Quantum walk is a powerful tool for quantum computing. Inspired by classical random walks, both discrete- [1, 2] and continuous-time [9] quantum walks have been applied to computation. Here we consider continuous-time quantum walk on a graph, which is generated by Schrödinger time evolution with time-independent Hamiltonian given by the adjacency matrix of the graph.

Certain continuous-time quantum walks can be viewed as scattering processes. This connection has been used to develop algorithms [9, 8] and to establish universality of models of computation based on quantum walk [4, 6].

In the scattering framework, we consider infinite graphs obtained by attaching semi-infinite paths to a finite graph $\hat{G}$ at a subset of vertices called terminals, as shown in Figure 1. A particle can be initialized in a state that moves toward $\hat{G}$ on one of the semi-infinite paths under the Schrödinger time evolution. After some time the particle has scattered; it moves away from $\hat{G}$ and, in general, has some outgoing amplitude on each of the semi-infinite paths. With a carefully designed graph, such a scattering process can perform a quantum computation.

A discrete version of scattering theory can be used to compute the amplitude scattered into each path. The theory of scattering on graphs was introduced by Farhi and Gutmann in the setting with two semi-infinite paths [9]; Childs presented an application with an arbitrary number of semi-infinite

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Figure 1. (a) A finite graph $\hat{G}$ with $N$ semi-infinite paths attached. (b) A momentum switch. A particle moving toward vertex 1 with momentum $k$ transmits perfectly to the upper path (through vertex 2), while a particle with momentum $p$ transmits to the lower path (through vertex 3).
paths \cite{4}. Other work has described further basic properties of scattering on graphs \cite{12}, classified the scattering properties of some small graphs using a computer search \cite{3}, established a discrete analog of Levinson’s Theorem \cite{7, 5}, and proved completeness of the scattering and bound states \cite{5}.

While it is straightforward to compute the scattering behavior of a given graph, it is considerably more difficult to design a graph that implements some desired scattering behavior. In this paper we construct graphs with particular scattering behavior and also show that certain behaviors cannot occur. We hope that these ideas will ultimately prove useful in the development of scattering algorithms.

We focus on a scattering gadget called a momentum switch. A momentum switch has three terminals (i.e., has the form of Figure 1 with $N = 3$) and has special scattering properties for (at least) two momenta $k$ and $p$. A particle with momentum $k$ transmits perfectly between paths 1 and 2, whereas a particle with momentum $p$ transmits perfectly between paths 1 and 3. Thus a momentum switch routes a particle in a direction that depends on its momentum, as shown in Figure 1. A switch between momenta $-\frac{\pi}{3}$ and $-\frac{2\pi}{3}$ was a key tool in the multi-particle quantum walk universality construction \cite{6}.

**Construction of momentum switches.** We construct momentum switches between various pairs of momenta. Our construction proceeds by considering a closely-related type of graph called a reflection/transmission (R/T) gadget. An R/T gadget is a graph with two terminals (as in Figure 1 with $N = 2$) such that some momenta transmit perfectly between the two paths, whereas other momenta perfectly reflect. The set of all momenta that perfectly transmit is called the transmission set of the gadget, while those that perfectly reflect are contained in the reflection set. The momentum switches we construct are built by combining R/T gadgets in a prescribed way.

We examine R/T gadgets of a restricted form, which correspond to attaching a finite graph $G_0$ to a single vertex of an infinite path. We discuss how the reflection and transmission sets of such gadgets are related to eigenstates of $G_0$. By analyzing the eigenstates of certain basic graphs (such as paths and cycles), we show how to construct R/T gadgets from them.

In some cases we show how, starting from an R/T gadget associated with a graph $G_0$, one can build a modified graph $G_0^{+\leftrightarrow}$ which is associated with an R/T gadget where the reflection and transmission sets are interchanged.

Using these two graphs, we construct a momentum switch by attaching $G_0$ and $G_0^{+\leftrightarrow}$ to the leaves of a claw. By construction, one gadget perfectly reflects and the other perfectly transmits at each relevant momentum of $G_0$. At each such momentum, one leaf of the claw is forced to have zero amplitude (corresponding to perfect reflection), while the other has amplitude of norm one (corresponding to perfect transmission). The resulting scattering eigenstate corresponds exactly to that of a momentum switch.

For example, we instantiate this construction by creating a momentum switch between $k = -\frac{\pi}{3}$ and $p = -\frac{2\pi}{3}$ as shown in Figure 2.


**Impossibility results.** While our results provide some hope for constructing general momentum switches, we also prove that that some pairs of momenta do not admit a momentum switch. In particular, we prove that there is no switch between momenta \(-\frac{\pi}{4}\) and \(-\frac{3\pi}{4}\). (These momenta are relevant because a switch between them would simplify a multi-particle universality construction along the lines of [6], but our proof technique also works for some other pairs of momenta.)

Our proof again uses the concept of R/T gadgets. In particular, a switch between two momenta implies the existence of an R/T gadget between those momenta (which can be constructed by simply removing one of the semi-infinite paths of the switch). Hence, by showing that no R/T gadget exists between \(-\frac{\pi}{4}\) and \(-\frac{3\pi}{4}\), we also show that no momentum switch exists between them.

By examining the finite matrices that arise when constructing the scattering states for a 2-terminal gadget and observing that every term in the corresponding eigenvalue equations is from the field \(\mathbb{Q}(\sqrt{2})\), we show that the scattering eigenstate at momentum \(-\frac{\pi}{4}\) can be written as

\[
|\text{sc}_j(-\frac{\pi}{4})\rangle = \alpha (H + \sqrt{2}) |a\rangle,
\]

where \(H\) is the adjacency matrix of the graph, \(|a\rangle\) is a 2-eigenvector of \(H^2\) with only rational amplitudes, and \(\alpha \in \mathbb{C}\). By replacing \(\sqrt{2}\) with \(-\sqrt{2}\), we then construct an eigenstate at momentum \(-\frac{3\pi}{4}\) with similar amplitudes to that of \(|\text{sc}_j(-\frac{\pi}{4})\rangle\) (in particular, those vertices with no amplitude are the same for both states). If a gadget perfectly reflects at \(-\frac{\pi}{4}\), we then have a scattering state at momentum \(-\frac{3\pi}{4}\) with no amplitude along one path, implying that the gadget also perfectly reflects at momentum \(-\frac{3\pi}{4}\). Hence, an R/T gadget cannot exist between these two momenta, and neither can a momentum switch.

**Approximate switches.** While the non-existence of a momentum switch between \(-\frac{\pi}{4}\) and \(-\frac{3\pi}{4}\) is unfortunate, we also show that it is not insurmountable: we construct a sequence of gadgets that approximates such a switch arbitrarily well. This approximate construction can be viewed as a kind of interferometry: we split an incoming wave packet into an equal superposition, apply a momentum-dependent phase along one of the paths, and then recombine the wave packet into one of two output paths. To split and recombine the wave packet, we use the basis-changing graph from the universality construction [4]. We also construct a new graph \(g_0\) with perfect transmission and an irrational phase factor at both momenta of interest. By using multiple copies of \(g_0\) in series, we can apply the momentum-dependent phase gate with arbitrarily good (but not perfect) precision, where the precision determines the requisite number of copies of \(g_0\).

**Extensions and open questions.** We hope that these results facilitate the construction of scattering algorithms. Our results could be used to design variants of the multi-particle quantum walk construction with different logical encodings. Alternatively, momentum switches might be useful for a scattering algorithm with information encoded into many different momenta, so as to selectively apply unitaries.

Along different lines, exact implementation of an S-matrix by scattering on an unweighted graph is analogous to exact synthesis of unitary operations using a finite set of gates [11, 10]. It might be interesting to further explore the set of S-matrices that can be realized by scattering on graphs, and perhaps to characterize the set of momentum switches that can be implemented.

Our construction only works for gadgets of a restricted form. It would be more satisfying to determine necessary and sufficient conditions for a graph to be a momentum switch (or even an R/T gadget) without restricting the form of the gadget.

More generally, one might consider the problem of designing scattering gadgets with other restrictions on the allowed Hamiltonian. Here we have assumed that the Hamiltonian is the adjacency matrix of a simple graph. One might also consider, say, Laplacians of graphs. Another natural model would allow matrices whose entries are unrestricted, but that can have at most some number of nonzero entries in each row (i.e., whose underlying graphs have bounded degree).
References


