Quantum Information and Computation, Vol. 15, No. 7&8 (2015) 0601–0621

MOMENTUM SWITCHES

ANDREW M. CHILDS DAVID GOSSET
Department of Combinatorics & Optimization, University of Waterloo
Institute for Quantum Computing, University of Waterloo
amchilds@uwaterloo.ca dngosset@gmail.com

DANIEL NAGAJ
Faculty of Physics, University of Vienna
Institute of Physics, Slovak Academy of Sciences
daniel.nagaj@univie.ac.at

MOUKTIK RAHA
Institute for Quantum Computing, University of Waterloo
Department of Physics and Meteorology, Indian Institute of Technology Kharagpur
mouktikraha@gmail.com

ZAK WEBB
Institute for Quantum Computing, University of Waterloo
Department of Physics & Astronomy, University of Waterloo
zakwwebb@gmail.com

Received June 27, 2014
Revised October 24, 2014

Certain continuous-time quantum walks can be viewed as scattering processes. These processes can perform quantum computations, but it is challenging to design graphs with desired scattering behavior. In this paper, we study and construct momentum switches, graphs that route particles depending on their momenta. We also give an example where there is no exact momentum switch, although we construct an arbitrarily good approximation.

Keywords: quantum walk, scattering theory

Communicated by: R Cleve & R de Wolf

1 Introduction

Quantum walk is a powerful tool for quantum computation. In particular, the concept of scattering on graphs has been used to develop algorithms [1, 2] and to establish universality of models of computation based on quantum walk [3, 4].

In the scattering framework, we consider an infinite graph obtained by attaching semi-infinite paths to some of the vertices of a finite graph $\hat{G}$, as shown in Figure 1. (The vertices to which semi-infinite paths are attached are called *terminals*.) A particle is initialized in a state that moves toward $\hat{G}$ on one of the semi-infinite paths. After some time the particle has scattered; it moves away from $\hat{G}$ and, in general, has some outgoing amplitude on each

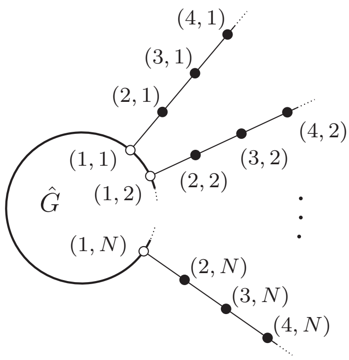

Fig. 1. An infinite graph G obtained from a finite graph $\hat{G}$ by attaching N semi-infinite paths. The open circles are *terminals*, vertices of $\hat{G}$ to which semi-infinite paths are attached. The internal vertices of $\hat{G}$ are not shown.

of the semi-infinite paths. By choosing the graph carefully, such a scattering process can be designed to 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 [1]; Childs presented an application with an arbitrary number of semi-infinite paths [3]. Other work has described further basic properties of scattering on graphs [5], classified the scattering properties of some small graphs using a computer search [6], established a discrete analog of Levinson's Theorem [7, 8], and proved completeness of the scattering and bound states [8].

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. Our goal in this paper is to develop tools for constructing scattering gadgets. We hope that these ideas will ultimately prove useful in the design 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 2.

A switch between momenta $-\frac{\pi}{2}$ and $-\frac{\pi}{4}$ was used as a tool in the multi-particle quantum walk universality construction [4]. In this paper, we construct switches between other pairs of momenta 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 momentum switches we construct in this paper are built by combining R/T gadgets in a prescribed way.

We also show 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 two particular momenta are relevant not only because they provide a concrete limitation on the construction

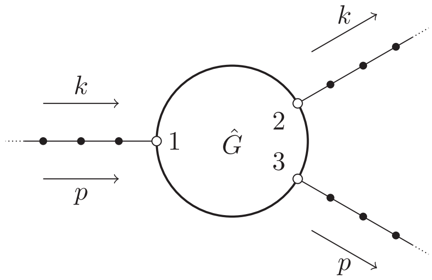

Fig. 2. A momentum switch. A particle moving toward vertex 1 with momentum k transmits perfectly to the upper path (through vertex 2), while a particle with momentum p transmits to the lower path (through vertex 3).

of momentum switches, but because they both support the universal gates constructed in [3], so a momentum switch between them would simplify a multi-particle universality construction along the lines of [4].) Nevertheless, we exhibit graphs that approximate a momentum switch at these two momenta to arbitrarily high precision.

The remainder of this paper is organized as follows. In Section 2 we review scattering theory on graphs. Then in Section 3 we define momentum switches and R/T gadgets. In Section 4 we give some explicit constructions of R/T gadgets, and in Section 5 we describe how to construct a momentum switch starting from a specific type of R/T gadget. Using this construction, we obtain a large class of momentum switches. In Section 6 we prove that there is no perfect momentum switch between $-\frac{\pi}{4}$ and $-\frac{3\pi}{4}$, and in Section 7 we describe approximate momentum switches between these momenta. We conclude in Section 8 with a discussion of the results and some directions for future work.

2 Continuous-time quantum walk and scattering theory

The continuous-time quantum walk on an unweighted graph G describes a particle moving (in superposition) between adjacent vertices of G. Specifically, the walk lives in the Hilbert space $\{|v\rangle : v \in V(G)\}$ and is generated by a time-independent Hamiltonian equal to the adjacency matrix of G.

As a motivating example, first consider the case where G is an infinite path. Then the Hamiltonian is

$$H = \sum_{x\in\mathbb{Z}} \big(|x\rangle\langle x+1| + |x+1\rangle\langle x|\big).$$

As with a free particle in one dimension (in the continuum), this Hamiltonian does not have any normalized eigenvectors. However, if we allow unnormalized states, then we can solve the eigenvalue equation and obtain eigenvectors $|\tilde{k}\rangle$ for each $k \in [-\pi, \pi)$, defined by $\langle x|\tilde{k}\rangle = e^{-ikx}$. These states satisfy $\langle x|H|\tilde{k}\rangle = E(k)\langle x|\tilde{k}\rangle$, where

$$E(k) = 2\cos(k).$$

We call these momentum states; the number $k \in [-\pi, \pi)$ is the corresponding momentum. While a momentum state is spread over the entire path, we can create a localized state, called a *wave packet*, by taking a superposition of states with similar momenta. A wave packet consisting of momenta near k moves with speed $\left|\frac{dE}{dk}\right| = |2\sin(k)|$ (see [4] for a formal discussion of how wave packets move).

Now consider the more general setup shown in Figure 1. An infinite graph G is obtained by attaching semi-infinite paths to N terminals of a finite graph $\hat{G}$. In this setting one can prepare a wave packet with momentum near k on the semi-infinite path labeled $j \in [N] := \{1, \ldots, N\}$; if $k \in (-\pi, 0)$, the particle moves toward $\hat{G}$. After some time the particle will have scattered off $\hat{G}$ and will be in a superposition of states that move away from $\hat{G}$ on the semi-infinite paths. Scattering theory provides tools for understanding such a process.

In particular, the dynamics of scattering off $\hat{G}$ are closely related to certain eigenvectors of G. For any $k \in (-\pi, 0)$ and any semi-infinite path $j \in [N]$, G has an *incoming scattering state* $|\mathrm{sc}_j(k)\rangle$ satisfying $H|\mathrm{sc}_j(k)\rangle = 2\cos(k)|\mathrm{sc}_j(k)\rangle$. Label vertices on the semi-infinite paths by (x, j'), where $j' \in [N]$ labels the path and $x \in \mathbb{Z}^+ := \{1, 2, \ldots\}$ labels the location on the path. The incoming scattering states have the form

$$\langle x, j'|\mathrm{sc}_j(k)\rangle = \delta_{j',j}e^{-ikx} + S_{j',j}(k)e^{ikx} \tag{1}$$

on the semi-infinite paths, where $S(k)$ is a unitary matrix called the S-matrix [8]. Although the S-matrix is defined through the scattering eigenstates of the Hamiltonian, it is a nontrivial fact that this matrix describes the dynamics of wave packet scattering (see, e.g., Theorem 1 of [4]). Specifically, the matrix element $S_{j',j}(k)$ can be interpreted as the amplitude for a wave packet with momentum k to scatter from the jth semi-infinite path to the j'th.

For any fixed momentum $k \in (-\pi, 0)$, the S-matrix can be computed by solving a system of linear equations. Any state of the form (1) on the semi-infinite paths satisfies the eigenvalue equation $\langle v|H|\mathrm{sc}_j(k)\rangle = 2\cos(k)\langle v|\mathrm{sc}_j(k)\rangle$ for all vertices $v \in V(G) \setminus V(\hat{G})$, independent of the form of $S(k)$. Suppose $\hat{G}$ has $m \geq N$ vertices, including N terminals and $m - N$ *internal vertices* (vertices to which semi-infinite paths are not attached). Then the m conditions $\langle v|H|\mathrm{sc}_j(k)\rangle = 2\cos(k)\langle v|\mathrm{sc}_j(k)\rangle$ for vertices $v \in V(\hat{G})$ constrain the N parameters $S_{j',j}(k)$ for $j' \in [N]$ as well as the $m - N$ amplitudes $\langle v|\mathrm{sc}_j(k)\rangle$ for internal vertices v.

There is a subtle technical point here that is reflected in the terminology used in the remainder of the paper. Generically these m equations completely determine the m unknown parameters and hence the state $|\mathrm{sc}_j(k)\rangle$, but in special cases these equations have more than one solution. This occurs only if there are one or more *confined bound states*, eigenstates of H with no amplitude on the semi-infinite paths [8]. Given a confined bound state $|\psi_c\rangle$ with eigenvalue $2\cos(k)$, any state of the form $|\mathrm{sc}_j(k)\rangle + \alpha|\psi_c\rangle$ also satisfies the eigenvalue equation. Although $|\mathrm{sc}_j(k)\rangle$ is specified uniquely by demanding orthogonality to the confined bound states [8], all states of the form $|\mathrm{sc}_j(k)\rangle + \alpha|\psi_c\rangle$ have the same amplitudes on the semi-infinite paths and hence the same S-matrix (since a confined bound state $|\psi_c\rangle$ has no amplitude on the semi-infinite paths). In the remainder of the paper, we use the term scattering state to describe any state of the form $|\mathrm{sc}_j(k)\rangle + \alpha|\psi_c\rangle$.

Note that H may have eigenstates that are neither scattering states nor confined bound states [8], but they are not relevant here since they cannot have the same eigenvalue as a scattering state.

A compact formula for the S-matrix and the states $|\mathrm{sc}_j(k)\rangle$ appears in reference [8]. Write the adjacency matrix of $\hat{G}$ in block form

$$\begin{pmatrix} A & B^\dagger \\ B & D \end{pmatrix} \tag{2}$$

where the first block corresponds to the terminals and the second to the internal vertices. Define the matrix

$$\gamma(z) = \begin{pmatrix} zA - \mathbb{I} & zB^\dagger \\ zB & zD - (1+z^2)\mathbb{I} \end{pmatrix}.$$

Then one can show that [8, Eq. (3.1)]

$$\begin{pmatrix} S(k) & 0 \\ e^{-ik}\Psi(k) & -e^{-2ik}\mathbb{I} \end{pmatrix} = -\gamma(e^{ik})^{-1}\gamma(e^{-ik})$$

where $\Psi(k)$ is an $(m-N)\times N$ matrix with $\langle v|\Psi(k)|j\rangle = \langle v|\mathrm{sc}_j(k)\rangle$ for all internal vertices v and all $j \in [N]$. If for some k_0 there is a confined bound state with eigenvalue $2\cos(k_0)$, then $\gamma(e^{ik_0})$ is singular and one should take the limit as $k \to k_0$ in the above equation. Another expression for the S-matrix is given by [8, Eq. (2.8)]

$$S(k) = -Q(e^{ik})^{-1}Q(e^{-ik}) \tag{3}$$

where

$$Q(z) = \mathbb{I} - z\big(A + B^\dagger[(z+\tfrac{1}{z})\mathbb{I} - D]^{-1}B\big).$$

For values of z on the unit circle, $[Q(z), Q(z^{-1})] = 0$ [8]. Using this fact and equation (3), one can show that the S-matrix is unitary. Since $Q(z)$ is a symmetric matrix, one can also show that the S-matrix is symmetric.

3 Momentum switches and reflection/transmission gadgets

As discussed in Section 1, a momentum switch is a special type of gadget that can be used to route a particle depending on its momentum. This property is naturally described in terms of the S-matrix.

For example, Figure 3 shows the momentum switch used in reference [4]. The S-matrix of this graph has a special form at momenta $-\frac{\pi}{4}$ and $-\frac{\pi}{2}$:

$$S_{\text{switch}}(-\tfrac{\pi}{4}) = \begin{pmatrix} 0 & 0 & e^{-i\pi/4} \\ 0 & -1 & 0 \\ e^{-i\pi/4} & 0 & 0 \end{pmatrix} \qquad S_{\text{switch}}(-\tfrac{\pi}{2}) = \begin{pmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

This equation says that a particle with momentum $-\frac{\pi}{4}$ traveling towards the graph along path 1 transmits perfectly to path 3 (i.e., the amplitude for this process has unit magnitude), whereas a particle with momentum $-\frac{\pi}{2}$ traveling along path 1 transmits perfectly to path 2. In other words, this graph is a momentum switch between momenta $-\frac{\pi}{4}$ and $-\frac{\pi}{2}$.

Generalizing this example, a finite graph $\hat{G}$ with three terminals (labeled $1,2,3$) is a momentum switch between two (disjoint) sets of momenta $\mathcal{D}, \mathcal{D}' \subset (-\pi, 0)$ if its S-matrix has perfect transmission from terminal 1 to terminal 2 at each momentum $k \in \mathcal{D}$ and perfect transmission from terminal 1 to terminal 3 at each momentum $p \in \mathcal{D}'$ (i.e., $|S_{1,2}(k)| = |S_{1,3}(p)| = 1$ for $k \in \mathcal{D}$ and $p \in \mathcal{D}'$). See Figure 2 for an illustration.

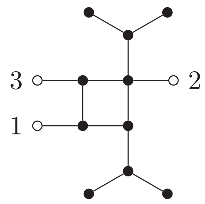

Fig. 3. The momentum switch from [4].

Momentum switches are closely related to another class of graphs that we call reflection/transmission (R/T) gadgets. An R/T gadget is a finite graph with two terminals. In addition, there exist two sets of momenta $\mathcal{R}, \mathcal{T} \subset (-\pi, 0)$ such that the gadget perfectly reflects (from both terminals) at all $k \in \mathcal{R}$ and perfectly transmits (between the two terminals) at all $p \in \mathcal{T}$ (i.e., $|S_{1,1}(k)| = |S_{1,2}(p)| = 1$ for $k \in \mathcal{R}$ and $p \in \mathcal{T}$).

There is a simple connection between R/T gadgets and momentum switches. While a momentum switch has three terminals and an R/T gadget only has two, we now show that by downgrading a terminal of a momentum switch $\hat{G}$ to an internal vertex (i.e., by removing the corresponding semi-infinite path from G), we can obtain an R/T gadget between the momenta separated by the switch.

Let $\hat{G}$ be a momentum switch and fix $k \in \mathcal{D}$ and $p \in \mathcal{D}'$. The S-matrix takes the form

$$S_{\text{switch}}(k) = \begin{pmatrix} 0 & T & 0 \\ T & 0 & 0 \\ 0 & 0 & R \end{pmatrix} \qquad S_{\text{switch}}(p) = \begin{pmatrix} 0 & 0 & T' \\ 0 & R' & 0 \\ T' & 0 & 0 \end{pmatrix}$$

where R, T, R', T' have unit magnitude, i.e., the switch connects paths 1 and 2 at momentum k and paths 1 and 3 at momentum p. Using equation (1), we see that the states $|\text{sc}_1(k)\rangle$, $|\text{sc}_2(k)\rangle$, and $|\text{sc}_2(p)\rangle$ have no amplitude on path 3.

Let G' be the graph obtained from G by removing the semi-infinite path connected to terminal 3, i.e., now we only attach semi-infinite paths to terminals 1 and 2. Since the states $|\text{sc}_1(k)\rangle$, $|\text{sc}_2(k)\rangle$, and $|\text{sc}_2(p)\rangle$ have no amplitude on the removed vertices, they remain eigenstates of G', and in particular they are still scattering states. Thus we can infer the S-matrix of G' from these states using (1), giving

$$S_{\text{R/T}}(k) = \begin{pmatrix} 0 & T \\ T & 0 \end{pmatrix} \qquad S_{\text{R/T}}(p) = \begin{pmatrix} R'' & T'' \\ 0 & R' \end{pmatrix},$$

where R'' and T'' need to be determined. Unitarity implies $T'' = 0$ and thus

$$S_{\text{R/T}}(p) = \begin{pmatrix} R'' & 0 \\ 0 & R' \end{pmatrix}.$$

Hence G' is an R/T gadget with $\mathcal{D} \subseteq \mathcal{T}$ and $\mathcal{D}' \subseteq \mathcal{R}$. The same construction can be used to obtain an R/T gadget with $\mathcal{D}' \subseteq \mathcal{T}$ and $\mathcal{D} \subseteq \mathcal{R}$ (by downgrading terminal 2 instead of terminal 3).

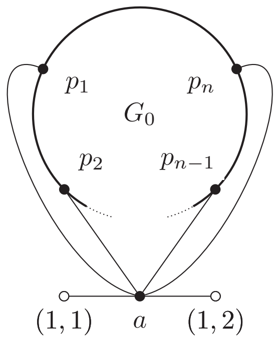

Fig. 4. A type 1 R/T gadget. Vertices of G_0 that are not part of the periphery $P = \{p_1, \ldots, p_n\}$ are not shown. The induced subgraph on vertices $V(G_0) \setminus P$ is denoted g_0.

4 Constructing R/T gadgets

In this Section we show how to design R/T gadgets between certain sets of momenta. We consider scattering on graphs obtained by attaching a finite graph G_0 to one vertex of an infinite path. The corresponding gadget, called a *type 1 R/T gadget*, is shown in Figure 4. We focus on such gadgets because their scattering properties are closely related to the eigenvectors of the subgraph G_0.

We refer to the graph shown in Figure 4 as $\hat{G}$, and we write G for the full graph obtained by attaching two semi-infinite paths to terminals $(1,1)$ and $(1,2)$. As shown in the Figure, the graph $\hat{G}$ for a type 1 gadget is determined by a finite graph G_0 and a subset $P = \{p_1, \ldots, p_n\} \subseteq V(G_0)$ of its vertices, called the *periphery*. Each vertex in the periphery is connected to a vertex denoted a, and a is also connected to two terminals $(1,1)$ and $(1,2)$. A type 1 R/T gadget with $n = 1$ has only one edge between G_0 and a; in this special case we also call it a *type 2 R/T gadget* (see Figure 5).

Looking at the eigenvalue equation for the scattering state $|\mathrm{sc}_1(k)\rangle$ at vertices $(1,1)$ and $(1,2)$, we see that the amplitude at vertex a satisfies

$$\langle a|\mathrm{sc}_1(k)\rangle = 1 + R(k) = T(k).$$

Thus perfect reflection at momentum k occurs if and only if $R(k) = -1$ and $\langle a|\mathrm{sc}_1(k)\rangle = 0$, while perfect transmission occurs if and only if $T(k) = 1$ and $\langle a|\mathrm{sc}_1(k)\rangle = 1$. Using this fact, we now derive conditions on the graph G_0 that determine when perfect transmission and reflection occur.

For type 1 gadgets, we give a necessary and sufficient condition for perfect reflection: G_0 should have an eigenvector for which the sum of amplitudes on the periphery is nonzero.

Lemma 1. *Let $\hat{G}$ be a type 1 R/T gadget. A momentum $k \in (-\pi, 0)$ is in the reflection set $\mathcal{R}$ if and only if G_0 has an eigenvector $|\chi_k\rangle$ with eigenvalue $2\cos(k)$ satisfying*

$$\sum_{i=1}^{n} \langle p_i|\chi_k\rangle \neq 0. \tag{4}$$

Proof. First suppose that $\hat{G}$ has perfect reflection at momentum k, i.e., $R(k) = -1$ and $\langle a|\mathrm{sc}_1(k)\rangle = 0$. Since $\langle (1,1)|\mathrm{sc}_1(k)\rangle = e^{-ik} - e^{ik} \neq 0$ and $\langle (1,2)|\mathrm{sc}_1(k)\rangle = 0$, to satisfy the eigenvalue equation at vertex a, we have

$$\sum_{j=1}^{n} \langle p_j|\mathrm{sc}_1(k)\rangle = e^{ik} - e^{-ik} \neq 0.$$

Further, since G_0 only connects to vertex a and the amplitude at this vertex is zero, the restriction of $|\mathrm{sc}_1(k)\rangle$ to G_0 must be an eigenvector of G_0 with eigenvalue $2\cos(k)$. Hence the condition is necessary for perfect reflection.

Next suppose that G_0 has an eigenvector $|\chi_k\rangle$ with eigenvalue $2\cos(k)$ satisfying (4), with the sum equal to some nonzero constant c. Define a scattering state $|\psi_k\rangle$ on the Hilbert space of the full graph G with amplitudes

$$\langle v|\psi_k\rangle = \frac{e^{ik} - e^{-ik}}{c} \langle v|\chi_k\rangle$$

for all $v \in V(G_0)$, $\langle a|\psi_k\rangle = 0$, and

$$\langle (x,j)|\psi_k\rangle = \begin{cases} e^{-ikx} - e^{ikx} & j = 1 \\ 0 & j = 2 \end{cases}$$

for all $x \in \mathbb{Z}^+$.

We claim that $|\psi_k\rangle$ is an eigenvector of G with eigenvalue $2\cos(k)$. The state clearly satisfies the eigenvalue equation on the semi-infinite paths since it is a linear combination of states with momentum $\pm k$. At vertices of G_0, the state is proportional to an eigenvector of G_0, and since the state as no amplitude at a, the eigenvalue equation is also satisfied at these vertices. It remains to see that the eigenvalue equation is satisfied at a, but this follows immediately by a simple calculation.

Since $|\psi_k\rangle$ has the form of a scattering state with perfect reflection, we see that $R(k) = -1$ and $T(k) = 0$ as claimed. □

The following Lemma gives a sufficient condition for perfect transmission (which is also necessary for type 2 gadgets). Let g_0 denote the induced subgraph on $V(G_0) \setminus P$ where $P = \{p_i : i \in [n]\}$ is the periphery.

Lemma 2. *Let $\hat{G}$ be a type 1 R/T gadget and let $k \in (-\pi, 0)$. Suppose $|\xi_k\rangle$ is an eigenvector of g_0 with eigenvalue $2\cos k$ and with the additional property that, for all $i \in [n]$,*

$$\sum_{\substack{v \in V(g_0): \\ (v,p_i) \in E(G_0)}} \langle v|\xi_k\rangle = c \neq 0 \tag{5}$$

for some constant c that does not depend on i. Then k is in the transmission set $\mathcal{T}$. If $\hat{G}$ is a type 2 R/T gadget, then this condition is also necessary.

Proof. If g_0 has a suitable eigenvector $|\xi_k\rangle$ satisfying (5), define a scattering state $|\psi_k\rangle$ on the full graph G, with amplitudes $\langle a|\psi_k\rangle = 1$,

$$\langle v|\psi_k\rangle = \begin{cases} -\frac{1}{c}\langle v|\xi_k\rangle & v \in V(g_0) \\ 0 & v \in P \end{cases} \tag{6}$$

in the graph G_0, and

$$\langle (x,j)|\psi_k\rangle = \begin{cases} e^{-ikx} & j=1 \\ e^{ikx} & j=2 \end{cases}$$

for $x \in \mathbb{Z}^+$. As in the proof of Lemma 1, the state $|\psi_k\rangle$ is clearly satisfies the eigenvalue equation (with eigenvalue $2\cos(k)$) at vertices on the semi-infinite paths and vertices of g_0. The factor of $-\frac{1}{c}$ in (6) is chosen so that the eigenvalue condition is satisfied at vertices in P. It is easy to see that the eigenvalue condition is also satisfied at a.

Since $|\psi_k\rangle$ is a scattering eigenvector of G with eigenvalue $2\cos(k)$ and perfect transmission, we have $T(k) = 1$.

Now suppose $\hat{G}$ is a type 2 R/T gadget (as shown in Figure 5), with $P = \{p\}$. Perfect transmission along with the eigenvalue equation at vertex a implies

$$\langle p|\mathrm{sc}_1(k)\rangle = 0,$$

so the restriction of $|\mathrm{sc}_1(k)\rangle$ to g_0 must be an eigenvector (since p is the only vertex connected to g_0). The eigenvalue equation at p gives

$$\langle a|\mathrm{sc}_1(k)\rangle + \sum_{w\colon (w,p)\in E(G_0)} \langle w|\mathrm{sc}_1(k)\rangle = 0 \quad \Longrightarrow \quad \sum_{w\colon (w,p)\in E(G_0)} \langle w|\mathrm{sc}_1(k)\rangle = -1.$$

Hence the restriction of $|\mathrm{sc}_1(k)\rangle$ to $V(g_0)$ is an eigenvector of the induced subgraph, with the additional property that the sum of the amplitudes at vertices connected to p is nonzero. □

4.1 Reflection/transmission set reversal

We now show how to switch the reflection and transmission sets for a type 2 gadget. In particular, for any such gadget with transmission set $\mathcal{T}$ and reflection set $\mathcal{R}$, we construct another (type 1) gadget with transmission set $\mathcal{T}'$ and reflection set $\mathcal{R}'$ such that $\mathcal{R} \subseteq \mathcal{T}'$ and $\mathcal{T} \subseteq \mathcal{R}'$.

The new R/T gadget $\hat{G}^{\leftrightarrow}$ is depicted in Figure 6. It is obtained by taking two copies of the subgraph g_0 from Figure 5, connecting both to a new vertex u, and connecting one copy of g_0 to the infinite path. More concretely, let $w_1, \ldots, w_r$ be the vertices of G_0 adjacent to p, as shown in Figure 5. For each vertex $v \in V(g_0)$ there are two corresponding vertices $v^{(1)}, v^{(2)} \in V(\hat{G}^{\leftrightarrow})$; in particular, for each vertex w_j there are two vertices $w_j^{(1)}, w_j^{(2)}$ in Figure 5, as shown in Figure 6. The vertex $u \in V(\hat{G}^{\leftrightarrow})$ is connected to the vertices $w_1^{(1)}, \ldots, w_n^{(1)}$ and $w_1^{(2)}, \ldots, w_n^{(2)}$. Vertices $w_1^{(1)}, \ldots, w_n^{(1)}$ are also connected to a vertex $a \in V(\hat{G}^{\leftrightarrow})$, and a is also connected to the two terminals $(1,1), (1,2) \in V(\hat{G}^{\leftrightarrow})$.

Lemma 3. *Let $\hat{G}$ be a type 2 R/T gadget with transmission set $\mathcal{T}$ and reflection set $\mathcal{R}$. The type 1 R/T gadget $\hat{G}^{\leftrightarrow}$ defined above has transmission set $\mathcal{T}' \supseteq \mathcal{R}$ and reflection set $\mathcal{R}' \supseteq \mathcal{T}$.*

Proof. First consider a momentum $k \in \mathcal{T}$. Using the condition derived in Lemma 2, we see that g_0 has an eigenvector $|\xi_k\rangle$ with eigenvalue $2\cos(k)$ where the sum of the amplitudes on vertices $w_1, \ldots, w_r$ is nonzero. Now consider the induced subgraph $G_0^{\leftrightarrow}$ of Figure 6 obtained by removing vertices $(1,1)$, $(1,2)$, and a. This subgraph has an eigenvector $|\chi_k^{\leftrightarrow}\rangle$ with eigenvalue $2\cos(k)$ given by

$$\langle v^{(i)}|\chi_k^{\leftrightarrow}\rangle = (-1)^i \langle v|\xi_k\rangle \quad \text{and} \quad \langle u|\chi_k^{\leftrightarrow}\rangle = 0$$

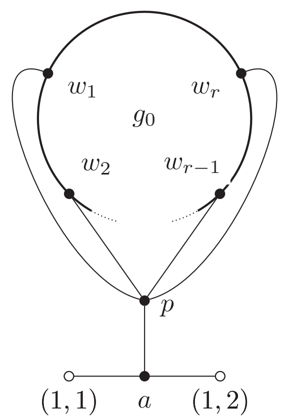

Fig. 5. A type 2 R/T gadget, i.e., a type 1 gadget with $|P| = 1$.

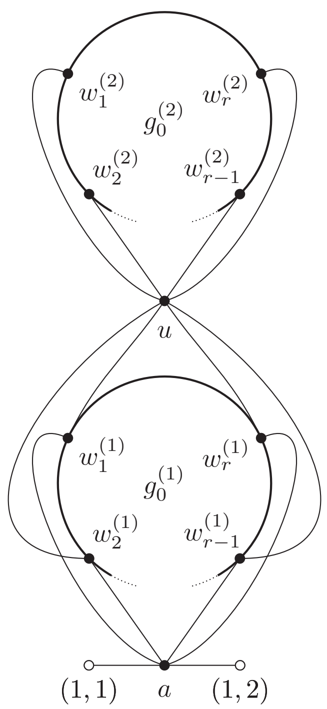

Fig. 6. The R/T gadget $\hat{G}^{\leftrightarrow}$ reversing the reflection and transmission sets of Figure 5.

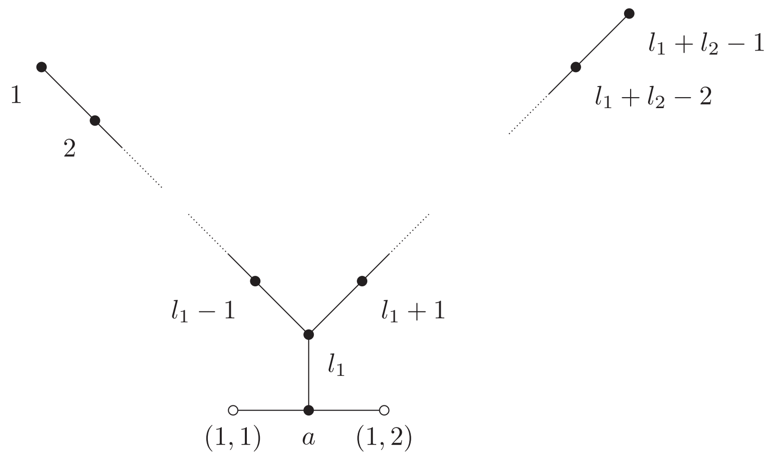

Fig. 7. An R/T gadget built from a path of length $l_1 + l_2 - 2$.

for all vertices $v \in V(g_0)$ and for $i \in \{1,2\}$. The fact that $|\chi_k^{\leftrightarrow}\rangle$ is an eigenvector follows because $|\xi_k\rangle$ is an eigenvector of g_0. Also, since $\sum_{j=1}^{r} \langle w_j|\xi_k\rangle \neq 0$, we have $\sum_{j=1}^{r} \langle w_j^{(1)}|\chi_k^{\leftrightarrow}\rangle \neq 0$. Using Lemma 1 we see that perfect reflection occurs at momentum k, so $\mathcal{T} \subseteq \mathcal{R}'$.

Next suppose $k \in \mathcal{R}$. Lemma 1 states that G_0 has an eigenvector $|\chi_k\rangle$ with eigenvalue $2\cos(k)$ such that $\langle p|\chi_k\rangle \neq 0$. Now consider the induced subgraph $g_0^{\leftrightarrow}$ of Figure 6 obtained by removing vertices $(1,1)$, $(1,2)$, a, and $w_1^{(1)}, \ldots, w_r^{(1)}$. This graph has an eigenvector $|\xi_k^{\leftrightarrow}\rangle$ with eigenvalue $2\cos(k)$ defined by

$$\langle v|\xi_k^{\leftrightarrow}\rangle = \begin{cases} \langle v|\chi_k\rangle & \text{for } v \in V(g_0^{(2)}) \\ \langle p|\chi_k\rangle & v = u \\ 0 & \text{otherwise.} \end{cases}$$

To see that this is an eigenvector, observe that $g_0^{\leftrightarrow}$ is a disconnected graph and $|\chi_k\rangle$ is an eigenvector of one of its components. Using this and Lemma 2 (since u is the only vertex adjacent to the periphery of $\hat{G}^{\leftrightarrow}$ with non-zero amplitude), we see that $k \in \mathcal{T}'$, so $\mathcal{R} \subseteq \mathcal{T}'$. □

4.2 Examples

We now present some examples of simple type 2 R/T gadgets.

4.2.1 Paths

As a first example, suppose G_0 is a finite path of length $l_1 + l_2 - 2$ connected to a at the l_1th vertex, as shown in Figure 7. We determine the reflection and transmission sets as a function of l_1 and l_2.

Using Lemma 1, we see that perfect reflection occurs at momentum $k \in (-\pi, 0)$ if and only if the path has an eigenvector with eigenvalue $2\cos(k)$ with non-zero amplitude on vertex l_1. Recall that the path of length L (where the length of a path is its number of edges) has

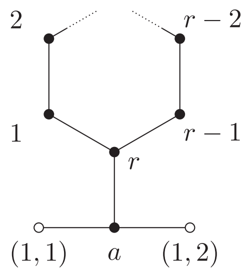

Fig. 8. An R/T gadget built from an r-cycle.

eigenvectors $|\psi_j\rangle$ for $j \in [L+1]$ given by

$$\langle x|\psi_j\rangle = \sin\left(\frac{\pi j x}{L+2}\right) \tag{7}$$

with eigenvalues $\lambda_j = 2\cos(\pi j/(L+2))$. Hence

$$\mathcal{R}_{\text{path}} = \left\{-\frac{\pi j}{l_1+l_2} : j \in [l_1+l_2-1] \text{ and } \frac{j l_1}{l_1+l_2} \notin \mathbb{Z}\right\}.$$

To characterize the momenta at which perfect transmission occurs, consider the induced subgraph obtained by removing the l_1th vertex from the path of length l_1+l_2-2 (a path of length l_1-2 and a path of length l_2-2). We can choose bases for the eigenspaces of this induced subgraph so that each eigenvector has all of its support on one of the two paths, and has nonzero amplitude on one of the vertices l_1-1 or l_1+1. Thus Lemma 2 implies that $\hat{G}$ perfectly transmits for all momenta in the set

$$\mathcal{T}_{\text{path}} = \left\{-\frac{\pi j}{l_1} : j \in [l_1-1]\right\} \cup \left\{-\frac{\pi j}{l_2} : j \in [l_2-1]\right\}.$$

For example, setting $l_1 = l_2 = 2$, we get $\mathcal{T}_{\text{path}} = \{-\frac{\pi}{2}\}$ and $\mathcal{R}_{\text{path}} = \{-\frac{\pi}{4}, -\frac{3\pi}{4}\}$.

4.2.2 Cycles

Suppose G_0 is a cycle of length r. Labeling the vertices by $x \in [r]$, where $x = r$ is the vertex attached to the path (as shown in Figure 8), the eigenvectors of the r-cycle are

$$\langle x|\phi_m\rangle = e^{2\pi i x m/r}$$

with eigenvalue $2\cos(2\pi m/r)$, where $m \in [r]$. For each momentum $k = -2\pi m/r \in (-\pi, 0)$, there is an eigenvector with nonzero amplitude on the vertex r (i.e., $\langle r|\phi_m\rangle \neq 0$), so Lemma 1 implies that perfect reflection occurs at each momentum in the set

$$\mathcal{R}_{\text{cycle}} = \left\{-\frac{\pi j}{r} : j \text{ is even and } j \in [r-1]\right\}.$$

To see which momenta perfectly transmit, we use Lemma 2. Consider the induced subgraph obtained by removing vertex r. This subgraph is a path of length $r-2$ and has eigenvalues $2\cos(\pi m/r)$ for $m \in [r-1]$ as discussed in the previous section. Using the expression (7) for the eigenvectors, we see that the sum of the amplitudes on the two ends is nonzero for odd values of m. Perfect transmission occurs for each of the corresponding momenta:

$$\mathcal{T}_{\text{cycle}} = \left\{ -\frac{\pi j}{r} : j \text{ is odd and } j \in [r-1] \right\}.$$

For example, the 4-cycle (i.e., square) has $\mathcal{T}_{\text{cycle}} = \{-\frac{\pi}{4}, -\frac{3\pi}{4}\}$ and $\mathcal{R}_{\text{cycle}} = \{-\frac{\pi}{2}\}$.

5 Constructing momentum switches

We now construct a momentum switch between the reflection and transmission sets $\mathcal{R}$ and $\mathcal{T}$ of a type 2 R/T gadget. We attach the gadget and its reversal (defined in Section 4.1) to the leaves of a claw, as shown in Figure 9. Specifically, given a type 2 R/T gadget $\hat{G}$, the corresponding momentum switch $\hat{G}^{\prec}$ consists of a copy of G_0, a copy of $G_0^{\leftrightarrow}$, and a claw. The three leaves of the claw are the terminals. Vertex p of G_0 is connected to leaf 2 of the claw, and vertices $w_1^{(1)}, \ldots, w_r^{(1)}$ of $G_0^{\leftrightarrow}$ are each connected to leaf 3 of the claw.

The high-level idea of the switch construction is as follows. For momenta in the transmission set, the gadget perfectly transmits while its reversal perfectly reflects, so the claw is effectively a path connecting terminals 1 and 2. For momenta in the reflection set, the roles of transmission and reflection are reversed, so the claw is effectively a path connecting terminals 1 and 3.

Lemma 4. *Let $\hat{G}$ be a type 2 R/T gadget with reflection set $\mathcal{R}$ and transmission set $\mathcal{T}$. The gadget $\hat{G}^{\prec}$ described above is a momentum switch between $\mathcal{R}$ and $\mathcal{T}$.*

Proof. We construct a scattering eigenstate for each momentum $k \in \mathcal{T}$ with perfect transmission from path 1 to path 2, and similarly construct a scattering eigenstate for each momentum $k' \in \mathcal{R}$ with perfect transmission from 1 to 3. These eigenstates show that $S_{2,1}(k) = 1$ and $S_{3,1}(k') = 1$. Since the S-matrix is symmetric and unitary, this gives the complete form of the S-matrix for all momenta in $\mathcal{R} \cup \mathcal{T}$. In particular, this shows that $\hat{G}^{\prec}$ is a momentum switch between $\mathcal{R}$ and $\mathcal{T}$.

We first construct the scattering states for momenta $k \in \mathcal{T}$. Lemma 2 shows that the graph g_0 has a $2\cos(k)$-eigenvector $|\xi_k\rangle$ satisfying equation (5) with some nonzero constant c. We define a state $|\mu_k\rangle$ on $G^{\prec}$ and we show that it is a scattering eigenstate with perfect transmission between paths 1 and 2. The amplitudes of $|\mu_k\rangle$ on the semi-infinite paths and the claw are

$$\langle (x,1)|\mu_k\rangle = e^{-ikx} \qquad \langle 0|\mu_k\rangle = 1 \qquad \langle (x,2)|\mu_k\rangle = e^{ikx} \qquad \langle (x,3)|\mu_k\rangle = 0.$$

The rest of the graph consists of the three copies of the subgraph g_0 and the vertices p and $u_{\leftrightarrow}$. The corresponding amplitudes are

$$\langle v|\mu_k\rangle = \begin{cases} -\frac{1}{c}\langle v|\xi_k\rangle & v \in V(g_0^{(1)}) \\ \frac{1}{c}\langle v|\xi_k\rangle & v \in V(g_0^{(2)}) \\ -\frac{e^{ik}}{c}\langle v|\xi_k\rangle & v \in V(g_0^{(3)}) \\ 0 & v = p \text{ or } v = u_{\leftrightarrow}. \end{cases}$$

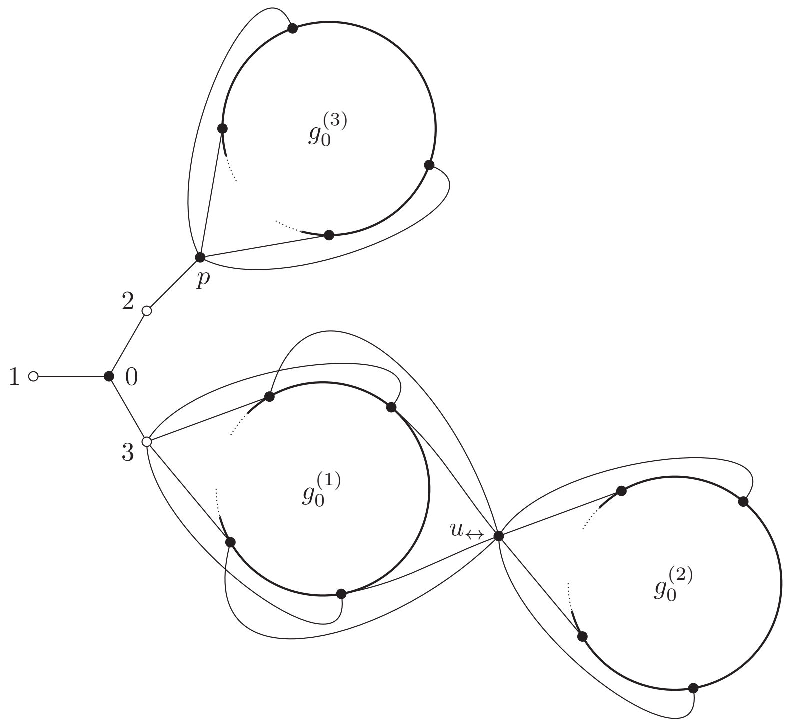

Fig. 9. A momentum switch $\hat{G}^{\prec}$ built from a type 2 R/T gadget and its reversal.

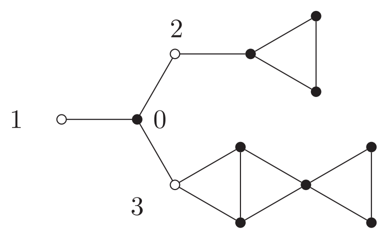

Fig. 10. A momentum switch between $-\frac{\pi}{3}$ and $-\frac{2\pi}{3}$.

We claim that $|\mu_k\rangle$ is an eigenstate of the Hamiltonian with eigenvalue $2\cos(k)$. As in previous proofs, the state clearly satisfies the eigenvalue condition on the semi-infinite paths and at the vertices of G_0 and $G_0^{\leftrightarrow}$, and the factors of $\frac{1}{c}$ in the above equation are chosen so that it also satisfies the eigenvalue condition at vertices p and $u_{\leftrightarrow}$. Since $|\mu_k\rangle$ is a scattering state with perfect transmission from path 1 to path 2, we see that $S_{2,1}(k) = 1$.

Finally, we construct an eigenstate $|\nu_{k'}\rangle$ with perfect transmission from path 1 to path 3 for each momentum $k' \in \mathcal{R}$. This state has the form

$$\langle (x,1)|\nu_{k'}\rangle = e^{-ik'x} \qquad \langle 0|\nu_{k'}\rangle = 1 \qquad \langle (x,2)|\nu_{k'}\rangle = 0 \qquad \langle (x,3)|\nu_{k'}\rangle = e^{ik'x}$$

on the semi-infinite paths and the claw. Lemma 1 shows that G_0 has a $2\cos(k')$-eigenstate $|\chi_{k'}\rangle$ with $\langle p|\chi_{k'}\rangle \neq 0$, which determines the form of $|\nu_{k'}\rangle$ on the remaining vertices:

$$\langle v|\nu_{k'}\rangle = \begin{cases} -\frac{1}{\langle p|\chi_{k'}\rangle}\langle v|\chi_{k'}\rangle & v \in V(G_0) \\ -\frac{e^{ik'}}{\langle p|\chi_{k'}\rangle}\langle v|\chi_{k'}\rangle & v \in V(g_0^{(2)}) \\ -e^{ik'} & v = u^{\leftrightarrow} \\ 0 & \text{otherwise.} \end{cases}$$

As before, it is easy to check that this a momentum-k' scattering state with perfect transmission from path 1 to path 3, so $S_{3,1}(k') = 1$.

Thus the gadget from Figure 9 is a momentum switch between $\mathcal{R}$ and $\mathcal{T}$. □

Using this construction, we can obtain a momentum switch from any of the examples discussed in Section 4.2. For example, using the R/T gadget built from the 3-cycle, we get a momentum switch between $-\frac{\pi}{3}$ and $-\frac{2\pi}{3}$, as shown in Figure 10. More generally, using an r-cycle, we obtain a switch between momenta of the form $-\frac{\pi j}{r}$ with odd or even values of j. As another example, using a path of length 4 connected at the center vertex, we obtain a switch between $-\frac{\pi}{4}$ and $-\frac{\pi}{2}$ that differs from the one shown in Figure 3.

6 Impossibility of a momentum switch between $-\frac{\pi}{4}$ and $-\frac{3\pi}{4}$

In this Section we prove that there does not exist a momentum switch between momenta $-\frac{\pi}{4}$ and $-\frac{3\pi}{4}$. We begin by proving that there is a basis for the space of scattering states with momentum $k = -\frac{\pi}{4}$ or $k = -\frac{3\pi}{4}$ where each basis vector has entries in $\mathbb{Q}(\sqrt{2})$. We then use this to prove that there is no R/T gadget between these two momenta. Since any momentum switch can be converted into an R/T gadget between the momenta it separated (as shown in Section 3), this implies that no momentum switch exists between $-\frac{\pi}{4}$ and $-\frac{3\pi}{4}$.

6.1 Basis vectors with entries in $\mathbb{Q}(\sqrt{2})$

Recall the general setup shown in Figure 1: N semi-infinite paths are attached to a finite graph $\hat{G}$. Consider an eigenvector $|\tau_k\rangle$ of the adjacency matrix of G with eigenvalue $2\cos(k)$ for $k \in (-\pi, 0)$. In general this eigenspace is spanned by incoming scattering states with momentum k and confined bound states [8] (which have zero amplitude on the semi-infinite paths). We can thus write the amplitudes of $|\tau_k\rangle$ on the semi-infinite paths as

$$\langle (x,j)|\tau_k\rangle = \kappa_j \cos(k(x-1)) + \sigma_j \sin(k(x-1))$$

for $x \in \mathbb{Z}^+$, $j \in [N]$, and $\kappa_j, \sigma_j \in \mathbb{C}$, and the amplitudes on the internal vertices as

$$\langle w|\tau_k\rangle = \iota_w$$

for $\iota_w \in \mathbb{C}$, where w indexes the internal vertices. We write the adjacency matrix of $\hat{G}$ as a block matrix as in (2). Since the state $|\tau_k\rangle$ satisfies the eigenvalue equation on the semi-infinite paths, it remains to satisfy the conditions specified by the block matrix equation

$$\begin{pmatrix} A & B^\dagger \\ B & D \end{pmatrix} \begin{pmatrix} \kappa \\ \iota \end{pmatrix} + \cos(k) \begin{pmatrix} \kappa \\ 0 \end{pmatrix} + \sin(k) \begin{pmatrix} \sigma \\ 0 \end{pmatrix} = 2\cos(k) \begin{pmatrix} \kappa \\ \iota \end{pmatrix}.$$

Hence, the nullspace of the matrix

$$M = \begin{pmatrix} A - \cos(k)\mathbb{I} & \sin(k)\mathbb{I} & B^\dagger \\ 0 & 0 & 0 \\ B & 0 & D - 2\cos(k)\mathbb{I} \end{pmatrix}$$

is in one-to-one correspondence with the $2\cos(k)$-eigenspace of the infinite matrix (here the first block corresponds to κ, the second to σ, and the third to ι). Further, M only has entries in $\mathbb{Q}(\cos(k), \sin(k))$, so its nullspace has a basis with amplitudes in $\mathbb{Q}(\cos(k), \sin(k))$, as can be seen using Gaussian elimination.

We are interested in the specific cases $2\cos(k) = \pm\sqrt{2}$ corresponding to $k = -\frac{\pi}{4}$ or $k = -\frac{3\pi}{4}$. In these cases $\mathbb{Q}(\cos(k), \sin(k)) = \mathbb{Q}(\sqrt{2})$, and we may choose a basis for the nullspace of M with amplitudes from $\mathbb{Q}(\sqrt{2})$. Furthermore, $\cos(kx), \sin(kx) \in \mathbb{Q}(\sqrt{2})$ for all $x \in \mathbb{Z}^+$, so with such a choice of basis, each amplitude of $|\tau_k\rangle$ is also an element of $\mathbb{Q}(\sqrt{2})$.

As noted above, the spectrum of G may include confined bound states [8] with eigenvalue $\pm\sqrt{2}$. However, any such states are eigenstates of the adjacency matrix of $\hat{G}$ subject to the additional (rational) constraints that the amplitudes on the terminals are zero. As such, the confined bound states have a basis over $\mathbb{Q}(\sqrt{2})$. We can use this basis to restrict attention to those states orthogonal to confined bound states using only constraints over $\mathbb{Q}(\sqrt{2})$, so there exists a basis over $\mathbb{Q}(\sqrt{2})$ for the N-dimensional subspace of scattering states with energy $\pm\sqrt{2}$ that are orthogonal to the confined bound states. Finally, since $\mathbb{Q}(\sqrt{2})$ can be seen as a two-dimensional vector space over $\mathbb{Q}$, note that for any member of this basis $|\tau_k\rangle$ there exist rational vectors $|u_k\rangle, |w_k\rangle$ such that $|\tau_k\rangle = |u_k\rangle + \sqrt{2}|w_k\rangle$. Since $H^2|\tau_k\rangle = 2|\tau_k\rangle$, we have $H|u_k\rangle = \pm 2|w_k\rangle$ and $H|w_k\rangle = \pm|u_k\rangle$, so

$$|\tau_k\rangle = (H \pm \sqrt{2}\mathbb{I})|w_k\rangle. \tag{8}$$

6.2 No R/T gadget and hence no momentum switch

Recall from Section 3 that a momentum switch between two momenta k and p can always be converted into an R/T gadget between k and p. Here we show that if an R/T gadget perfectly reflects at momentum $-\frac{\pi}{4}$, then it must also perfectly reflect at momentum $-\frac{3\pi}{4}$. This implies that no R/T gadget exists between these two momenta, and thus no momentum switch exists.

We use the following basic fact about two-terminal gadgets several times:

Fact 1. *If a two-terminal gadget has a momentum-k scattering state $|\phi\rangle$ with zero amplitude along path 2, then the gadget perfectly reflects at momentum k.*

Proof. Without loss of generality, we may assume that $|\phi\rangle$ is orthogonal to all confined bound states. If $|\phi\rangle$ has zero amplitude along path 2, then there exist some $\mu, \nu \in \mathbb{C}$ such that

$$\langle (x,2)|\phi\rangle = \mu\langle (x,2)|\text{sc}_2(k)\rangle + \nu\langle (x,2)|\text{sc}_1(k)\rangle = \mu e^{-ikx} + \mu R e^{ikx} + \nu T e^{ikx} = 0$$

for all $x \in \mathbb{Z}^+$. Since this holds for all x, we have $\mu = \mu R + \nu T = 0$. Since μ and ν cannot both be zero, we have $T = 0$. □

For an R/T gadget, the scattering states (at some fixed momentum) that are orthogonal to the confined bound states span a two-dimensional space. As shown in Section 6.1, we can expand each scattering eigenstate at momentum $k = -\frac{\pi}{4}$ in a basis with entries in $\mathbb{Q}(\sqrt{2})$, where each basis vector takes the form (8). This gives

$$|\text{sc}_1(-\tfrac{\pi}{4})\rangle = (H + \sqrt{2}\mathbb{I})(\alpha|a\rangle + \beta|b\rangle)$$

where $\alpha, \beta \in \mathbb{C}$, $\alpha \neq 0$, and $|a\rangle$ and $|b\rangle$ are rational 2-eigenvectors of H^2.

If $T(-\frac{\pi}{4}) = 0$, then for all $x \geq 0$,

$$\langle x, 2|\text{sc}_1(-\tfrac{\pi}{4})\rangle = 0 = \langle x, 2|(H + \sqrt{2}\mathbb{I})(\alpha|a\rangle + \beta|b\rangle).$$

Dividing through by α and rearranging, we get that for all $x \geq 0$,

$$\frac{\beta}{\alpha}(\langle x, 2|H|b\rangle + \sqrt{2}\langle x, 2|b\rangle) = -\langle x, 2|H|a\rangle - \sqrt{2}\langle x, 2|a\rangle.$$

If the left-hand side is not zero, then $\beta/\alpha \in \mathbb{Q}(\sqrt{2})$ since H, $|a\rangle$, and $|b\rangle$ are rational. If the left-hand side is zero, then $(H+\sqrt{2}\mathbb{I})|a\rangle$ is an eigenstate at energy $2\cos(k)$ with no amplitude along path 2, so $\beta = 0$ (using Fact 1), and again $\beta/\alpha \in \mathbb{Q}(\sqrt{2})$.

Now write $\beta/\alpha = r + s\sqrt{2}$ with $r, s \in \mathbb{Q}$, and consider the rational 2-eigenvector of H^2

$$|c\rangle := |a\rangle + (r + sH)|b\rangle.$$

Note that

$$\alpha(H + \sqrt{2}\mathbb{I})|c\rangle = \alpha(H + \sqrt{2}\mathbb{I})|a\rangle + \alpha(rH + r\sqrt{2} + sH^2 + sH\sqrt{2})|b\rangle.$$

Since $|b\rangle$ is a 2-eigenvector of H^2 and $\beta/\alpha = r + s\sqrt{2}$, this simplifies to

$$\alpha(H + \sqrt{2}\mathbb{I})|c\rangle = \alpha(H + \sqrt{2}\mathbb{I})|a\rangle + \beta(H + \sqrt{2}\mathbb{I})|b\rangle = |\text{sc}_1(-\tfrac{\pi}{4})\rangle,$$

so $|\text{sc}_1(-\frac{\pi}{4})\rangle$ can be written as $\alpha(H + \sqrt{2}\mathbb{I})$ times a rational 2-eigenvector of H^2.

Since $\langle x, 2|\text{sc}_1(-\frac{\pi}{4})\rangle = 0$ for all $x \geq 1$ (and $\alpha \neq 0$), we have

$$\langle x, 2|(H + \sqrt{2}\mathbb{I})|c\rangle = \langle x, 2|H|c\rangle + \sqrt{2}\langle x, 2|c\rangle = 0.$$

As H is a rational matrix and $|c\rangle$ is a rational vector, the rational and irrational components must both be zero, implying $\langle x, 2|c\rangle = \langle x, 2|H|c\rangle = 0$ for all $x \geq 1$. Furthermore, since $|\text{sc}_1(-\frac{\pi}{4})\rangle$ is a scattering state with zero amplitude on path 2, it must have some nonzero amplitude on path 1 and thus there is some $x_0 \in \mathbb{Z}^+$ for which $\langle x_0, 1|c\rangle \neq 0$ or $\langle x_0, 1|H|c\rangle \neq 0$.

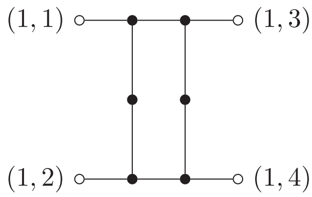

Fig. 11. A graph G_{bc} that implements a basis-changing gate at $-\frac{\pi}{4}$ and $-\frac{3\pi}{4}$.

Now consider the state obtained by replacing $\sqrt{2}$ with $-\sqrt{2}$:

$$|\overline{\mathrm{sc}}_1(-\tfrac{\pi}{4})\rangle := \alpha(H - \sqrt{2}\mathbb{I})|c\rangle.$$

This is a $-\sqrt{2}$-eigenvector of H, which can be confirmed using the fact that $|c\rangle$ is a 2-eigenvector of H^2. As $\langle x,2|H|c\rangle = \langle x,2|c\rangle = 0$ for all $x \geq 1$, $\langle x,2|\overline{\mathrm{sc}}_1(-\frac{\pi}{4})\rangle = 0$ for all $x \geq 1$. Furthermore the amplitude at vertex $(x_0, 1)$ is nonzero, i.e., $\langle x_0, 1|\overline{\mathrm{sc}}_1(-\frac{\pi}{4})\rangle \neq 0$, and hence $|\overline{\mathrm{sc}}_1(-\frac{\pi}{4})\rangle$ has a component orthogonal to the space of confined bound states (which have zero amplitude on both semi-infinite paths). Hence, there exists a scattering state with eigenvalue $-\sqrt{2}$ with no amplitude on path 2. By Fact 1, the gadget perfectly reflects at momentum $-\frac{3\pi}{4}$. It follows that no perfect R/T gadget (and hence no perfect momentum switch) exists between these momenta.

This proof technique can also establish non-existence of momentum switches between other pairs of momenta k and p. For example, a slight modification of the above proof shows that no momentum switch exists between $k = -\frac{\pi}{6}$ and $p = -\frac{5\pi}{6}$.

7 An approximate switch between $-\frac{\pi}{4}$ and $-\frac{3\pi}{4}$

Although no perfect switch exists between momenta $-\frac{\pi}{4}$ and $-\frac{3\pi}{4}$, in this Section we construct a sequence of graphs that approximates such a switch arbitrarily well. At a high level, the switch works by splitting an incoming wave packet into two pieces, applying a momentum-dependent relative phase, and recombining the pieces.

The first ingredient in our construction is the graph G_{bc} shown in Figure 11, which was used in the single- and multi-particle universality constructions to implement a basis-changing gate [3, 4]. At momenta $k = -\frac{\pi}{4}$ and $-\frac{3\pi}{4}$, the S-matrix of this graph has the form

$$S(-\tfrac{\pi}{4}) = \begin{pmatrix} 0 & U_{\mathrm{bc}} \\ U_{\mathrm{bc}} & 0 \end{pmatrix} \qquad S(-\tfrac{3\pi}{4}) = \begin{pmatrix} 0 & -U_{\mathrm{bc}}^* \\ -U_{\mathrm{bc}}^* & 0 \end{pmatrix},$$

where each block has size 2×2 and

$$U_{\mathrm{bc}} = -\frac{1}{\sqrt{2}} \begin{pmatrix} i & 1 \\ 1 & i \end{pmatrix}.$$

The second ingredient, which we use to apply a momentum-dependent phase, is the graph G_{ph} shown in Figure 12. This graph has perfect transmission at both momenta of interest, with transmission coefficients $T(-\frac{\pi}{4}) = -e^{i\phi}$ and $T(-\frac{3\pi}{4}) = e^{i\phi}$, where

$$e^{i\phi} = \frac{2\sqrt{2}}{3} + \frac{i}{3} = e^{i \arctan \frac{1}{2\sqrt{2}}}. \tag{9}$$

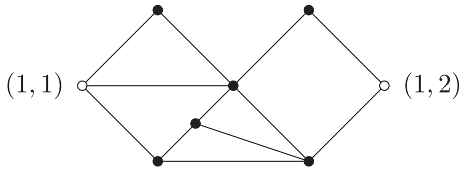

Fig. 12. A graph G_{ph} with perfect transmission and irrational argument at $-\frac{\pi}{4}$ and $-\frac{3\pi}{4}$.

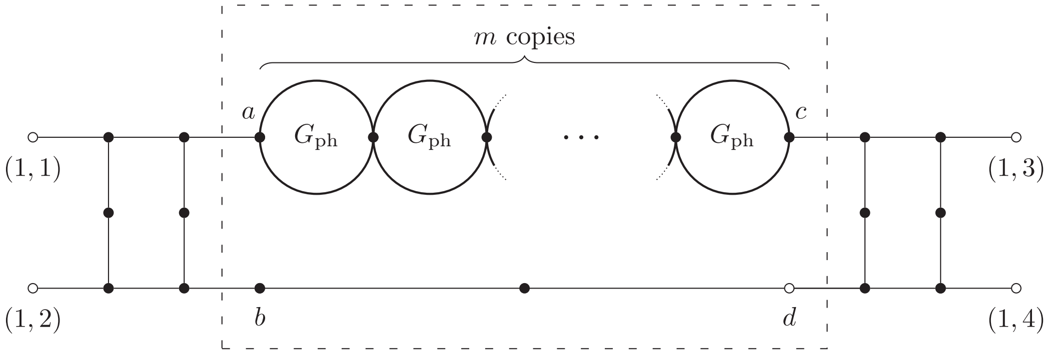

Fig. 13. An approximate momentum switch between $-\frac{\pi}{4}$ and $-\frac{3\pi}{4}$ (for suitable values of m).

We construct an approximate momentum switch from G_{ph} and G_{bc} as shown in Figure 13. Here we use m copies of G_{ph} for some odd m that depends on the precision required in the approximation. To understand the scattering matrix of this graph, we use the following fact. Suppose graphs G_1 and G_2 each have one input terminal and one output terminal, and both have perfect transmission at some fixed momentum k, i.e., $|T_1(k)| = |T_2(k)| = 1$. Now consider the gadget obtained by merging G_1 with G_2 by identifying the output vertex of G_1 with the input vertex of G_2 (now the input terminal is that of G_1 and the output terminal is that of G_2). Then the resulting graph has perfect transmission with transmission coefficient $e^{2ik}T_1(k)T_2(k)$.

Using this fact and equation (9) we see that the graph obtained by merging m copies of G_{ph} in this way (with m odd) has transmission coefficients $T(-\frac{3\pi}{4}) = -T(-\frac{\pi}{4}) = i^{(m-1)}e^{im\phi}$. Now look at the induced subgraph of Figure 13 on vertices contained within the dotted box, and consider attaching semi-infinite paths to vertices labeled a, b, c, d. Using the fact that the path with two edges has perfect transmission with coefficient 1 (at any momentum), we see that the S-matrix of this gadget is

$$\begin{pmatrix} 0 & U_m(k) \\ U_m(k) & 0 \end{pmatrix}$$

where

$$U_m(-\tfrac{\pi}{4}) = \begin{pmatrix} -i^{(m-1)}e^{im\phi} & 0 \\ 0 & 1 \end{pmatrix} \qquad U_m(-\tfrac{3\pi}{4}) = \begin{pmatrix} i^{(m-1)}e^{im\phi} & 0 \\ 0 & 1 \end{pmatrix}.$$

The full graph shown in Figure 13 is obtained from this subgraph by merging it with two copies of G_{bc} in a similar way to the merging procedure described above. Since each of the subgraphs being merged has perfect transmission from input terminals (on the left) to output terminals (on the right), their S-matrices compose in a simple way. At both momenta $k \in \{-\frac{\pi}{4}, -\frac{3\pi}{4}\}$, the overall S-matrix has perfect transmission from the input paths on the left-hand side to the output paths on the right-hand side, and takes the form

$$\begin{pmatrix} 0 & V(k) \\ V(k) & 0 \end{pmatrix}$$

where

$$V(-\tfrac{\pi}{4}) = -U_{\rm bc}U_m(-\tfrac{\pi}{4})U_{\rm bc} = -\frac{1}{2}\begin{pmatrix} -i^{m+1}e^{im\phi}+1 & -i^m e^{im\phi}+i \\ -i^m e^{im\phi}+i & -i^{m-1}e^{im\phi}-1 \end{pmatrix}$$
$$V(-\tfrac{3\pi}{4}) = -U^*_{\rm bc}U_m(-\tfrac{3\pi}{4})U^*_{\rm bc} = -\frac{1}{2}\begin{pmatrix} i^{m+1}e^{im\phi}+1 & -i^m e^{im\phi}-i \\ -i^m e^{im\phi}-i & i^{m-1}e^{im\phi}-1 \end{pmatrix}$$

assuming m is odd. Since $i^{m+1} = -i^{m-1} = \pm 1$, we can see from these expressions that if either $e^{im\phi} \approx 1$ or $e^{im\phi} \approx -1$, then the graph is close to a momentum switch at these momenta. (More precisely, since a momentum switch is a three-terminal gadget and this graph has four terminals, we obtain an approximate momentum switch from this graph by downgrading the terminal vertex $(1,2)$ to an internal vertex). Since $\arctan(2^{-3/2})$ is an irrational multiple of π, the set $\{e^{2ij\phi} \colon j \in \mathbb{Z}^+\}$ is dense on the unit circle, so for any $\epsilon > 0$ and choice of sign $\pm$, there exists some $j \in \mathbb{Z}^+$ such that $|e^{i(2j+1)\phi} \pm 1| = |e^{2ij\phi} \pm e^{-i\phi}| < \epsilon$. Taking $m = 2j+1$ copies of $G_{\rm ph}$, this lets us approximate a momentum switch between $-\frac{\pi}{4}$ and $-\frac{3\pi}{4}$ to any desired precision. In particular, $m = 37$ gives an approximation with

$$\left\| V(-\tfrac{\pi}{4}) - \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \right\| \approx 0.0076 \approx \left\| V(-\tfrac{3\pi}{4}) - \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix} \right\|.$$

The next value of m yielding a better approximation is $m = 379$, with an error of approximately 0.0071.

8 Discussion

In this work we have constructed momentum switches that route a quantum walker along a path that depends on its momentum. Our results could be used to design variants of the multi-particle quantum walk universality construction that use qubits encoded as particles with different momenta (the original construction [4] used momenta $-\frac{\pi}{4}$ and $-\frac{\pi}{2}$). More broadly, we hope that tools for designing scattering gadgets will be useful for developing new quantum algorithms based on continuous-time quantum walk.

We also gave an example showing that (perfect) momentum switches cannot always be constructed. 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 [9, 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.

Other avenues for research also remain open. Many of our results only apply to graphs in a restricted family. In particular, our understanding of R/T gadgets is mostly limited to those of type 1 (although our result concerning non-existence of an R/T gadget between momenta $-\frac{\pi}{4}$ and $-\frac{3\pi}{4}$ is more general). It would be more satisfying to determine necessary and sufficient conditions for a graph to be an R/T gadget (or a momentum switch) without restricting its form.

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).

Acknowledgments

This work was supported in part by NSERC; the Ontario Ministry of Research and Innovation; the Ontario Ministry of Training, Colleges, and Universities; the US ARO; and the Slovak Research and Development Agency grant APVV-0808-12 QIMABOS.

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