a_i a_j + a_j a_i = 0, \quad \{a_i^\dagger, a_j^\dagger\} = 0, \quad \{a_i, a_j^\dagger\} = \delta_{ij} I. \quad (6)$$

The annihilation and creation operators act on computational basis states in the following manner, consistent with the anticommutation relations:

$$\begin{aligned} a_i |x_0, \dots, x_i, \dots, x_{n-1}\rangle \\ = \delta_{x_i, 1} e^{i\pi \sum_{m=0}^{i-1} x_m} |x_0, \dots, \bar{x}_i, \dots, x_{n-1}\rangle \end{aligned} \quad (7)$$

and

$$\begin{aligned} a_i^\dagger |x_0, \dots, x_i, \dots, x_{n-1}\rangle \\ = \delta_{x_i, 0} e^{i\pi \sum_{m=0}^{i-1} x_m} |x_0, \dots, \bar{x}_i, \dots, x_{n-1}\rangle. \end{aligned} \quad (8)$$

Given these definitions, we can transform the Pauli operators in Eqs. (2)–(4) to creation and annihilation operators of fermions by a Jordan-Wigner transformation [7,8]. This is done by first defining the operators $\sigma_i^\pm = \frac{1}{2}(X_i \pm iY_i)$ that relate to the annihilation and creation operators as

$$\sigma_j^+ = \exp\left(i\pi \sum_{m=0}^{j-1} a_m^\dagger a_m\right) a_j^\dagger, \quad \sigma_j^- = \exp\left(i\pi \sum_{m=0}^{j-1} a_m^\dagger a_m\right) a_j. \quad (9)$$

With these rules, the three types of interactions H_1 , H_2 , and H_3 can be rewritten as (we omit terms that are proportional to I since they will only add irrelevant phase factors to the quantum state of the computer)

$$H_1 = 2\alpha_1 a_i^\dagger a_i + 2\beta_1 a_{i+1}^\dagger a_{i+1}, \quad (10)$$

$$H_2 = \alpha_2 (a_i^\dagger - a_i)(a_{i+1}^\dagger + a_{i+1}) - \beta_2 (a_i^\dagger + a_i)(a_{i+1}^\dagger - a_{i+1}), \quad (11)$$

and

$$\begin{aligned} H_3 = & -i\alpha_3 (a_i^\dagger - a_i)(a_{i+1}^\dagger - a_{i+1}) \\ & -i\beta_3 (a_i^\dagger + a_i)(a_{i+1}^\dagger + a_{i+1}). \end{aligned} \quad (12)$$

Thus we see that the total Hamiltonian $H = H_1 + H_2 + H_3$ is a sum of nearest-neighbor fermionic interactions that are quadratic in the fermion creation and annihilation operators, i.e., we can obtain any real linear combination of the Hermitian operators $a_i^\dagger a_i$, $a_{i+1}^\dagger a_{i+1}$, $a_i^\dagger a_{i+1} - a_i a_{i+1}^\dagger$, $i(a_i^\dagger a_{i+1} + a_i a_{i+1}^\dagger)$, $a_i^\dagger a_{i+1}^\dagger - a_i a_{i+1}$, and $i(a_i^\dagger a_{i+1}^\dagger + a_i a_{i+1})$. Fermionic systems that evolve according to such a quadratic Hamiltonian are referred to as “noninteracting,” because a canonical transformation (change of basis) exists that brings the Hamiltonian into a standard form involving a sum of terms each of which acts only on a single mode.

We note that if the initial gate set in terms of Pauli matrices did not have the nearest-neighbor restriction, then the

¹Note that the gate that swaps pairs of qubits is *not* included in the set defined by Eq. (1), because of the restriction to $SU(2)$ [rather than $U(2)$] submatrices; therefore, the distinction between nearest-neighbor and farther-neighbor gates that we make here is meaningful.

corresponding fermion interaction would not have been quadratic: this is due to the nonlocal “sign” part in the Jordan-Wigner transformation, Eq. (9). It has been found that these nonlocal signs are not a problem when one considers the question of simulating the dynamics of fermionic systems on a quantum computer: fermion dynamics can be simulated efficiently on a quantum computer, see Refs. [9–11]. Furthermore, it has been shown in Ref. [10] that universal quantum computation can be obtained by fermionic interactions that include Hamiltonians that are *quartic* in the annihilation and creation operators. Terms with an odd number of fermion operators are unphysical (they could transform an isolated fermion into an isolated boson), but they have some interesting mathematical features; see the discussion, Sec. VI.

III. PRESERVING THE NUMBER OF FERMIONS

Before we discuss how a fermionic circuit involving H_1 , H_2 , and H_3 can be simulated classically, we show how this simulation is done in the more restricted case when the gates preserve the number of fermions. Thus we consider a circuit on n fermionic modes where each elementary gate U corresponds to an interaction between modes i and j , and can be written as $U = \exp(iH_g)$ where the gate Hamiltonian is written generally as

$$H_g = b_{ii}a_i^\dagger a_i + b_{jj}a_j^\dagger a_j + b_{ij}a_i^\dagger a_j + b_{ij}^*a_j^\dagger a_i. \quad (13)$$

Note that the coefficients $b_{\alpha\beta}$ form a 2×2 Hermitian matrix; we will consider these coefficients to be part of an $n \times n$ matrix \mathbf{b} , which is only nonzero for matrix elements involving modes i and j . Here and later in Sec. IV we impose no restriction that i and j be nearest-neighbor modes, unlike the case that Valiant introduced. We will abbreviate the vacuum state $|00 \dots 0\rangle$ as $|\mathbf{0}\rangle$. Let $U = U_{\text{poly}(n)} \dots U_2 U_1$ be a sequence of two-qubit gates representing the quantum circuit. We consider

$$Ua_i^\dagger|\mathbf{0}\rangle = Ua_i^\dagger U^\dagger U|\mathbf{0}\rangle = Ua_i^\dagger U^\dagger|\mathbf{0}\rangle, \quad (14)$$

since $U|\mathbf{0}\rangle = |\mathbf{0}\rangle$ due to fermion number preservation. U acts by conjugation as

$$Ua_i^\dagger U^\dagger = \sum_m V_{im} a_m^\dagger. \quad (15)$$

When U corresponds to a gate operation as in Eq. (13), the matrix V is given by $V = \exp(i\mathbf{b})$. This result is proved by making a canonical transformation that diagonalizes \mathbf{b} . By group composition, the matrix V for the entire circuit U is given by matrix multiplication of the V 's for each gate. This evaluation of V is polynomially efficient in n if the circuit contains $\text{poly}(n)$ gates (in fact, we could replace the individual two-qubit gates by an arbitrary quadratic fermion-number-preserving Hamiltonian and the matrix V of the total circuit could still be evaluated efficiently).

We will first show how to evaluate efficiently the matrix element $\langle y|U|x\rangle$ where $|x\rangle$ and $|y\rangle$ are arbitrary input and output bitstrings. Since U preserves the number of fermions,

$\langle y|U|x\rangle = 0$ if x and y have different Hamming weight. Let U act on a state $|x\rangle$ with k fermions in certain positions:

$$U|x\rangle = Ua_{i_1}^\dagger a_{i_2}^\dagger \dots a_{i_k}^\dagger |\mathbf{0}\rangle, \quad (16)$$

where $i_1 < i_2 < \dots < i_k$ by convention. Using Eqs. (14) and (15), we can write

$$U|x\rangle = \sum_{p_1, \dots, p_k} V_{i_1, p_1} V_{i_2, p_2} \dots V_{i_k, p_k} a_{p_1}^\dagger a_{p_2}^\dagger \dots a_{p_k}^\dagger |\mathbf{0}\rangle. \quad (17)$$

The output state equals $\langle y| = \langle \mathbf{0}| a_{l_1} \dots a_{l_k}$, where $l_1 < l_2 < \dots < l_k$. Using the anticommutation rules Eq. (6), we see that contributions to the inner product $\langle y|U|x\rangle$ only arise when $p_1 \dots p_k$ is some permutation π of the indices $l_1 \dots l_k$. Furthermore, we get an overall sign for every term corresponding to the number of interchanges of creation operators that we have to perform in order to rewrite the state $a_{\pi(l_1)}^\dagger \dots a_{\pi(l_k)}^\dagger |\mathbf{0}\rangle$ as $a_{l_1}^\dagger \dots a_{l_k}^\dagger |\mathbf{0}\rangle$. After this reordering no more sign changes will take place, since $\langle \mathbf{0}| a_{l_k} \dots a_{l_1} a_{l_1}^\dagger \dots a_{l_k}^\dagger |\mathbf{0}\rangle = \langle \mathbf{0}| a_{l_k} a_{l_k}^\dagger \dots a_{l_1} a_{l_1}^\dagger |\mathbf{0}\rangle = 1$. Thus

$$\langle y|U|x\rangle = \sum_{\pi} \text{sgn}(\pi) V_{i_1, \pi(l_1)} V_{i_2, \pi(l_2)} \dots V_{i_k, \pi(l_k)}. \quad (18)$$

If \tilde{V} is defined as the matrix V where we have selected rows i_1, \dots, i_k and columns l_1, \dots, l_k , then we see that $\langle y|U|x\rangle = \det(\tilde{V})$. The determinant of a $k \times k$ matrix, $k \leq n$, is computable in polynomial time in n .

Simulating measurements

Next we consider how to simulate classically the outcomes of measurements on arbitrary subsets of qubits at the end of the computation. We will show how to calculate the probability that a certain subset of qubits is in a particular state y^* [item (2) in Theorem 1]. With those probabilities in hand, one can sample the probability distribution as given by quantum mechanics [item (3) of Theorem 1].

The Hermitian operator $a_i^\dagger a_i$ counts the number of fermions in mode i . Thus its expectation value with respect to a density matrix ρ , $\text{Tr} a_i^\dagger a_i \rho$, is the probability that mode i is in state $|1\rangle$. Similarly, the expectation value of $a_i a_i^\dagger = I - a_i^\dagger a_i$ is the probability that mode i is in state $|0\rangle$. So in order to evaluate the probability that, given an input state $|x\rangle$, a certain subset of k modes is in state $|y^*\rangle$ we calculate

$$\begin{aligned} p(y^*|x) &= \text{Tr} a_{j_1} a_{j_1}^\dagger \dots a_{j_k} a_{j_k}^\dagger U|x\rangle \langle x| U^\dagger \\ &= \langle x| U^\dagger a_{j_1} a_{j_1}^\dagger \dots a_{j_k} a_{j_k}^\dagger U|x\rangle, \end{aligned} \quad (19)$$

with $j_1 \neq j_2 \neq \dots \neq j_k$ and we use $a_i^\dagger a_i$ or $a_i a_i^\dagger$ when $y_i^* = 1$ or 0, respectively. [Equation (19) illustrates a case where $y_{j_1}^* = 0$ and $y_{j_k}^* = 1$.] Again we write $|x\rangle = a_{p_1}^\dagger \dots a_{p_l}^\dagger |\mathbf{0}\rangle$. We have to evaluate the expression

TABLE I. The matrix $M(i, j)$ for $i < j$.

		j			
		a_{p_β}	a_{n_β}	$a_{m_\beta}^\dagger$	$a_{p_\beta}^\dagger$
i	a_{p_α}	0	0	$V_{j_\beta, p_\alpha}^\dagger$	$\delta_{\alpha, \beta}$
	a_{n_α}	X	$\sum_{n_\alpha, n_\beta} V_{n_\alpha, j_\alpha} V_{n_\beta, j_\beta} \overline{a_{n_\alpha}^\dagger} a_{n_\beta} = 0$	$\sum_{n_\alpha, m_\beta} V_{n_\alpha, j_\alpha} V_{j_\beta, m_\beta}^\dagger \overline{a_{n_\alpha}^\dagger} a_{m_\beta}^\dagger = \delta_{\alpha, \beta}$	V_{p_β, j_α}
	$a_{m_\alpha}^\dagger$	X	$\sum_{m_\alpha, n_\beta} V_{j_\alpha, m_\alpha}^\dagger V_{n_\beta, j_\beta} \overline{a_{m_\alpha}^\dagger} a_{n_\beta} = 0$	$\sum_{m_\alpha, m_\beta} V_{j_\alpha, m_\alpha}^\dagger V_{j_\beta, m_\beta}^\dagger \overline{a_{m_\alpha}^\dagger} a_{m_\beta}^\dagger = 0$	0
	$a_{p_\alpha}^\dagger$	X	X	X	0

$$p(y^*|x) = \sum_{m_1, n_1, \dots, m_k, n_k} V_{j_1, m_1}^\dagger V_{n_1, j_1} \dots V_{j_k, m_k}^\dagger V_{n_k, j_k} \times \langle \mathbf{0} | a_{p_1} \dots a_{p_1} (a_{n_1} a_{m_1}^\dagger \dots a_{m_k}^\dagger a_{n_k}) a_{p_1}^\dagger \dots a_{p_1}^\dagger | \mathbf{0} \rangle. \quad (20)$$

We will invoke Wick's theorem [12(a)] (described in quantum many-body or quantum field theory textbooks such as Ref. [13]) to rewrite this formula [12(b)]. Wick's theorem states that we can rewrite a string of annihilation and creation operators $A_1 \dots A_n$ as

$$A_1 \dots A_n = :A_1 \dots A_n: + \sum_{k=1}^{\lfloor n/2 \rfloor} C_k, \quad (21)$$

with

$$C_1 = : \overline{A_1 A_2} \dots A_n : + : \overline{A_1 A_2 A_3} \dots A_n : + \dots, \\ C_2 = : \overline{A_1 A_2 A_3 A_4} A_5 \dots A_n : + : \overline{A_1 A_2 A_3 A_4 A_5} \dots A_n : + \dots, \quad (22)$$

etc. Here $:A_1 \dots A_n:$ denotes the so-called normal ordered form of the sequence of operators $A_1 \dots A_n$. $:A_1 \dots A_n:$ is equal to the reordered sequence of operators $A_{\pi(1)} \dots A_{\pi(n)}$ where all the creation operators are moved to the left (but not reordered among each other), and the quantity is negated when the number of interchanges of creation and annihilation operators to achieve this form is odd. The object $\overline{A_i A_j}$ is called a contraction and is defined as

$$\overline{A_i A_j} = A_i A_j - :A_i A_j:. \quad (23)$$

The terms C_k in Eq. (21) are each a sum over every possible choice of k contractions in the normal ordered product.

From the anticommutation rules for creation and annihilation operators, it follows that

$$\overline{a_i^\dagger a_j} = \overline{a_i^\dagger} a_j = \overline{a_i} a_j = 0, \quad \overline{a_i a_j^\dagger} = \delta_{ij}. \quad (24)$$

The normal-ordered form is extremely convenient when evaluating an object such as $\langle \mathbf{0} | A_1 \dots A_n | \mathbf{0} \rangle$ since the

vacuum expectation value of any normal-ordered sequence of operators vanishes $\langle \mathbf{0} | A_{i_1} \dots A_{i_k} | \mathbf{0} \rangle = 0$. Therefore, when we evaluate the vacuum expectation value of Eq. (22), the only terms that remain come from $C_{\lfloor n/2 \rfloor}$ (n even), in which every operator A_i is contracted (or matched) with another operator A_j . The last step is to bring the fully contracted terms to a form in which contracted operators are adjacent; that is, we have

$$\langle \mathbf{0} | : A_1 A_2 A_3 A_4 A_5 \dots A_i \dots A_{n-1} A_n : | \mathbf{0} \rangle \\ = \text{sgn}(\pi) \langle \mathbf{0} | : \overline{A_1 A_3 A_2 A_5 A_4 A_i} \dots \overline{A_{n-1} A_n} : | \mathbf{0} \rangle \\ = \text{sgn}(\pi) \overline{A_1 A_3 A_2 A_5 A_4 A_i} \dots \overline{A_{n-1} A_n}, \quad (25)$$

where $\text{sgn}(\pi)$ is -1 (1) when the number of crossings of the contraction lines is odd (even). Evidently, what emerges is the Pfaffian $\text{Pf}(M)$ of $M(i, j)$, an $n \times n$ antisymmetric matrix [i.e., $M(i, j) = -M(j, i)$]. The Pfaffian $\text{Pf}(M)$ is 0 when n is odd, and for even n it is defined as [18]

$$\text{Pf}(M) = \sum_{\pi} \text{sgn}(\pi) M_{\pi(1), \pi(2)} \dots M_{\pi(n-1), \pi(n)}, \quad (26)$$

where the sum over π is restricted to permutations on the indices $1, 2, \dots, n$ such that $\pi(2k-1) < \pi(2k)$ and $\pi(1) < \pi(3) < \pi(5) \dots$. Equations (20), (25), (26) tell us that

$$p(y^*|x) = \text{Pf}(M), \quad (27)$$

where M can be constructed from Eq. (20) and the contraction identities, Eq. (24), in the following manner. The matrix elements $M(i, j)$ for $1 \leq i < j \leq 2(k+l)$ are obtained from Table I: The indices $i, j = 1, \dots, 2(k+l)$ are assigned to the ordered sequence of creation and annihilation operators in Eq. (20). To determine $M(i, j)$ ($i < j$) we find what type of operator the indices i and j correspond to and then read off the matrix element $M(i, j)$ from the table. We use unitarity of V and the contraction rules to determine each entry of the table. The Xs in the table indicate that these entries do not occur.

The Pfaffian of an $n \times n$ antisymmetric matrix M can be computed in $\text{poly}(n)$ time, since $\text{Pf}(M)^2 = \det M$. The simulation procedure that was formulated in Ref. [1] very simi-

larly relies on the evaluation of a Pfaffian. At the moment it is not clear to us how the representation of the quantum circuit in Ref. [1] using matchgates corresponds to the fermionic representation developed here.

IV. GENERAL NONINTERACTING FERMIONS

We are now ready to consider the classical simulation of a quantum circuit consisting of gates that are built from general quadratic fermionic interactions. These interactions only preserve the parity of the fermion number. In order to deal with these general interactions, we transform the set of fermion annihilation and creation operators to a new set of Hermitian operators (associated with so-called Majorana fermions [10,14]):

$$c_{2i} = a_i + a_i^\dagger, \quad c_{2i+1} = -i(a_i - a_i^\dagger), \quad (28)$$

where $i = 0, \dots, n-1$. The anticommutation relation for this new set of operators is

$$\{c_k, c_l\} = 2\delta_{kl}I. \quad (29)$$

Note that operators c_{2i} and c_{2i+1} are in some sense the fermionic version of conjugate variables p and q that are obtained from linearly combining bosonic annihilation and creation operators. It is clear that the Hamiltonians H_1 , H_2 , and H_3 of Eqs. (2)–(4) will be quadratic in these new operators. Let U be a sequence of two-qubit gates each composed of interactions that are quadratic in the operators c_i ; i.e., each of the gates corresponds to a Hamiltonian H

$$H = \frac{i}{4} \sum_{k \neq l} \alpha_{kl} c_k c_l. \quad (30)$$

We again have omitted any term proportional to I . Hermiticity of H requires only that $\text{Im}(\alpha_{kl}) = \text{Im}(\alpha_{lk})$. It is conventional to choose the α matrix to be real and antisymmetric, so that $i\alpha$ is a Hermitian $n \times n$ matrix. For the interactions we have introduced, the α matrix will only be nonzero in a 4×4 subblock, but this restriction is not necessary for the following procedure to work. Similar to the number-conserving case, a sequence of gates $U = U_{\text{poly}(n)} \dots U_2 U_1$ acts by conjugation as

$$U c_i U^\dagger = \sum_j R_{ij} c_j, \quad (31)$$

where $R \in \text{SO}(2n)$. We will establish this important result by explicitly computing the matrix R for a single gate $U = e^{iH}$. The result is not so well known as for the number-conserving case (although it has been mentioned in [10]), so we will give some of the details of the derivation. We follow the notation of [14(a)]. First, the Hamiltonian of Eq. (30), with α chosen to be a real antisymmetric matrix, can be brought into canonical form

$$H = \frac{i}{2} \sum_{j=0}^{n-1} \epsilon_j b'_j b''_j. \quad (32)$$

b' and b'' are given by the real orthogonal transformation [14(b)]

$$\begin{pmatrix} b'_0 \\ b''_0 \\ \vdots \\ b'_{n-1} \\ b''_{n-1} \end{pmatrix} = W \begin{pmatrix} c_0 \\ c_1 \\ \vdots \\ c_{2n-2} \\ c_{2n-1} \end{pmatrix}. \quad (33)$$

The $2n \times 2n$ orthogonal matrix W diagonalizes α into 2×2 blocks:

$$W\alpha W^T = \begin{pmatrix} 0 & \epsilon_0 & & & & \\ -\epsilon_0 & 0 & & & & \\ & & \ddots & & & \\ & & & 0 & \epsilon_{n-1} & \\ & & & & -\epsilon_{n-1} & 0 \end{pmatrix}. \quad (34)$$

The b' 's and b'' 's have the same anticommutation relations as the original Majorana fermion operators. Note that $\pm \epsilon_j$ are the eigenvalues of the matrix $i\alpha$. We now write Eq. (31) using the canonical transformation

$$U c_i U^\dagger = \sum_j \exp\left(-\frac{1}{2} \sum_m \epsilon_m b'_m b''_m\right) (W_{2j,i} b'_j + W_{2j+1,i} b''_j) \exp\left(\frac{1}{2} \sum_m \epsilon_m b'_m b''_m\right). \quad (35)$$

Because the Hamiltonian in this canonical form is a sum of commuting terms, the exponentials here can be factorized; the factors with $m \neq j$ commute through and disappear, and we obtain

$$U c_i U^\dagger = \sum_j \exp\left(-\frac{1}{2} \epsilon_j b'_j b''_j\right) (W_{2j,i} b'_j + W_{2j+1,i} b''_j) \exp\left(\frac{1}{2} \epsilon_j b'_j b''_j\right). \quad (36)$$

The remaining exponential factors can be expanded and simplified:

$$\begin{aligned} \exp\left(\frac{1}{2} \epsilon_j b'_j b''_j\right) &= \sum_{k=0}^{\infty} \frac{(\epsilon_j/2)^k}{k!} (b'_j b''_j)^k \\ &= \sum_{k=0}^{\infty} \frac{(\epsilon_j/2)^{2k}}{2k!} (-1)^k + \sum_{k=0}^{\infty} \frac{(\epsilon_j/2)^{2k+1}}{(2k+1)!} \\ &\quad \times (-1)^k b'_j b''_j \\ &= \cos(\epsilon_j/2) + b'_j b''_j \sin(\epsilon_j/2). \end{aligned} \quad (37)$$

Plugging this form into Eq. (36) and simplifying, we obtain Eq. (31), where R is given by $R = W^T M W$, with the matrix M having the 2×2 block form

$$M = \begin{pmatrix} \cos \epsilon_0 & -\sin \epsilon_0 & & & & \\ \sin \epsilon_0 & \cos \epsilon_0 & & & & \\ & & \ddots & & & \\ & & & \cos \epsilon_{n-1} & -\sin \epsilon_{n-1} & \\ & & & \sin \epsilon_{n-1} & \cos \epsilon_{n-1} & \end{pmatrix}. \quad (38)$$

As before, given a quantum circuit with $\text{poly}(n)$ two-mode noninteracting fermion gates, that is, involving four Majorana fermions per gate, we can construct the total $2n \times 2n$ matrix R in polynomial time by straightforward matrix multiplication of the individual R matrices corresponding to the gates.

We again consider the probabilities with which certain measurement outcomes are obtained, i.e., $p(y^*|x)$ in Eq. (19), and show that as before these quantities are equal to the Pfaffian of some antisymmetric matrix.

As before, we consider an input state $|x\rangle = a_{p_1}^\dagger \dots a_{p_l}^\dagger |\mathbf{0}\rangle$, which we will now write as $c_{2p_1} \dots c_{2p_l} |\mathbf{0}\rangle$ with $p_1 < p_2 < \dots < p_l$. Thus we would like to evaluate

$$p(y^*|x) = \langle \mathbf{0} | c_{2p_1} \dots c_{2p_l} U^\dagger a_{j_1} U U^\dagger a_{j_1}^\dagger U \dots U^\dagger \times a_{j_k}^\dagger U U^\dagger a_{j_k} U c_{2p_1} \dots c_{2p_l} |\mathbf{0}\rangle, \quad (39)$$

The pattern of a and a^\dagger is again determined by the state $|y^*\rangle$. We need a formula for how our general (non-number conserving) U acts by conjugation on the creation and destruction operators. We can use Eq. (31):

$$\begin{aligned} U^\dagger a_i U &= \frac{1}{2} U^\dagger (c_{2i} + i c_{2i+1}) U = \frac{1}{2} \sum_j (R_{2i,j}^T + i R_{2i+1,j}^T) c_j \\ &= \sum_j T_{ij} c_j, \end{aligned} \quad (40)$$

and similarly

$$U^\dagger a_i^\dagger U = \sum_j T_{ij}^* c_j. \quad (41)$$

This defines the $n \times 2n$ matrix T . We then obtain for the measurement probability

$$\begin{aligned} p(y^*|x) &= \sum_{m_1, n_1, \dots, m_k, n_k} T_{j_1, m_1} T_{j_1, n_1}^* \dots T_{j_k, n_k}^* T_{j_k, m_k} \\ &\times \langle \mathbf{0} | c_{2p_1} \dots c_{2p_l} c_{m_1} c_{n_1} \dots c_{n_k} c_{m_k} c_{2p_1} \dots c_{2p_l} | \mathbf{0} \rangle. \end{aligned} \quad (42)$$

Again we can use Wick's theorem to evaluate the vacuum matrix element. This is done by writing the Majorana operators in terms of the fermion creation and annihilation operators. Expanding gives a large number of terms, to each of which Wick's theorem applies. Each term normal orders differently, but in every case only the fully contracted terms

TABLE II. The matrix $N(i, j)$ for $i < j$.

		j		
		c_{m_β}	c_{n_β}	c_{2p_β}
i	c_{m_α}	$(THT^T)_{j_\alpha, j_\beta}$	$(THT^\dagger)_{j_\alpha, j_\beta}$	$(TH)_{j_\alpha, 2p_\beta}$
	c_{n_α}	$(T^*HT^T)_{j_\alpha, j_\beta}$	$(T^*HT^\dagger)_{j_\alpha, j_\beta}$	$(T^*H)_{j_\alpha, 2p_\beta}$
	c_{2p_α}	$(HT^T)_{2p_\alpha, j_\beta}$	$(HT^\dagger)_{2p_\alpha, j_\beta}$	$\delta_{\alpha, \beta}$

survive. All of these fully contracted terms are generated by contractions directly over the Majorana operators, defined by linear extension:

$$\overline{c_{2i} c_{2j+1}} = -i(\overline{a_i a_j} - \overline{a_i a_j^\dagger} + \overline{a_i^\dagger a_j} - \overline{a_i^\dagger a_j^\dagger}) = i \delta_{ij}. \quad (43)$$

and similarly,

$$\overline{c_{2i+1} c_{2j}} = -i \delta_{ij}, \quad \overline{c_{2i} c_{2j}} = \overline{c_{2i+1} c_{2j+1}} = \delta_{ij}. \quad (44)$$

Here we have used Eq. (24). Then, the vacuum expectation value is written as the sum of all fully contracted expressions over the Majorana operators, with the usual fermionic sign. Thus, we can say that Wick's theorem applies in the same way to the Majorana fermion operators as it does to ordinary fermion creation and annihilation operators; we emphasize that this is only true for the vacuum expectation value, it is *not* true as an operator identity (normal ordering is not defined for the Majorana operators).

□ We can summarize these contraction rules by writing $c_i c_j = H_{ij}$ where H is a $2n \times 2n$ Hermitian matrix consisting of 2×2 blocks:

$$H = \begin{pmatrix} 1 & i & & & \\ -i & 1 & & & \\ & & \ddots & & \\ & & & 1 & i \\ & & & -i & 1 \end{pmatrix}. \quad (45)$$

Applying Wick's theorem again leads to a Pfaffian expression. In Table II we give entries that permit the $2(l+k) \times 2(l+k)$ matrix N to be constructed such that $p(y^*|x) = \text{Pf}(N)$. Again, the entire evaluation is clearly doable in polynomial time.

V. INTERMEDIATE MEASUREMENTS AND CLASSICALLY CONDITIONED OPERATIONS

We now extend our quantum circuit of noninteracting fermions by allowing intermediate complete von Neumann measurements in the computational basis on subset of qubits, which then determine the subsequent choices of unitary gates and measurements on the remaining qubits. We will show here that a fermionic circuit with these resources can still be simulated efficiently with a classical algorithm. Care has to be taken in specifying which intermediate and final measurements are allowed in our model; we restrict ourselves to complete von Neumann measurement in the computational

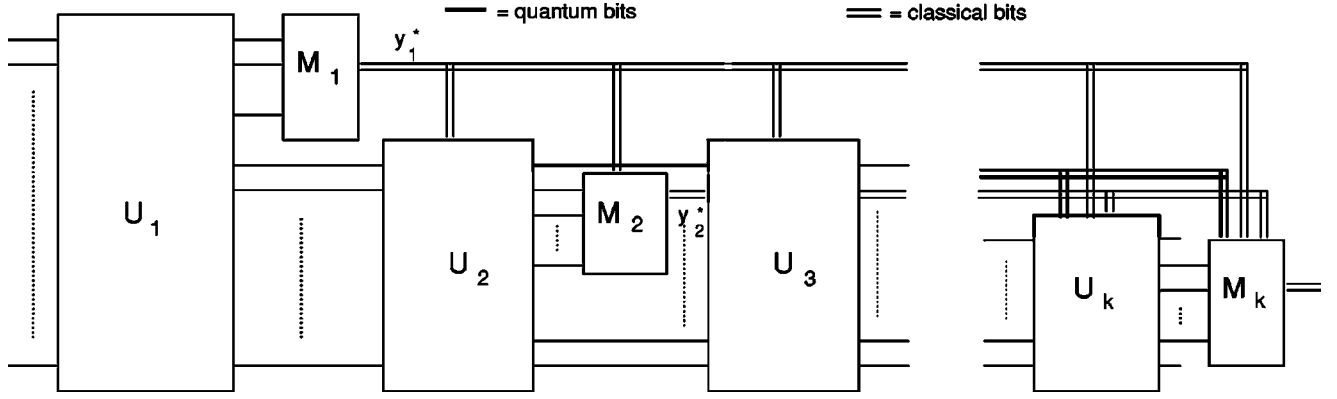


FIG. 1. A quantum circuit with classically conditioned gates.

basis; i.e., the outcomes of the measurement are either “no fermion present in this mode” or “one fermion present in this mode.” A lot of added power can be hidden in the kind of measurement that one is allowed to do; for example, it has been shown in Ref. [10] that universal quantum computation can be achieved by noninteracting fermion gates plus a non-destructive eigenvalue measurement of the quartic operator $c_j c_k c_r c_s$.

A general quantum circuit employing our set of resources is depicted in Fig. 1. Every time a measurement is made on a subset of qubits, these qubits are no longer used in any later steps of the computation. Our classical simulation will be constructed in the following manner. Measurements M_1, \dots, M_k on subsets S_1, \dots, S_k will take place at “times” t_1, \dots, t_k . The total unitary evolution until the measurement M_1 is denoted as U_1 , the conditional unitary evolution between M_k and M_{k+1} is denoted as $U_{k+1}(y_1^*, y_2^*, \dots, y_k^*)$ where the labels $y_1^*, y_2^*, \dots, y_k^*$ correspond to the outcomes of the measurements M_1, \dots, M_k . The choice of measurements themselves may depend on earlier measurement outcomes, i.e., $M_l = M_l(y_1^*, \dots, y_{l-1}^*)$. Even though the later time-evolution operators will not act on the qubits that are already measured, we keep the dimension of these matrices the same as the initial matrix U_1 ; i.e., these are $2^n \times 2^n$ matrices when the total number of fermionic modes is n .

We can calculate the probability that at time t_1 subset S_1 is in the state $|y_1^*\rangle$ (and sample from this probability distribution) by the methods that we have developed in Secs. III and IV. If the quantum measurement gives $|y_1^*\rangle$, then the

remaining qubits are in the state

$$\rho_2 = \frac{U_2(y_1^*) P_{y_1^*} U_1 |x\rangle \langle x| U_1^\dagger P_{y_1^*} U_2(y_1^*)^\dagger}{\text{Tr} P_{y_1^*} U_1 |x\rangle \langle x| U_1^\dagger}, \quad (46)$$

where the projector $P_{y_1^*}$ is of the form $a_{j_1} a_{j_1}^\dagger \dots a_{j_{|S_1|}} a_{j_{|S_1|}}^\dagger$ where $j_1, \dots, j_{|S_1|} \in S_1$, and whether the factor $a_{j_i} a_{j_i}^\dagger$ or $a_{j_i}^\dagger a_{j_i}$ appears depends on whether $(y_1^*)_{j_i}$ is 0 or 1, respectively. Let us assume that we have sampled the measurement probability distribution at time t_1 and have found a particular outcome y_1^* . To sample from the probability distribution of measurement M_2 , we will have to be able to evaluate

$$p(y_2^* | y_1^*, x) = \text{Tr} P_{y_2^*} \rho_2. \quad (47)$$

$P_{y_2^*}$, like $P_{y_1^*}$, is again a product of creation and annihilation operators; e.g., $a_{i_1}^\dagger a_{i_1} \dots a_{i_{|S_2|}}^\dagger a_{i_{|S_2|}}$ where $i_1, \dots, i_{|S_2|} \in S_2$ and the pattern of creation and annihilation operators depends on the bits of y_2^* . The denominator in Eq. (46) is already determined when simulating the first measurement, so we will focus on calculating

$$\begin{aligned} p(y_1^*, y_2^* | x) &= \text{Tr} P_{y_2^*} U_2(y_1^*) P_{y_1^*} U_1 |x\rangle \langle x| U_1^\dagger P_{y_1^*} U_2(y_1^*)^\dagger \\ &= \langle x | U_1^\dagger P_{y_1^*} U_2(y_1^*)^\dagger P_{y_2^*} U_2(y_1^*) P_{y_1^*} U_1 |x\rangle. \end{aligned} \quad (48)$$

 TABLE III. The matrix $O(i, j)$ for $i < j$.

		j				
		$c_{(a f)\beta}$	$c_{(b g)\beta}$	$c_{d\beta}$	$c_{e\beta}$	$c_{2p\beta}$
i	$c_{(a f)\alpha}$	$(T^1 H T^{1T})_{j_\alpha, j_\beta}$	$(T^1 H T^{1\dagger})_{j_\alpha, j_\beta}$	$(T^1 H T^{12T})_{j_\alpha, i_\beta}$	$(T^1 H T^{12\dagger})_{j_\alpha, i_\beta}$	$(T^1 H)_{j_\alpha, 2p_\beta}$
	$c_{(b g)\alpha}$	$(T^{1*} H T^{1T})_{j_\alpha, j_\beta}$	$(T^{1*} H T^{1\dagger})_{j_\alpha, j_\beta}$	$(T^{1*} H T^{12T})_{j_\alpha, i_\beta}$	$(T^{1*} H T^{12\dagger})_{j_\alpha, i_\beta}$	$(T^{1*} H)_{j_\alpha, 2p_\beta}$
	$c_{d\alpha}$	$(T^{12} H T^{1T})_{i_\alpha, j_\beta}$	$(T^{12} H T^{1\dagger})_{i_\alpha, j_\beta}$	$(T^{12} H T^{12T})_{i_\alpha, i_\beta}$	$(T^{12} H T^{12\dagger})_{i_\alpha, i_\beta}$	$(T^{12} H)_{i_\alpha, 2p_\beta}$
	$c_{e\alpha}$	$(T^{12*} H T^{1T})_{i_\alpha, j_\beta}$	$(T^{12*} H T^{1\dagger})_{i_\alpha, j_\beta}$	$(T^{12*} H T^{12T})_{i_\alpha, i_\beta}$	$(T^{12*} H T^{12\dagger})_{i_\alpha, i_\beta}$	$(T^{12*} H)_{i_\alpha, 2p_\beta}$
	$c_{2p\alpha}$	$(H T^{1T})_{2p_\alpha, j_\beta}$	$(H T^{1\dagger})_{2p_\alpha, j_\beta}$	$(H T^{12T})_{2p_\alpha, i_\beta}$	$(H T^{12\dagger})_{2p_\alpha, i_\beta}$	$\delta_{\alpha, \beta}$
	$c_{(a f)\beta}$	$(T^1 H T^{1T})_{j_\alpha, j_\beta}$	$(T^1 H T^{1\dagger})_{j_\alpha, j_\beta}$	$(T^1 H T^{12T})_{j_\alpha, i_\beta}$	$(T^1 H T^{12\dagger})_{j_\alpha, i_\beta}$	$(T^1 H)_{j_\alpha, 2p_\beta}$

This equation has basically the same form as Eq. (39), except that (1) we have more annihilation and creation operators and (2) we conjugate different sets of operators by different unitary matrices. The important fact here is that we can again express the probability as the Pfaffian of some antisymmetric matrix. Let us see how we construct this matrix.

At this point we simplify the notation somewhat.

$$\begin{aligned}
p(y_1^*, y_2^* | x) = & \sum_{\substack{a_1, b_1, f_1, g_1, \dots, a_{|S_1|}, b_{|S_1|}, f_{|S_1|}, g_{|S_1|} \\ d_1, e_1, \dots, d_{|S_2|}, e_{|S_2|}}} T_{j_1, a_1}^1 T_{j_1, b_1}^{1*} \dots T_{j_{|S_1|}, b_{|S_1|}}^{1*} T_{j_{|S_1|}, a_{|S_1|}}^1 T_{i_1, e_1}^{12*} T_{i_1, d_1}^{12} \dots T_{i_{|S_2|}, e_{|S_2|}}^{12*} T_{i_{|S_2|}, d_{|S_2|}}^{12} T_{j_1, f_1}^1 \\
& \times T_{j_1, g_1}^{1*} \dots T_{j_{|S_1|}, g_{|S_1|}}^{1*} T_{j_{|S_1|}, f_{|S_1|}}^1 \langle \mathbf{0} | c_{2p_1} \dots c_{2p_1} (c_{a_1} c_{b_1} \dots c_{b_{|S_1|}} c_{a_{|S_1|}}) (c_{e_1} c_{d_1} \dots c_{e_{|S_2|}} c_{d_{|S_2|}}) \\
& \times (c_{f_1} c_{g_1} \dots c_{g_{|S_1|}} c_{f_{|S_1|}}) c_{2p_1} \dots c_{2p_1} | \mathbf{0} \rangle.
\end{aligned} \tag{49}$$

In Table III we show how to construct the matrix O of dimension $2(l + 2|S_1| + |S_2|)$ for which $p(y_1^*, y_2^* | x) = \text{Pf}(O)$. The notation $c_{(a/f)_\alpha}$ indicates that the c operator can be either a c_{a_α} or a c_{f_α} ; the reason is that these operators have identical T prefactors.

It is clear that we can extend this procedure to the case of a circuit that contains $k = \text{poly}(n)$ instances of measurements on subsets that determine the next choice of unitary evolution. In general, when we express a probability such as Eq. (48), we see that P_1 gets conjugated by U_1 , P_2 by U_{12} , P_3 by U_{123}, \dots , and P_k by $U_{12\dots k}$, the total unitary evolution. When we write $p(y_1^*, y_2^* \dots y_k^* | x) = \text{Pf}(X)$, the dimension of the matrix X is $2(l + |S_k| + 2\sum_{i=1}^{k-1} |S_i|)$. The entries of this matrix can be determined by calculating particular matrix elements (specified by the measured sets of qubits) of at most $(2k+1)^2$ matrices of the form $T^i H T^{j\dagger}$, etc., where i and j are labels that can be $1, 12, 123, \dots, 123\dots k$.

Let us summarize the simulation algorithm.

Classical simulation of a quantum circuit with noninteracting fermions and fermion counting measurements; see Fig. 1:

(i) Compute the $n \times 2n$ matrix T^1 corresponding to U_1^\dagger , Eq. (40).

(ii) Simulate measurement M_1 : sample from the probability distribution $p(y_1^* | x)$ using the measurement theorem in Ref. [1] and the fact that $p(y^* | x) = \text{Pf}(O_1) = \sqrt{\det O_1}$ where O_1 is a $2(l+k) \times 2(l+k)$ matrix with k equal to the Hamming weight of input string x and l equal to the number of bits in y_1^* .

(iii) Let y_1^* be the outcome of this measurement M_1 , and let U_2 be the corresponding unitary evolution. Compute T^{12} corresponding to $U_1^\dagger U_2^\dagger$.

(iv) Simulate measurement M_2 : sample from the probability distribution $p(y_2^* | y_1^*, x) = p(y_1^*, y_2^* | x) / p(y_1^* | x)$, where we use the fact that we can evaluate $p(y_1^*, y_2^* | x) = \text{Pf}(O_2)$. O_2 depends on T^{12} and T^1 as in Table III.

Let $U_2(y_1^*) = U_2$, $P_{y_1^*} = P_1$, and $P_{y_2^*} = P_2$. We put in $U_1 U_1^\dagger$ and $U_2 U_2^\dagger$ terms in the appropriate places in Eq. (48), so that operators in the first (from the left) P_1 get conjugated by U_1^\dagger , operators in P_2 get conjugated by $U_{12}^\dagger \equiv U_1^\dagger U_2^\dagger$, and the last P_1 gets conjugated by U_1^\dagger again. Let T^k , $k=1, 12$, be defined by $U_k^\dagger a_i U_k = \sum_j T_{ij}^k c_j$. We obtain

(v) Let y_2^* be the outcome of the measurement M_2 and let U_3 be the corresponding unitary evolution, possibly also depending on the first outcome y_1^* . Calculate T^{123} corresponding to $U_1^\dagger U_2^\dagger U_3^\dagger$.

(vi) Simulate measurement M_3 : sample from the probability distribution $p(y_3^* | y_1^*, y_2^*, x) = [p(y_1^*, y_2^*, y_3^* | x)] / [p(y_1^*, y_2^* | x)]$, where we use the fact that we can evaluate $p(y_1^*, y_2^*, y_3^* | x) = \text{Pf}(O_3)$. O_3 depends on T^{123} , T^{12} and T^1 .

(vii) Repeat steps (v) and (vi) for the subsequent evolutions U_4, \dots, U_k , finding expressions for $T^{123\dots k}$, and finally simulate the last measurement M_k by sampling from the distribution $p(y_k^* | y_1^*, y_2^*, \dots, y_{k-1}^*, x) = p(y_1^*, y_2^*, \dots, y_k^* | x) / p(y_1^*, y_2^*, \dots, y_{k-1}^* | x)$.

It is evident that this procedure is polynomial when the number of stages k of the compute/measure procedure of Fig. 1 is $\text{poly}(n)$: the largest matrix whose Pfaffian must be computed has dimension bounded by $4kn$.

VI. DISCUSSION

The present work opens a set of very interesting questions concerning the boundary between classical and quantum computation. For fermionic quantum circuits we may ask, what is the effect of adding circuit elements beyond those considered above (those associated with a noninteracting fermion model)? Three outcomes are possible: (1) the circuit can perform universal quantum computation, (2) the circuit remains efficiently simulatable by a classical computation, or (3) some intermediate case. For example, one could explore the effect of adding (unphysical) linear terms to the gate Hamiltonians. These terms $a_i + a_i^\dagger$ and $i(a_i - a_i^\dagger)$ will be somewhat similar, but not identical to one-qubit gates in terms of Pauli matrices; they are nonlocal gates, as can be seen from the Jordan-Wigner transformation, Eq. (9). It can in fact be shown [4] that these linear interactions can be incorporated in purely quadratic fermion interactions by add-

ing a new fermionic mode, which we may label “ -1 ,” and changing the linear interactions on, say, mode i to quadratic interactions between mode i and mode -1 . Another line of investigation could be into some known physical models (e.g., the Anderson model and the Kondo model [15]) that involve more general fermionic interactions at a single site (meaning two fermionic modes), many of whose properties are computable.

Valiant’s work shows that some terms added to the fermion model (or some gates added to the circuit model) still result in a classically simulatable system; these new terms are to act on the first two fermionic modes only. These new gates (if they exist) do not preserve the parity of the number of fermions, and thus involve either linear or cubic terms in the annihilation and creation operators. (This follows from the fact that any gate that obeys the five matchgate identities in Ref. [1] and preserves the parity of the number of fermions is automatically quadratic in the number of fermions.) See Ref. [4] for a more extensive treatment of these additional gates.

The case of adding power by intermediate measurements is also quite interesting: between the case of complete von Neumann measurements that are classically simulatable, and the quartic-operator basis measurements of Bravyi and Kitaev [10], which give universal quantum computation, there are many possible positive operator valued measure measurement scenarios that have not been analyzed. We are hopeful that further analysis will be able to identify more scenarios as definitely classical or definitely quantum.

This classical-quantum boundary is remarkably different for fermionic and bosonic systems. A model quadratic in bosonic operators describes the “linear optics” scenario of quantum computation; formally, this model only differs from the noninteracting-fermion model in that bosons are characterized by commutation rather than anticommutation relations:

$$[a_i, a_j] \equiv a_i a_j - a_j a_i = 0, \quad [a_i^\dagger, a_j^\dagger] = 0, \quad [a_i, a_j^\dagger] = \delta_{ij} I. \quad (50)$$

Nevertheless, the exact parallel to the model we analyzed above, in which quadratic Hamiltonians can be interspersed with complete von Neumann measurements, is fully “quantum” in the bosonic case [2] despite being “classical” for fermions.

We would like to emphasize again that this quantum/classical distinction may not be perfectly sharp; being able to efficiently compute some properties of a circuit classically does not mean that every aspect of the quantum dynamics of this circuit is also efficiently computable. This is shown when we try to carry out the analysis in Secs. III and IV for bosons, to see where the parallels between the two cases break down. In fact, one can go surprisingly far before any differences appear. An equation of the form of Eq. (15) still applies for bosons, where V can be shown to be any element in $U(n)$ [16]. That is, a canonical transformation exists in both the boson and fermion cases that permits a representation of the system as a set of noninteracting particles.

It might have been thought that this easy diagonalization leads to an easy computation of all possible properties, but this does not appear to be the case. An essential difference is that no sign changes occur when we interchange the bosonic creation operators among each other. This causes an expression such as $\langle y|U|x\rangle$ in Sec. III to be equivalent to the *permanent* of some matrix, if we analyze the case when $|x\rangle$ and $|y\rangle$ both contain no more than one boson per mode. The permanent is a much harder object to calculate exactly than the determinant of the fermion case; in fact, this has been proved to be a $\#P$ -complete problem [17]. Our methods will therefore fail to evaluate these bosonic matrix elements efficiently.

In summary, our results on the classical simulatability of noninteracting fermions leave some interesting questions unanswered about the computational power of various physical models of quantum computation. While Valiant’s analysis turns out to conform largely to a “known” area of physics, his work shows that mathematical approaches to these problems are possible that have never been envisioned in many-body physics.

ACKNOWLEDGMENTS

We are grateful for the support of the National Security Agency and the Advanced Research and Development Activity through Army Research Office Contract Nos. DAAG55-98-C-0041 and DAAD19-01-C-0056. We thank M. Devoret, E. Knill, and R. Laflamme for helpful discussions. We also thank E. Knill for showing us his unpublished work on fermions and matchgates.

-
- [1] L. Valiant, in *Proceedings of the ACM Symposium on the Theory of Computing* (ACM Press, New York, 2001), p. 114; see <http://www.deas.harvard.edu/~valiant>.
- [2] E. Knill, R. Laflamme, and G. Milburn, *Nature* (London) **409**, 46 (2001).
- [3] D. Gottesman, *Group 22: Proceedings of the XXII International Colloquium on Group Theoretical Methods in Physics*, edited by S. P. Corney, R. Delbourgo, and D. Jarvis (1999), p. 32; e-print [quant-ph/9807006](http://arxiv.org/abs/quant-ph/9807006).
- [4] E. Knill, e-print [quant-ph/0108033](http://arxiv.org/abs/quant-ph/0108033).
- [5] D. Bacon, J. Kempe, D. P. DiVincenzo, D. A. Lidar, and K. B.

- Whaley, in *Proceedings of the 1st International Conference on Experimental Implementation of Quantum Computation*, edited by R. G. Clark (Rinton Press, Princeton, 2001), p. 257; e-print [quant-ph/0102140](http://arxiv.org/abs/quant-ph/0102140).
- [6] A. Imamoglu, D. D. Awschalom, G. Burkard, D. P. DiVincenzo, D. Loss, M. Sherwin, and A. Small, *Phys. Rev. Lett.* **83**, 4204 (1999).
- [7] P. Jordan and E. Wigner, *Z. Phys.* **47**, 631 (1928).
- [8] M. Plischke and B. Bergersen, *Equilibrium Statistical Physics* (World Scientific, Singapore, 1994).
- [9] D. Abrams and S. Lloyd, *Phys. Rev. Lett.* **79**, 2586 (1997).

- [10] S. Bravyi and A. Kitaev, e-print quant-ph/0003137.
- [11] G. Ortiz, J. E. Gubernatis, E. Knill, and R. Laflamme, e-print quant-ph/0012334.
- [12] (a) G. C. Wick, Phys. Rev. **80**, 268 (1950). (b) We actually use Wick's theorem for ordinary operator products rather than for time-ordered operator products, which is the case analyzed in most standard treatments. The version of the theorem we are using is excellently set out in T. D. Crawford and H. F. Schaefer III, Rev. Comput. Chem. **14**, 33 (2000); see also http://zopyros.ccqc.uga.edu/lec_top/cc/html/node13.html.
- [13] R. D. Mattuck, *A Guide to Feynman Diagrams in the Many-Body Problem* (McGraw-Hill, New York, 1976).
- [14] (a) A. Kitaev, Usp. Fiz. Nauk (Suppl.) **171**(10), 131 (2001). e-print cond-mat/00010440. (b) See R. A. Horn and C. R. Johnson, *Matrix Analysis* (Cambridge University Press, Cambridge, 1985), p. 82, Theorem 2.3.4.
- [15] N. W. Ashcroft and N. D. Mermin, *Solid State Physics* (Saunders, Philadelphia, 1976).
- [16] M. Reck, A. Zeilinger, H. J. Bernstein, and P. Bertani, Phys. Rev. Lett. **73**, 58 (1994).
- [17] L. G. Valiant, Theor. Comput. Sci. **8**, 181 (1979).
- [18] For a discussion of Pfaffians via an exposition of Pfaff's 1815 paper introducing the construction, see T. Muir, *The Theory of Determinants in the Historical Order of Development* (Dover, New York, 1950), Vol. 1, pp. 396–401.