

# Universal computation by multi-particle quantum walk

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Quantum walk is a versatile and intuitive framework for developing quantum algorithms. Applications of quantum walk include an example of exponential speedup over classical computation [6] and optimal algorithms for element distinctness [3] and formula evaluation [8].

Quantum walk can also be viewed as a model of computation. From this perspective it is natural to ask which quantum computations can be performed efficiently by quantum walk. This question was answered in reference [5] where it was shown that any  $n$ -qubit quantum circuit  $\mathcal{C}$  can be efficiently simulated by a continuous-time quantum walk on a suitably designed sparse unweighted graph  $G_{\mathcal{C}}$ . This graph is exponentially large as a function of  $n$ , as required to account for the size of the Hilbert space. Although the quantum walk on such a graph can be efficiently simulated by a universal quantum computer [2], it may be no more natural to implement this walk than to perform a general quantum computation.

In this work we consider a generalization of quantum walk to systems with more than one walker on a graph. A continuous-time, multi-particle quantum walk is generated by a time-independent Hamiltonian with a term corresponding to a single-particle quantum walk for each particle, along with a term corresponding to an interaction between particles. We show that multi-particle quantum walk is capable of universal quantum computation. Specifically, we show that any  $n$ -qubit circuit with  $g$  gates can be simulated by the dynamics of  $\mathcal{O}(n)$  particles that interact for a time  $\text{poly}(n, g)$  on an unweighted planar graph of maximum degree 4 with  $\text{poly}(n, g)$  vertices. We present explicit universal constructions based on the Bose-Hubbard model, fermions with nearest-neighbor interactions, and distinguishable particles with nearest-neighbor interactions. We also show that almost any interaction between indistinguishable particles can be used to perform universal computation.

Because our graphs are exponentially smaller (as a function of  $n$ ) than those used in the single-particle universality construction, the multi-particle quantum walks we describe can be efficiently implemented using an architecture where vertices of the graph are represented by devices at different spatial locations. Recently, there has been considerable interest in experimentally implementing multi-particle quantum walk [4, 10, 11, 12] and these experiments can be viewed as first steps toward implementing our construction. However, these experiments only involve non-interacting particles; a nontrivial interaction appears necessary for universality [1, 13]. Our work serves to clarify the necessary resources for universal computation and provides a set of concrete goals for experimental implementation of multi-particle quantum walk.

Performing universal computation using quantum walk is nontrivial since the model is highly restricted. Not only must the computation be performed without time-dependent control, it must also be encoded entirely in the choice of a graph, with no ability to adjust edge weights to implement a desired gate. The previous single-particle universality construction was based on scattering a quantum walker through subgraphs that implement gates, but scattering is substantially more complicated in many-body interacting systems. To overcome this challenge, we design a multi-particle quantum walk that is well approximated by independent one- and two-particle scattering processes, and develop tools to make this approximation precise.

We have demonstrated the computational power of a broad class of many-body systems in the absence of time-dependent control. Since it is also possible to efficiently simulate a multi-particle quantum walk of the type we consider using a universal quantum computer, we have shown that this model exactly captures the power of quantum computation. Viewed from a different perspective, our result provides limitations on classical simulation of many-body interacting systems. For example, assuming quantum computers are more powerful than classical ones, our work implies that the dynamics of the Bose-Hubbard model on a sparse, planar graph cannot be efficiently simulated on a classical computer.

**Multi-particle quantum walk** In a multi-particle quantum walk, the particles interact on a given simple graph  $G$  with vertex set  $V(G)$  and edge set  $E(G)$ . The Hilbert space for  $m$  distinguishable particles on

$G$  is spanned by states  $|i_1, \dots, i_m\rangle$  where  $i_w \in V(G)$  is the location of the  $w$ th particle. A continuous-time, multi-particle quantum walk of  $m$  distinguishable particles on  $G$  is generated by a time-independent Hamiltonian

$$H_G^{(m)} = \sum_{w=1}^m \sum_{(i,j) \in E(G)} \left( |i\rangle\langle j|_w + |j\rangle\langle i|_w \right) + \sum_{i,j \in V(G)} \mathcal{U}_{ij}(\hat{n}_i, \hat{n}_j), \quad (1)$$

where the subscript  $w$  indicates that the operator acts on the location register for the  $w$ th particle (and as the identity on all other particles). Here  $\mathcal{U}_{ij}(\hat{n}_i, \hat{n}_j)$  is a function of the number operators  $\hat{n}_i$  and  $\hat{n}_j$  that count the numbers of particles located at vertices  $i$  and  $j$ , respectively (explicitly,  $\hat{n}_i = \sum_{w=1}^m |i\rangle\langle i|_w$ ).

The first term of (1) allows particles to move between adjacent sites, while the second term is an interaction between particles. We place some physically-motivated restrictions on the interaction terms that we consider (see the technical version [7] for more details). Our framework includes models with on-site interactions, nearest-neighbor interactions, and other types of local interaction terms.

States representing  $m$  indistinguishable particles can be represented in the distinguishable-particle basis as states that are either symmetric (if the particles are bosons) or antisymmetric (if the particles are fermions) under the interchange of any two particles. A notable example of a bosonic multi-particle quantum walk, the well-known Bose-Hubbard model, is obtained with on-site interaction term  $\mathcal{U}_{ij}(\hat{n}_i, \hat{n}_j) = (U/2)\delta_{i,j}\hat{n}_i(\hat{n}_i - 1)$  (here  $U$  is a constant that sets the strength of the interaction).

**Universal computation** In this section we describe (at a high level) how to simulate a quantum circuit using a multi-particle quantum walk of indistinguishable particles on an unweighted nonplanar graph. Extensions using planar graphs and distinguishable particles are given in the technical version [7].

We first transform the  $n$ -qubit quantum circuit  $\mathcal{C}$  that we want to simulate into an  $(n + 1)$ -qubit circuit  $\mathcal{C}'$  of a certain canonical form. We call the original  $n$  qubits *computational qubits*; the additional qubit is an ancilla qubit that we call the *mediator qubit*. All two-qubit gates in the circuit  $\mathcal{C}'$  are of the form  $C\theta = \text{diag}(1, 1, 1, e^{i\theta})$  acting between one of the computational qubits and the mediator qubit. For almost any value of  $\theta$ , we can approximate  $\mathcal{C}$  by a circuit  $\mathcal{C}'$  of this form. For our scheme the  $\theta$  we use depends on the particle statistics and interaction type as explained below.

Qubits are encoded as single-particle wave packets that move with momentum  $k$ . Each of the  $n+1$  qubits is represented in a dual-rail encoding using two paths that run through the graph, as shown in Figure 2. The computational basis states  $|0\rangle$  and  $|1\rangle$  are encoded as states with the particle moving along one of two paths. For the  $n$  computational qubits, we use wave packets with the same momentum ( $k = -\pi/4$ ), but the mediator is encoded with a different momentum ( $k = -\pi/2$ ).

To implement single-qubit unitaries on each of the encoded qubits, we design the graph so that the particles scatter through a sequence of small subgraphs while remaining far from one another. The specific subgraphs that we use for this purpose are given in the technical version [7].

Implementing two-qubit gates is more challenging since we must find a two-particle scattering process that is tractable to analyze. Using the symmetry of two indistinguishable particles interacting on a long path, we can show that two wave packets initially traveling toward each other on a long path will continue to travel after scattering as if no interaction occurred, except that the phase of the wave function is modified. We write  $e^{i\theta}$  for the phase acquired at the momenta relevant to our construction.

Figure 1(b) shows the graph used to implement the  $C\theta$  gate between a computational qubit (encoded using the paths labeled  $c$ ) and the mediator qubit (paths labeled  $m$ ). A key ingredient is a subgraph we call the *momentum switch*, as depicted in Figure 1(a).

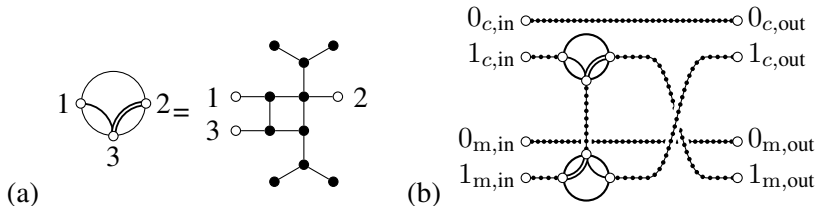


Figure 1: (a) Momentum switch. (b)  $C\theta$  gate.

The momentum switch has perfect transmission between vertices 1 and 3 at momentum  $-\pi/4$  and perfect transmission between vertices 2 and 3 at momentum  $-\pi/2$ . In other words, a particle with momentum  $-\pi/2$  follows the double line, while a particle with momentum  $-\pi/4$  follows the single line. To see why the graph in [Figure 1\(b\)](#) implements a  $C\theta$  gate, consider the movement of two particles as they pass through the graph. If either particle begins on the path  $0_{\text{in}}$ , it travels along a path to the output without interacting with the second particle. When the computational particle begins on the path  $1_{c,\text{in}}$ , it is routed downward as it passes through the top momentum switch. It travels down the vertical path and then is routed to the right as it passes through the bottom switch. Similarly, when the mediator particle begins on the path  $1_{m,\text{in}}$ , it is routed upward through the vertical path at the bottom switch and then to the right at the top switch. If both particles begin on the path  $1_{\text{in}}$ , then they interact on the vertical path. In this case, as the two particles move past each other, the wave function acquires a phase  $e^{i\theta}$  arising from this interaction.

To illustrate how these ingredients are put together, a graph corresponding to a simple quantum circuit  $\mathcal{C}'$  with two computational qubits and a mediator qubit is depicted in [Figure 2](#). Here the placeholders labeled  $B, H, T$  represent subgraphs that implement specific single-qubit gates. In this example, to initialize the system we prepare two single-particle wave packets with momentum  $-\pi/4$  and a single-particle wave packet with momentum  $-\pi/2$ , with support on the paths on the left-hand side of the figure. We then allow the quantum system to evolve for a total time  $T$  using the multi-particle quantum walk Hamiltonian (the technical version [\[7\]](#) describes how  $T$  is chosen). A subsequent measurement of the locations of the particles gives the result of the computation.

**Bounding the error** To prove that our construction works, we further develop the theory of scattering on graphs [\[9\]](#). Notable previous applications of such scattering include the quantum algorithm for the Hamiltonian NAND tree [\[8\]](#) and the single-particle universality construction [\[5\]](#).

Whereas the previous single-particle universality construction was analyzed using the method of stationary phase, we develop new techniques to analyze multi-particle scattering. We prove a theorem that approximates the time evolution of a single-particle wave packet incident on an arbitrary finite graph with any number of semi-infinite paths attached. We also prove a theorem that approximates the time-evolved state for two-particle wave packet scattering on an infinite path. These two theorems make statements about scattering of finite wave packets on infinite graphs. We also prove a “truncation lemma” that lets us apply our two theorems when the relevant scattering process takes place on a finite subgraph of a larger graph.

The bounds we prove using these tools are sufficient to establish universality with only polynomial overhead, but are almost certainly not optimal. For example, in the Bose-Hubbard model and models with nearest-neighbor interactions, we prove that the error can be made arbitrarily small by choosing the total number of vertices in the graph to be  $\mathcal{O}(n^{13}g^5)$  and the total evolution time to be  $\mathcal{O}(n^{12}g^5)$  (recall that  $n$  is the number of qubits and  $g$  is the number of gates in the circuit to be simulated).

**Conclusions** We have shown that a large class of quantum many-body systems defined on graphs are capable of universal computation. An intriguing open question is to determine the complexity of the analog of the local Hamiltonian problem for such models. Taking (say) the Bose-Hubbard model on a finite graph, one can ask if it is QMA-complete to approximate the ground state energy. Another avenue for future research is to develop new quantum algorithms based on multi-particle quantum walk.

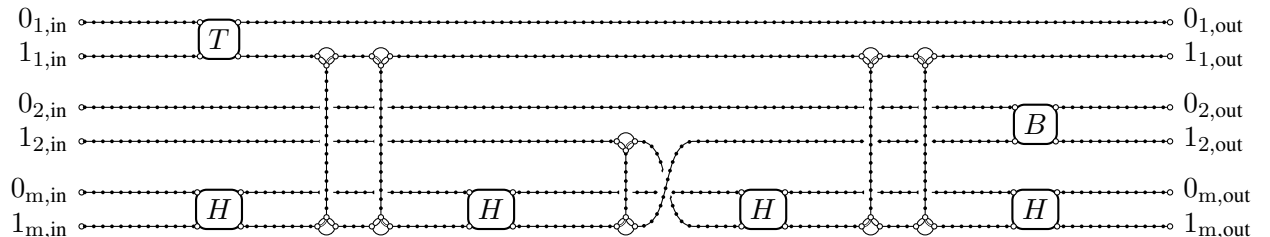


Figure 2: Schematic depiction of a graph implementing 5  $C\theta$  gates and 6 single qubit gates.

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