Universal Quantum Computation by Scattering in the Fermi-Hubbard Model

Ning Bao, Patrick Hayden, Grant Salton, and Nathaniel Thomas
Stanford Institute for Theoretical Physics, Stanford University, Stanford, CA 94305

The Hubbard model may be the simplest model of particles interacting on a lattice, but simulation of its dynamics remains beyond the reach of current numerical methods. In our work, we show that general quantum computations can be encoded into the physics of wave packets propagating through a planar graph, with scattering interactions governed by the fermionic Hubbard model. Therefore, simulating the model on planar graphs is as hard as simulating quantum computation. We give two different arguments, demonstrating that the simulation is difficult both for wave packets prepared as excitations of the fermionic vacuum, and for hole wave packets at filling fraction one-half in the limit of strong coupling. In the latter case, which is described by the t-J model, there is only reflection and no transmission in the scattering events, as would be the case for classical hard spheres. In that sense, the construction provides a quantum mechanical analog of the Fredkin-Toffoli billiard ball computer.

I. Introduction

The aim of quantum Hamiltonian complexity theory is to categorize the basic questions of physics by how difficult they are to resolve computationally [1]. Thanks to the Trotter expansion [2] and the phase estimation algorithm [3, 4], simulating the dynamics of a quantum system is often easier than estimating its ground state energy [5, 6]. Over the past 15 years, increasingly sophisticated methods have been developed for simulating the physics of spin systems and even quantum field theories on quantum computers [7, 8]. In most cases then, the question is not whether a given system can be efficiently simulated but whether that simulation even requires the full power of quantum computation. Free fermion systems, for example, can be efficiently simulated on a classical computer [9] while free boson systems appear to be hard to simulate classically while falling short of being able to encode arbitrary quantum computations [10].

In recent work, Childs *et al.* demonstrated that a wide class of quantum systems, including the Bose-Hubbard model, is *universal* for quantum computation, in the sense that is is possible to encode arbitrary quantum computations into their dynamics if their interactions are arranged between the vertices of a particular computation-dependent planar graph [11]. Since the Bose-Hubbard model can be simulated on a quantum computer and can simulate arbitrary quantum computations, the complexity of simulating the model is therefore *precisely* the power of quantum computation.

In our work, we prove an analogous result for the Fermi-Hubbard model – a broadly applicable model with relevance to phenomena ranging from the Mott insulator transition to high-temperature superconductivity [12–14]. Along the way, we also established the universality of the t-J model, thus demonstrating that two widely studied and physically relevant fermionic Hamiltonians are universal for quantum computation. While the techniques of [11] apply to some systems of anti-commuting scalars, spin is an integral part of the Fermi-Hubbard model and its universality for quantum computation is not resolved by the earlier results. The most natural way to realize anticommuting scalars using spin-$1/2$ fermions is to polarize all the fermions in the same direction, thereby freezing out the spin degree of freedom. In that case, however, any spin-spin interactions vanish and the resulting dynamics classically simulatable [9]. A different strategy, such as the one we employ, is therefore required to achieve universality in the Fermi-Hubbard and t-J models.

We are interested in performing arbitrary quantum computations without the use of any time-dependent control. Moreover, we do not permit the Hamiltonian to be tailored to the task at hand: all sites interact in the same way although we allow the sites to be arranged in computation-specific planar configuration. These restrictions tie the hands of any experimentalist to the point that this approach may be unlikely to yield practical schemes for quantum computation. Our objective, instead, is to assess the inherent computational power of the Fermi-Hubbard model.

Our approach, as in Childs *et al.* [11], is to encode the quantum circuit representing the computation as a planar graph, with the Hamiltonian governing interactions between adjacent vertices. The computation then proceeds by sending a collection of wave packets into the graph, allowing them to scatter, and then observing the transmitted particles. Unlike in [11], however, the computation's quantum information is stored not in the location of the wave packet but, rather, in the spin degrees of freedom of the fermions. To implement gates, we adapt a result of DiVincenzo *et al.* on the universality of the controlled Heisenberg interaction [15], emulating controlled interactions using repeated scattering processes.

II. The Fermi-Hubbard and t-J models

The Fermi-Hubbard Hamiltonian on a graph $\mathcal{G} = (V, E)$ is given by

$$H = -t \sum_{\sigma\in\{\uparrow,\downarrow\}} \sum_{\{i,j\}\in E} (c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i\sigma}) + U \sum_{i\in V} n_{i\uparrow} n_{i\downarrow}, \tag{1}$$

where c_i are fermionic operators and $n_{i\sigma} \equiv c^\dagger_{i\sigma} c_{i\sigma}$ (no sum) is the number operator [11, 13]. The parameters of this model are t and U (the onsite Coulomb repulsion strength).

The Fermi-Hubbard Hamiltonian near half-filling and in the limit of large positive U can be transformed perturbatively into the t-J Hamiltonian [13]. We do this by identifying the Fermi-Hubbard creation operators $c^\dagger_i$ with t-J annihilation operators a_i, the Fermi-Hubbard half-filling state with the no-particle state of the t-J model, and $J = 4t^2/U$. Note that this identifies the large U limit with the small J limit. The new Hamiltonian is then

$$H = \sum_{\{i,j\}\in E} P_S \left[-t \sum_{\sigma\in\{\uparrow,\downarrow\}} (a^\dagger_{i\sigma} a_{j\sigma} + a^\dagger_{j\sigma} a_{i\sigma}) + J\left(\vec{S}_i \cdot \vec{S}_j - \frac{n_i n_j}{4}\right)\right] P_S, \tag{2}$$

where $P_S \equiv I - \sum_{i\in V} n_{i\uparrow} n_{i\downarrow}$ is the projector onto the single particle state and prohibits hopping of two t-J particles onto the same site, regardless of their spin. The physical interpretation of this condition is that there cannot be a negative number of fermions on a site (interpreting t-J excitations as holes in the Fermi-Hubbard model at half-filling).

III. One- and two-particle scattering

If we restrict our attention to a system containing only one particle, then the Hamiltonian corresponds to a quantum walk of the wave packet over the graph $\mathcal{G}$. We focus on graphs that consist of a finite portion connected to one or more semi-infinite lines. States that scatter in from one of the semi-infinite lines, through the finite portion, and then out through the semi-infinite lines can be identified as stationary states of the Hamiltonian. The associated eigenvalue problem was studied in [16] and [11, Appendix A]. Each incoming semi-infinite line is referred to as a "rail".

A one-particle scattering problem of particular importance in the present context is scattering through a graph known as a "momentum switch". Momentum switches are subgraphs that are engineered to shunt single particle wave packets based on their momenta, and they were studied extensively by Childs *et al.* [11, 17]. For particular incoming momenta, these subgraphs have perfect transmission or reflection between wave packets traveling with momenta $|k_1| = \pi/4$ and $|k_2| = \pi/2$. Such a graph is shown in left panel of fig. 1.

Returning to two-particle scattering, our strategy for building unitary gates will be to selectively route pairs of wave packets into an interaction region, as shown in the right panel of fig. 1, and scatter them off one another. We take care to ensure that no more than two particles are in the interaction region at any given time. In the limit of infinitely long wave packets, scattering of two particles in this interaction region induces a unitary g on the two-spin subspace that will, in general, entangle the two spins in the controlled phase operation. For the t-J model, this unitary is

$$g = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & e^{i\theta(p_1,p_2,J)} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \tag{3}$$

in the basis $\{|\uparrow\uparrow\rangle, |T_0\rangle, |S\rangle, |\downarrow\downarrow\rangle\}$, where $\theta(p_1, p_2, J) = \mathrm{Arg}\left[-e^{2ip_2}\left(\frac{J-2\cos(p_1/2)e^{-ip_2}}{J-2\cos(p_1/2)e^{ip_2}}\right)\right]$, $|T_0\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$, $|S\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$, $p_1 = -(k_1 + k_2)$, and $p_2 = (k_2 - k_1)/2$.

IV. Universality

Our goal was to build a universal quantum gate set using only the two aforementioned processes: momentum switches that can be used to shunt wave packets depending on their momenta, and induced unitaries on the spin subspace of two colliding particles. Following DiVincenzo *et al.* [15], each logical qubit is encoded in the $S = 1/2$, $S_z = +1/2$ subspace of three physical rails. In parituclar, qubits are encoded in the logical basis $\left\{|0_L\rangle = |S\rangle|\uparrow\rangle, \quad |1_L\rangle = \sqrt{\frac{2}{3}}|\uparrow\uparrow\downarrow\rangle - \frac{1}{\sqrt{3}}|T_0\rangle|\uparrow\rangle\right\}$.

DiVincenzo *et al.* [15] showed that the exchange interaction is universal when it can be dynamically controlled. In particular, the authors established universality of a unitary spin-spin interaction of the form

$$\tilde{U} \equiv e^{i\gamma t \vec{S}_1 \cdot \vec{S}_2} = \exp\left[i\frac{\gamma t}{4}\right] \exp\left[-i\gamma t\, |S\rangle\langle S|\right],$$

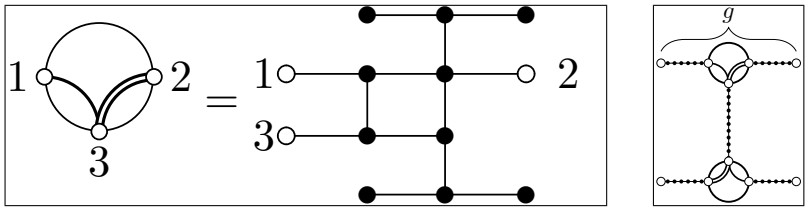

FIG. 1. A simple momentum switch subgraph **(left panel)**. Two-particle scattering implementing the unitary g **(right panel)**.

where t is a controllable time parameter. They used a computer search to determine interaction durations sufficient to produce a universal gate set, finding that a universal set of gates can be produced by systematically interacting qubits for one of fourteen numerically determined times, as needed.

In our case, the interaction timescale is determined by the wave packet width and momentum. In other words, unitary transformations of the spin subspace are implemented in discrete steps corresponding to individual collisions rather than through continuous time evolution. In order to reproduce a desired unitary, U, two wave packets need to be repeatedly scattered off one another until $\tilde{U}$ is sufficiently well approximated. This amounts to repeatedly stepping by a fixed amount through angles on a circle until a target angle (mod 2π) is reached to within a desired tolerance.

The final step in the universality construction is measurement. A simple and sufficient procedure for measuring the logical state of the triple rail qubit is to measure the third spin along the z direction. If the state is $|0_L\rangle$ then the outcome will always be $|\uparrow\rangle$, but if the state is $|1_L\rangle$ then the outcome will be $|\downarrow\rangle$ with probability $2/3$. Repeating the entire computation and using majority voting can then shrink the error probability exponentially as a function of the number of repetitions.

The scattering analysis is exact in the limit of infinite width wave packets, but for finite width wave packets, the induced transformation on the spin space is not even unitary. Nonetheless, our scheme is universal for finite wave packets of width polynomial in the number of gates and qubits. We find the same error bounds as Childs *et al.*: $L = \mathcal{O}(n^{12}m^4)$, $\mathcal{O}(n^{13}m^5)$ vertices, and $\mathcal{O}(n^{12}m^5)$ total evolution time, where L is the wave packet length, n is the number of logical qubits, and m is the number of logical gates used. We suspect that these bounds are overly conservative and that further analysis could significantly reduce the degree of these polynomials.

V. Universality in the Dilute Limit

Similar universality arguments to those given for the t-J model, which governs the Hubbard model at half-filling in the limit of large positive U, apply to the Hubbard model itself. In that case, the wave packets are excitations prepared above the fermionic vacuum, as defined by the Hubbard model annihilation operators $c_{i\sigma}$.

If we restrict to the $|S\rangle$ sector, the scattering problem becomes identical to the one solved in Appendix B of Childs *et al.* [11] for the Bose-Hubbard model, since the spatial part of the fermionic wavefunction must be symmetric in the $|S\rangle$ sector. The other sectors have no interaction and therefore trivial scattering. The scattering produces a phase in the spin singlet sector. As a result, two-particle scattering induces an entangling unitary operator of the same form as eq. (3), with the phase a function of U rather than J. As in our analysis of the t-J model, repeated use of such a unitary can be used to simulate controlled Heisenberg interactions and thereby build universal quantum computation.

VI. Discussion

The fermionic Hubbard model, despite its simplicity, captures many essential features of the physics of electrons in solids. In our work, we show that that rich variety of behavior extends to universal quantum computation: simulating the Hubbard model on an arbitrary graph, both just below half-filling and in the dilute limit, is as hard as simulating an arbitrary quantum computation. The graph itself encodes the computation to be performed. More specifically, it is possible in principle to perform arbitrary quantum computations by scattering wave packets through a graph, with interactions governed by the Hubbard model.

The approach we chose to encode these computations is to simulate the Heisenberg Hamiltonian with time-varying control by discrete scattering events, each of which have the same effect as a short period of Heisenberg interaction. As a simple special case of this procedure, our method can therefore obviously be used to simulate the Heisenberg Hamiltonian on a line or lattice.

In the case of strong coupling at half-filling, there is only reflection and no transmission in the scattering events, as would be the case for classical hard spheres. This provides an amusing echo of the Fredkin-Toffoli billiard ball computer that played an important role in the history of reversible computation [18].

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