Fermions in Quantum Complexity Theory

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Abstract

A brief survey of the role of fermions in quantum computation is presented, focusing on the Terhal-DiVincenzo result for noninteracting fermions. Creation and annihilation operators are used to formalize fermionic quantum computation, in order to derive in detail the relationship between classical computation of the determinant and the simulation of noninteracting fermions. Universal quantum computation using fermions is also discussed, including the use of interactions and the addition of charge measurement to free-electron systems.

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I. INTRODUCTION AND OVERVIEW

Introductory treatments of quantum computation typically deal with qubits that are distinguishable. That is, whatever their physical implementation may be, it is always possible to pick out a particular qubit and perform operations or make measurements upon it. The advantage of this assumption is that the quantum states describing such particles take on a particularly simple structure—that of a tensor product space—making the unitaries governing the computation easier to understand.

Such implementations of qubits could use, for example, multiple nuclear spins each with different nuclear masses or gyromagnetic ratios. Physically, such spins would be distinguishable as the particles are inherently different, and the total system would be described by a (mixed) state in the tensor product of the Hilbert spaces describing each spin individually. Using this physical assumption, we arrive at the familiar circuit model of quantum computation, for which we know universal quantum computation with a small set of gates is possible. This of course leads us directly to define the complexity class BQP corresponding to this model of distinguishable particles.

But yet another fundamental concept of quantum mechanics—often not even mentioned in an introductory treatment—is the notion of particle indistinguishability. Physically, particles of the same type (say, electrons or photons) within in a single quantum system are *indistinguishable*. Classically, we might imagine tracking their trajectories as a means of distinguishing otherwise identical particles. In quantum mechanics, however, this is not possible even in principle—after specifying every single degree of freedom in the particles, they remain indistinguishable. This remarkable fact can actually be derived from quantum field theory where particles are identified with identical excitations of a field, but in nonrelativistic quantum mechanics, it must be taken as an axiom. Far from being an isolated notion in theoretical physics, the indistinguishability of particles plays a dominant role in atomic physics and even in the consideration of some classical systems, as in the Gibbs paradox and mixing paradoxes in the statistical mechanics of ideal gases.

More precisely, we define the *exchange operator* P_{jk} to be the operator that exchanges the jth and kth qubits; its action on, say, two qubits would be $P_{12}|\psi\rangle|\phi\rangle = |\phi\rangle|\psi\rangle$. Then, particle indistinguishability means that the only physically meaningful states are the eigenstates of the exchange operator, for any pair of qubits. Since $P_{ij}^2 = I$ the identity, we deduce that the

only possible eigenvalues are ± 1, so that the states are either symmetric or antisymmetric under particle exchange. Particles whose states obey symmetry are called *bosons* (e.g., photons), and particles whose states obey antisymmetry are called *fermions* (e.g., electrons). It is another part of the axiom (alternatively, the spin-statistics theorem in quantum field theory) that all particles are either one or the other.

The main point of interest here for quantum complexity theory is relatively clear: what are the capabilities and limitations for a model of quantum computation based on a system of identical particles? A particularly interesting consideration is the case of *noninteracting* identical particles. Because identical particles obey special statistics (Bose-Einstein vs. Fermi-Dirac) due to the structure of their wavefunctions, nontrivial effects like exchange forces arise naturally in their physics, even in the absence of any coupling or external interactions. Thus, this motivates the question of the sorts of computing power afforded by restricting ourselves to measurements on noninteracting identical particles. It is relatively clear that any computation involving indistinguishable particles can be simulated efficiently by distinguishable qubits—this can be seen in the formalism we develop in the next section. The harder question is under what conditions the other direction is possible.

For bosons, a result by Knill, Laflamme, and Milburn in 2000 states that noninteracting bosons (in particular, photons in linear optics) with adaptive measurements are universal for quantum computation.[1] It is not known whether noninteracting bosons with nonadaptive measurements are universal, but it was shown in 2010 by Aaronson and Arkhipov that even an efficient, approximate classical sampling of such a system would result in the collapse of the polynomial hierarchy to the third level.[2]

This project, on the other hand, aims to survey the fundamental results along these lines for the case of fermions. We first present the language used to describe the quantum states of identical particles, in terms of creation and annihilation operators. Using this language, we survey the results of Terhal and DiVincenzo's 2002 paper that fermionic quantum computation with adaptive measurements can be efficiently classically simulated.[3] We explicitly derive the simulation for the special case where particle number is conserved, as this gives the key connection between classical computation of determinants, and noninteracting fermion statistics. Finally, we discuss a few universality results, both by introducing interaction terms[4] and by adding charge measurements to noninteracting electrons; the latter was shown to be universal by Beenakker, et al. in 2004.[5]

II. FERMIONIC QUANTUM COMPUTATION

Suppose that for a single particle, there are m possible eigenstates it can take on (which we will refer to as *modes*); these states span the m-dimensional Hilbert space $\mathcal{H}$ of that particle. For a system of n distinguishable particles, their quantum state simply lies in the 2^m-dimensional Hilbert space $\mathcal{H}_n = \mathcal{H}^{\otimes n}$, spanned by $|k_1\rangle|k_2\rangle$, for $1 \leq k_1, k_2 \leq m$.

For identical particles, however, we are required to either symmetrize or antisymmetrize. We note that this suggests a different way to describe the system: we need only say how many particles occupy each eigenstate, and the symmetrization requirement will uniquely dictate the valid state in the tensor-product representation.

Suppose there are n particles and m modes, and there are x_j particles in the jth mode. Our basis states in this representation take the form $|x_1, \ldots, x_m\rangle$, where $x_1 + \cdots + x_m = n$. These states span a subspace $\mathcal{F}_n$ consisting of all allowed n-particle states. The full space of indistinguishable particles, sometimes called *Fock space*, is given by a direct sum of these n-particle states: $\mathcal{F} = \mathcal{F}_0 \oplus \mathcal{F}_1 \oplus \cdots$. This is the setting in which indistinguishable particle dynamics take place.

To build a quantum state in Fock space, we start with the vacuum state of no particles, written as $|0, \ldots, 0\rangle$, spanning $\mathcal{F}_0$. To move into the other subspaces, we introduce *creation and annihilation operators*, $a_j^\dagger$ and a_j respectively, which add and subtract a particle from the jth mode. In general, these operators are neither Hermitian nor unitary, and for fermions, their action is defined through the following *anticommutation relations*:

$$\{a_j, a_k^\dagger\} \equiv a_j a_k^\dagger + a_k^\dagger a_j = \delta_{ij} I$$
$$\{a_j, a_k\} = \{a_j^\dagger, a_k^\dagger\} = 0$$

It is interesting to note that bosons follow the same relations, but with the *commutator* $[a_j, a_k^\dagger] \equiv a_j a_k^\dagger - a_k^\dagger a_j$. A state $|\psi\rangle$ with n fermions occupying modes $j_1, \ldots, j_n$ is obtained by acting on the vacuum state:

$$|\psi\rangle = \epsilon_{j_1,\ldots,j_n} a_{j_1}^\dagger \cdots a_{j_n}^\dagger |0, \ldots, 0\rangle$$

where $\epsilon_{j_1,\ldots,j_n}$ is the alternating symbol, to enforce the anticommutation sign convention. In this formalism, the number of particles in the jth mode is the eigenvalue of the number operator $N_j = a_j^\dagger a_j$. Note that $(a_j^\dagger)^2 = 0$, so that each mode contains exactly either zero or one fermion, giving rise to the *Pauli exclusion principle*. Thus, $\dim \mathcal{F}_n = \binom{m}{n}$.

To obtain unitary operators on $\mathcal{F}$, we can either build them out of $m \times m$ single-particle unitaries V acting on $\mathcal{F}$, or we can say that a unitary U is *generated* by a Hermitian operator (sometimes called the *Hamiltonian*), which is solely a function of the creation and annihilation operators. That is,

$$U = \exp\left[iH(a_1^\dagger, a_1, \ldots, a_m^\dagger, a_m)\right]$$

If H contains terms which are all quadratic (the product of at most two annihilation or creation operators), then we say that the operator U involves *noninteracting* fermions. Furthermore, if H contains the same number of a_j and $a_j^\dagger$ for each j, the number of particles is preserved. This is also not strictly physically necessary, what is required is that the parity of the number of particles is presevered, which is satisfied if H contains an even number of a_j or $a_j^\dagger$ per term. We will also see in the next section an example of how this formulation in terms of H relates to the single particle unitaries V.

III. SIMULATING NONINTERACTING FERMIONS

Here we discuss the central results of Terhal and DiVincenzo, where they showed that quantum computation using noninteracting fermions can be simulated classically, even with the addition of adaptive measurements. As they noted in their paper, their results turned out to be equivalent to a unitary subclass of Valiant's 2001 paper[6] on the classical simulation of matchgates.

First, let us consider the simpler case where the number of fermions stays constant. In this case, a computation step acting between modes α and β can be written as $U = \exp(iH)$, generated by

$$H = h_{\alpha\alpha} a_\alpha^\dagger a_\beta + h_{\beta\beta} a_\beta^\dagger a_\beta + h_{\alpha\beta} a_\alpha^\dagger a_\beta + h_{\alpha\beta}^* a_\beta^\dagger a_\alpha$$

The matrix h is Hermitian, and it in fact generates $V = \exp(ih)$, the single-particle unitary. For convenience, we consider it to be an $n \times n$ matrix instead, which is zero everywhere except along modes α and β.

Suppose now that U acts on a state with one fermion in mode j. We can compute that

$$U a_j^\dagger |0, \ldots, 0\rangle = U a_j^\dagger U^\dagger U |0, \ldots, 0\rangle = U a_j^\dagger U^\dagger |0, \ldots, 0\rangle \tag{1}$$

since U does nothing acting on the vacuum. Furthermore, conjugation by U gives the following linear superposition, seen from exponentiating h.

$$Ua_j^\dagger U^\dagger = \sum_k V_{jk} a_k^\dagger \tag{2}$$

We can now calculate, for arbitrary fermionic states $|x\rangle$ and $|y\rangle$ with the same number of particles, the inner product $\langle y|U|x\rangle$. Suppose $|x\rangle$ has particles in modes $j_1, \ldots, j_l$ and $|y\rangle$ has particles in modes $k_1, \ldots, k_l$, so that $|x\rangle = a_{j_1}^\dagger \cdots a_{j_l}^\dagger |0, \ldots, 0\rangle$ and $|y\rangle = a_{k_1}^\dagger \cdots a_{k_l}^\dagger |0, \ldots, 0\rangle$.

Using Equations 1 and 2, the action of U is

$$\begin{aligned} U|x\rangle &= Ua_{j_1}^\dagger U^\dagger \cdots Ua_{j_l}^\dagger U^\dagger |0, \ldots, 0\rangle \\ &= \sum_{p_1, \ldots, p_l} \left(V_{j_1,p_1} \cdots V_{j_l,p_l}\right) a_{p_1}^\dagger \cdots a_{p_l}^\dagger |0, \ldots, 0\rangle \end{aligned}$$

Acting on the left with $|y\rangle$, we get

$$\langle y|U|x\rangle = \sum_{p_1, \ldots, p_l} \left(V_{j_1,p_1} \cdots V_{j_l,p_l}\right) \langle 0|a_{k_l} \cdots a_{k_1} a_{p_1}^\dagger \cdots a_{p_l}^\dagger |0\rangle$$

We now see that because of the Pauli exclusion principle, the inner product is zero unless $p_1, \ldots, p_l$ is a permutation of $k_1, \ldots, k_l$. Once this is established, we can permute the annihilation and creation operators until we obtain $a_{k_l} a_{k_l}^\dagger \cdots a_{k_1} a_{k_1}^\dagger$, whose expectation value on $|0, \ldots, 0\rangle$ is one. However, we also pick up a number of minus signs equal to the sign of the permtuation. Altogether, then,

$$\langle y|U|x\rangle = \sum_{\sigma \in \mathcal{S}_l} \operatorname{sgn}(\sigma) V_{j_1,\sigma(k_1)} \cdots V_{j_l,\sigma(k_l)} = \det \widetilde{V} \tag{3}$$

where $\widetilde{V}$ is an $l \times l$ submatrix of V consisting of rows $j_1, \ldots, j_l$ and columns $k_1, \ldots, k_l$.

The determinant can, of course, be classically, in polynomial time in n, making the calculation of the amplitudes $\langle y|U|x\rangle$ easy to simulate classically. Thus, noninteracting fermions where the number of fermions is preserved is no stronger than classical computation.

Perhaps a more direct way of viewing the result is to see it as something like a determinental point process, where we have a matrix V and we wish to sample a submatrix $\widetilde{V}$ with probability given by $|\det \widetilde{V}|^2$. Viewed in this light, the output of the sampling algorithm would be a string of rows sampled, corresponding with $|y\rangle$; its probability would be $|\det \widetilde{V}|^2 = |\langle y|U|x\rangle|^2$, thus simulating the quantum algorithm.

An algorithm performing this sampling could be the following one.[7] We start with the matrix V which we wish to sample from, and consider the rows of V to be vectors $\mathbf{v}_j$.

1. Randomly pick a row k_1 with probability $\|\mathbf{v}_{k_1}\|^2/l$.

2. Set $\mathbf{v}_j \mapsto \mathbf{v}_j - (\mathbf{v}_{k_1} \cdot \mathbf{v}_j)\mathbf{v}_{k_1}$.

3. Sample k_2 with probability $\|\mathbf{v}_{k_2}\|/(l-1)$, and repeat until l rows have been sampled.

Due to the geometric projection performed in Step 2, the output of this algorithm would be the sampled rows $k_1, \ldots, k_l$, each picked with probability equal to the square of the determinant of the submatrix picked out. This is therefore a classical algorithm for sampling noninteracting fermions with a constant number of particles.

In addition to this important special case, Terhal and DiVincenzo also treat the cases where we introduce adaptive measurements and allow for the particle number to change. The idea is essentially the same—we permute the creation and annhilation operators until we get an expression involving a classically efficiently computable function of some matrix, which samples the quantum algorithm. We will not, however, go into the details, which are given in the original paper in [3].

To handle the case of changing particle number, Terhal and DiVincenzo introduce the Majorana fermion operators $c_{2j} = a_j + a_j^\dagger$ and $c_{2j+1} = -i(a_j - a_j^\dagger)$, which obey the anti-commutation relation $\{c_k, c_l\} = 2\delta_{kl}$. A more involved computation is needed, however, to obtain the analogue of Equation 2.

For intermediate measurements, it is important to restrict attention to complete measurements, which reveal whether or not there is a fermion in a specific mode. Terhal and DiVincenzo remark that a nondestructive eigenvalue measurement of the operator $c_j c_k c_r c_s$ for modes j, k, r, s will, as shown in [4], be universal for quantum computation.

IV. UNIVERSALITY RESULTS

To obtain universal quantum computation with fermions, an obvious approach would be to abandon noninteracting fermions and simply introduce an interaction term in the Hamiltonians generating the gates. This was accomplished early on in 2000 by Bravyi and Kitaev.[4] In their paper, they demonstrated that a universal set of gates for fermionic quantum computation is

$$\left\{\exp\left[i\frac{\pi}{4}a_0^\dagger a_0\right], \exp\left[i\frac{\pi}{4}\left(a_0^\dagger a_1 + a_1^\dagger a_0\right)\right], \exp\left[i\frac{\pi}{4}\left(a_1 a_0 + a_0^\dagger a_1^\dagger\right)\right], \exp\left[i\pi a_0^\dagger a_0 a_1^\dagger a_1\right]\right\}$$

The meaning of these terms are also offered: the first is the presence of an external potential, the second describes tunnelling, the third is a superconductor-like interaction term, and the last one, importantly, is a two-particle interaction. This set of unitary gates are sufficient for universal quantum computation for fermions.

Perhaps a more surprising result for universality, however, was given by Beenakker, et al. in 2004, where it was demonstrated that by introducing single-charge measurements to a noninteracting fermionic system, it is possible to construct a CNOT gate, which then allows free-electron quantum computation. A schematic of the main components of the gate are shown in Figure 1 below.

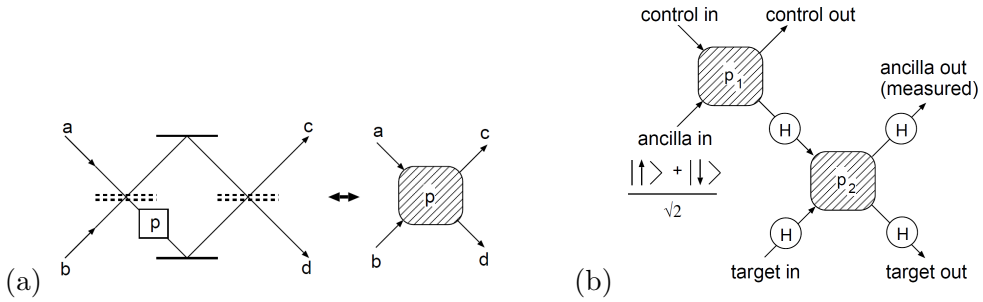

FIG. 1. Schematic of a deterministic CNOT designed from beamsplitters, single-charge detectors, and ancilla qubits. Figure (a) gives the design for a spin parity measurement. Electrons a and b pass through a polarizing beam splitter, which transmits spin up and reflects spin down. p denotes a measurement of the charge. Figure (b) shows how to use two spin parity measurements to implement a CNOT. H denotes a Hadamard gate. Correction Pauli operators are required to complete the CNOT at the end. Figures adapted from [5].

A measurement of the charge in a given mode results in the number operator N_j. Since this paper is concerned with both spatial and spin degrees of freedom, the possible occupation numbers for a spatial degree of freedom are 0, 1, and 2, the latter being possible for electrons with opposite spins occupying the same spatial mode.

The explicit calculation of the details behind the design are given in the appendix to [5]. Let us denote the control in with $|x\rangle$, the target in with $|y\rangle$, the control out with $|x'\rangle$ and the target out with $|y'\rangle$. The procedure also involves the parity measurements p_1, p_2 and the value of the ancilla out measured in the computational basis, z. The result of the circuit

in Figure 1 is

$$|x'\rangle|y'\rangle = (-1)^{x(p_2+1)}\,|x\rangle|x+y+z+p_1+1\rangle$$

after dropping input-independent overall phases. Thus, if $p_2 = 0$, we should apply X to the control, and if $z + p_1 + 1 = 1$, then we apply X to the target.

These results, as the figure designs indicate, are best suited for free-electron systems, where interactions are minimal and we have access only to linear elements such as beam-splitters. Since fermions that are close together typically strongly interact, pairwise interaction effects like those discussed above might be more convenient. Nevertheless, this result demonstrates that the analogue of linear optics quantum computation with bosons can be achieved with fermions as well, provided the addition of these charge measurements.

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