Modifying quantum walks: a scattering theory approach

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Abstract
We show how to construct discrete-time quantum walks on directed, Eulerian
graphs. These graphs have tails on which the particle making the walk
propagates freely, and this makes it possible to analyze the walks in terms
of scattering theory. The probability of entering a graph from one tail and
leaving from another can be found from the scattering matrix of the graph.
We show how the scattering matrix of a graph that is an automorphic image
of the original is related to the scattering matrix of the original graph, and we
show how the scattering matrix of the reverse graph is related to that of the
original graph. Modifications of graphs and the effects of these modifications
are then considered. In particular we show how the scattering matrix of a graph
is changed if we remove two tails and replace them with an edge or cut an
edge and add two tails. This allows us to combine graphs, that is if we connect
two graphs we can construct the scattering matrix of the combined graph from
those of its parts. Finally, using these techniques, we show how two graphs can
be compared by constructing a larger graph in which the two original graphs
are in parallel, and performing a quantum walk on the larger graph. This is a
kind of quantum walk interferometry.

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1. Introduction

Quantum walks are quantum versions of random walks. In both, a particle on a graph moves
through the graph as time progresses. In a classical random walk, the path that the particle
takes at a given time is determined by probabilities, while in a quantum walk it is governed by
probability amplitudes. The result is that in a classical random walk, the motion is diffusive,
while in a quantum walk, the motion is more akin to wave propagation. These walks were first
proposed and studied by Aharanov, Davidovich and Zagury [1]. They were later rediscovered

by a number of workers who were interested in them as possible sources of quantum algorithms [2–5]. The search for walk-based algorithms has been successful, and search algorithms [6], subset-finding algorithms [7, 8], a quantum algorithm that can solve a particular oracle problem exponentially faster than is possible with any classical algorithm [9], and, most recently, a quantum algorithm for evaluating the NAND tree [10, 11], have been found. There has now been considerable work on the properties of quantum walks, and some of it is summarized in two relatively recent reviews [12, 13].

Quantum walks come in two varieties, discrete and continuous. Here we shall consider only discrete walks. In these walks, there is a unitary operator that advances the walk one time step. In most versions of discrete-time walks, the particle making the walk is located on the vertices of the graph, and states corresponding to the particle being located at a particular vertex form an orthonormal basis for a Hilbert space $\mathcal{H}_v$, whose states describe the location of the particle. In order to guarantee the unitarity of the time-step operator, it is necessary to enlarge the Hilbert space by adding a quantum coin. For example, if the walk is taking place on the line, the coin space, $\mathcal{H}_c$ is two-dimensional. It is spanned by the orthonormal basis $\{|R\rangle, |L\rangle\}$, and if the coin is in the state $|R\rangle$ the particle moves to the right on its next step, and if the coin is in the state $|L\rangle$ it moves to the left. On a more complicated regular graph, the dimension of the coin space is larger, and it is spanned by an orthonormal basis, each of whose elements corresponds to a direction. The quantum walk takes place on the space $\mathcal{H}_v \otimes \mathcal{H}_c$.

Here we shall consider a discrete-time quantum walk in which the particle is located on the directed edges, rather than the vertices, of the graph. The properties of a class of walks of this type, in which for each directed edge going from a vertex v_1 to vertex v_2, there is a corresponding edge going from v_2 to v_1, were explored in [14] and [15]. They have the advantage that a coin space is unnecessary, and that it is simple to define them for any graph. In this case, the Hilbert space that describes the walk is spanned by an orthonormal basis whose elements correspond to directed edges. That is, there are two orthogonal states corresponding to each edge: one corresponding to the particle being on the edge going in one direction and the other to the particle being on the same edge but going in the opposite direction. In [15] we considered walks of this type on a general graph, G, connected to two tails. Each tail is a half line consisting of an infinite number of edges, with one end going off to infinity and the other attached to a vertex of G. The particle propagates freely on the tails, for example, if it is on one edge moving to the right at one step, after the next step it is on the edge to the right of the one it was on and still moving to the right. The motion of the particle in the graph G is more complicated. This arrangement allowed us to study quantum walks from the point of view of scattering theory. Scattering theory was first applied to quantum walks by Farhi and Gutman, in the case of continuous-time quantum walks [2]; in our case it is applied to discrete-time walks. A freely moving particle approaches G on one tail, scatters in G, and has some amplitude to be reflected from G back onto the tail from which it came and another amplitude to be transmitted through G onto the other tail. The properties of a walk in which a particle starts on one tail and is later measured to be on the other one can be found from a transmission function that is characteristic of the graph G. There is a corresponding reflection function that describes walks that begin and end on the same tail. Both are functions of a complex variable and are analytic in a region including the unit disc.

Here we would like to extend that work. We shall first consider graphs with directed edges in which there is not necessarily a directed edge from v_2 to v_1 if there is one from v_1 to v_2. The graphs will however be Eulerian, that is each vertex will have the same number of edges entering it as leaving it. Defining a quantum walk on a general directed graph is a problem we shall not address, but for an example of recent work in this area see [16]. In addition, we shall allow an arbitrary number of tails. This leads to a transmission matrix

instead of a transmission function. We shall then consider how the transmission matrix of the graph changes when the underlying graph changes. In particular, we shall see what happens when two tails are discarded and replaced by an edge connecting the two vertices to which they were attached or an edge is cut and replaced by two tails. The transmission matrix of the new graph can be calculated from the transmission matrix of the original graph. We shall also be able to combine graphs. In particular, if we have two graphs with tails, we can remove two tails, one from each graph, and replace them by a single edge that connects the vertices to which they were attached, thereby connecting the two graphs. The transmission matrix for the combined graph can be expressed in terms of the transmission matrices of the two original graphs. Finally, we shall show how two graphs can be compared by constructing a larger graph from them in which the two original graphs are in parallel. This allows us to do a kind of interferometry on graphs.

This approach has the advantage that it allows us to construct quantum walks on larger graphs from walks on smaller ones. A quantum walk is characterized by the transmission matrix of that graph. What we show how to do is computing the transmission matrix of a larger graph from those of smaller graphs that are its constituents.

2. Basic formalism

We shall begin by defining a graph in a rather general way. A graph G consists of a set V of vertices and a set E of directed edges, and two maps, $i : E \rightarrow V$ and $t : E \rightarrow V$. These maps associate with each edge, e a point $i(e)$, which we shall call the initial point, and a point $t(e)$, which we shall call the terminal or end point. We allow both loop edges in which $i(e) = t(e)$, and multiple edges, that is distinct edges with the same initial and terminal points. This type of ensemble is often called a digraph in the literature; all our graphs will be digraphs so we will drop the 'di'. This abstract definition has the obvious geometric realization in which we first embed the vertices as points in Euclidean three space, and embed the edges, each of which is a distinct copy $e = [0_e, 1_e]$ of the unit interval directed from 0_e to 1_e by mapping 0_e onto $i(e)$ and 1_e onto $t(e)$. In the geometric realization an edge becomes a path joining $i(e)$ to $t(e)$ and inherits its orientation from the unit interval. Thus loops carry an unambiguous orientation. For each $v \in V$ let $\omega_v = \{e | t(e) = v\}$ and $\tau_v = \{e | i(e) = v\}$. These are, respectively, the sets of incoming and outgoing edges at v. Note that the sets ω_{v_1} and ω_{v_2} are disjoint for $v_1 \neq v_2$, as are the sets τ_{v_1} and τ_{v_2}. We also have that $E = \bigcup_{v \in V} \omega_v = \bigcup_{v \in V} \tau_v$.

We shall be interested in graphs that satisfy the condition $|\omega_v| = |\tau_v|$. Graphs with this property are called Eulerian. If a graph is to be the underlying graph for the quantum walks we wish to study, it must be Eulerian.

The basic picture of our quantum walk is the following. The particle making the walk is located on the edges of the graph, and when it passes through a vertex it scatters. If the particle is on an edge between the vertices v_1 and v_2, it can either be going from v_1 to v_2 (corresponding to the directed edge with $i(e) = v_1$ and $t(e) = v_2$), or it can be going from v_2 to v_1 (corresponding to the directed edge with $i(e) = v_2$ and $t(e) = v_1$). If it is going from v_1 to v_2, the next time step will carry it through v_2 onto one of the edges leaving v_2. In order to define the walk we need a Hilbert space that describes a particle on the directed edges of the graph, and a unitary operator that advances the walk one time step. This operator is constructed from operators that describe the scattering at the individual vertices.

We first construct the Hilbert space for the quantum states of a particle moving on the graph. Let Ω_v and T_v be the Hilbert spaces generated by taking the elements of ω_v and τ_v, respectively, as orthonormal basis elements. Let $U_v : \Omega_v \rightarrow T_v$ be the local scattering operator, and we assume that U_v is an isometry. By combining these local operators we are

able to construct a unitary operator that advances the quantum walk one step. In particular, we define $U : L^2(E) \to L^2(E)$, where $L^2(E) = \bigoplus_{v \in V} \Omega_v = \bigoplus_{v \in V} T_v$, such that $U|\Omega_v = U_v$. We call such a unitary U a quantum structure on the Eulerian graph G.

Let $G = (V, E, i, t)$ be a graph. The reverse graph $G_R = (V_R, E_R, i_R, t_R)$ is a graph where the set $V_R = V$ and $E_R = E$, while $i_R(e) = t(e)$ and $t_R(e) = i(e)$. In this new graph G_R we have reversed the orientation on all the edges of the geometric realization of G. We see that $(\tau_R)_v = \omega_v$ and $(\omega_R)_v = \tau_v$. If the original graph G is Eulerian then so is G_R. If U is a quantum structure on G we will now define a reverse quantum structure U_R on G_R. Let $L^2(E_R)$ be the Hilbert space generated by taking the oriented edges of G_R as orthonormal basis elements. Define the conjugate linear map $R : L^2(E_R) \to L^2(E)$ so that if $|v_2, v_1\rangle \in L^2(E_R)$ is the basis element corresponding to the edge e considered as an edge of G_R, so that $i_R(e) = v_2$ and $t_R(e) = v_1$, then

$$R|v_2, v_1\rangle = |v_1, v_2\rangle, \tag{1}$$

where $|v_1, v_2\rangle$ is the basis element corresponding to e considered as an edge of G, so that $i(e) = v_1$ and $t(e) = v_2$. R is the orientation reversing map, and it is an isometry from $(\Omega_R)_v$ onto T_v and from $(T_R)_v$ onto Ω_v, for all $v \in V$. The reverse quantum structure on G_R is defined by

$$(U_R)_v = R^{-1} U^{-1} R, \tag{2}$$

which is a linear isometry from $(\Omega_R)_v$ onto $(T_R)_v$. The operator R defined here is closely related to the time-reversal operator for quantum walks defined in [15].

A graph $G = (V, E, i, t)$ possesses a pairing if there exists a fixed-point-free involution A on the edges E such that $t(Ae) = i(e)$ and $i(Ae) = t(e)$. The initial and terminal points of e are the terminal and initial points of Ae. A graph possessing a pairing is clearly Eulerian. The simplest case of such a graph is when each pair of vertices which are connected at all have exactly two edges joining them one in each direction, a divided highway. Such graphs are said to be simple. Quantum walks on simple graphs were treated in [15].

Let $G = (V, E, i, t)$ and $G' = (V', E', i', t')$ be a pair of graphs. Let $\phi = (f, F)$ be a pair of maps, $f : V \to V'$ and $F : E \to E'$. ϕ is a graph morphism if $i' \circ F = f \circ i$ and $t' \circ F = f \circ t$. If f and F are bijections we call ϕ a graph isomorphism. If ϕ is a graph morphism then $F : \omega_v \to \omega_{f(v)}$ and $F : \tau_v \to \tau_{f(v)}$. F thereby extends to a linear map also denoted by F which maps Ω_v into $\Omega_{f(v)}$ and also maps T_v into $T_{F(v)}$. Clearly $F : L^2(E) \to L^2(E')$ and $\|F\| \leqslant 1$. Let G have a quantum structure U and let G' have a quantum structure U'. A graph morphism ϕ is said to be a quantum graph morphism if

$$F \circ U = U' \circ F. \tag{3}$$

If ϕ is a graph isomorphism or a graph automorphism which commutes with quantum structures as above then we call them quantum isomorphisms or quantum automorphisms, respectively.

In order to apply scattering theory to our walk, we need regions where the particle propagates freely, and no scattering takes place. For this reason, we will attach semi-infinite lines, or tails, to our graph. Let G be a graph with a finite number of edges and vertices, and $\mathcal{H}_G$ be the Hilbert space spanned by the states corresponding to its directed edges. We shall single out two subsets of the vertices, $\{v_k | k = 1, \ldots, K\}$ and $\{u_l | l = 1, \ldots, L\}$, where we will attach incoming tails X_k and outgoing tails Y_l, respectively. We shall make no further assumptions on these vertices. A given vertex may appear many times in one or both lists. We want to be able to clearly identify the distinct incoming and outgoing tails. The vertices of the incoming tail X_j are denoted by k_j, where $k = 1, 2, \ldots$, and the directed edges are $|k_j, (k-1)_j\rangle = |k, k-1\rangle_j$ for $k \geqslant 2$ and the attaching edge is $|1_j, v_j\rangle$, which we shall often denote as $|1, 0\rangle_j$, in order to be consistent with the above notation for the directed edges on

the tail. The vertices of the outgoing tail Y_l are denoted by m_l, where $m = 1, 2, \ldots$. The oriented edges are $|m_l, (m+1)_l\rangle = |m, m+1\rangle_l$, and the attaching edge is $|u_l, 1_l\rangle$, which we shall often denote as $|0, 1\rangle_l$. In this way given G and the two sets of vertices we can construct a new graph $\Gamma = (G, (v_1, \ldots, v_K)(u_1, \ldots, u_L))$ where the vertices of the new graph are those of G, the vertices $k_j 1 \leqslant k < \infty$ for each tail X_k, and the vertices $(m)_l 1 \leqslant m < \infty$ for each outgoing tail Y_l. The edges of Γ are the edges of G and the edges $|k, k-1\rangle_j$, and $|m, m+1\rangle_l$ as above. In order that Γ be the underlying graph for a quantum structure it must be Eulerian , which implies that $K = L$, i.e. the number of incoming tails is the same as the number of outgoing tails. We call such a graph Γ an Eulerian graph with tails.

If we are given an Eulerian graph with tails Γ, we want to study quantum structures U on Γ with the additional property that

$$U|k+1, k\rangle_j = |k, k-1\rangle_j \tag{4}$$

on each edge of an incoming tail, and

$$U|m-1, m\rangle_l = |m, m+1\rangle_l \tag{5}$$

on each edge of an outgoing tail. We say such a quantum structure is free. The 'particle' freely propagates towards G along an incoming edge and freely propagates away from G along an outgoing edge.

We now want to consider eigenstates of U that correspond to the following situation. A particle approaches G on the tail X_k, scatters in G, and then has amplitudes to leave G on any of outgoing tails Y_l. A quantum state of this form is given by

$$|\psi_k(\theta)\rangle = \sum_{l=0}^{\infty} e^{-il\theta}|l+1, l\rangle_k + |\psi_{G,k}(\theta)\rangle + \sum_{l=1}^{K} t_l^{(k)}(\theta) \sum_{m=0}^{\infty} e^{im\theta}|m, m+1\rangle_l, \tag{6}$$

and satisfies the equation

$$U|\psi_k(\theta)\rangle = e^{-i\theta}|\psi_k(\theta)\rangle. \tag{7}$$

The first part of $|\psi_k(\theta)\rangle$ corresponds to the incoming particle, the second to the part of the state inside G and the final part to the outgoing particle. As we shall later show, the functions $t_l^{(k)}(\theta)$ and $|\psi_{G,k}(\theta)\rangle$ are restrictions to the unit circle of functions that are analytic for $|z| < 1 + \epsilon$, for some $\epsilon > 0$, while $|\psi_k(\theta)\rangle$ itself is the restriction to the unit circle of an analytic function from the punctured disc, $0 < |z| < 1 + \epsilon$ into $L^\infty(E)$.

In order to begin the extension of the above eigenstate into the complex plane, define

$$|\sigma_{j+}(z)\rangle = \sum_{l=0}^{\infty} z^l |l, l+1\rangle_j, \qquad |\sigma_{j-}(z)\rangle = \sum_{l=0}^{\infty} z^{-l}|l+1, l\rangle_j. \tag{8}$$

Note that

$$U|\sigma_{j+}(z)\rangle = \frac{1}{z}(|\sigma_{j+}(z)\rangle - |0, 1\rangle_j), \qquad U|\sigma_{j-}(z)\rangle = \frac{1}{z}|\sigma_{j-}(z)\rangle + U|1, 0\rangle_j. \tag{9}$$

We then define

$$|\psi_k(z)\rangle = |\sigma_{k-}(z)\rangle + |\psi_{G,k}(z)\rangle + \sum_{j=1}^{K} t_j^{(k)}(z)|\sigma_{j+}(z)\rangle, \tag{10}$$

such that it is the solution to the equation

$$zU|\psi_k(z)\rangle = |\psi_k(z)\rangle. \tag{11}$$

This equation will be satisfied if and only if

$$U(|\psi_{G,k}(z)\rangle + |1, 0\rangle_k) = \frac{1}{z}(|\psi_{G,k}(z)\rangle + \sum_{j=1}^{K} t_j^{(k)}(z)|0, 1\rangle_j). \tag{12}$$

This will be our key equation, and we shall now analyze it in more detail.

Let P_G be the orthogonal projection onto $\mathcal{H}_G$, and set

$$|w_k\rangle = P_G U|1, 0\rangle_k. \tag{13}$$

If we now apply P_G to both sides of equation (12), we have that

$$P_G U|\psi_{G,k}(z)\rangle + |w_k\rangle = \frac{1}{z}|\psi_{G,k}(z)\rangle. \tag{14}$$

Defining $U_G = P_G U$, let us consider the equation

$$(-zU_G + I)|\Phi(z)\rangle = z|w_k\rangle, \tag{15}$$

on $\mathcal{H}_G$. We find that

$$\begin{aligned}|\Phi(z)\rangle &= \sum_{n=0}^{\infty} z^{n+1} U_G^n|w_k\rangle \\ &= \sum_{n=1}^{\infty} z^n U_G^n|1, 0\rangle_k, \end{aligned} \tag{16}$$

which converges absolutely and uniformly on the disc $|z| < 1$, and hence $|\Phi(z)\rangle$ is analytic in the disc $|z| < 1$.

Let $\mathcal{H}_0$ be the subspace of $\mathcal{H}_G$ spanned by the L^2 eigenvectors of U that are contained in $\mathcal{H}_G$, i.e. eigenstates of U that have their support in the graph G. These are the analogs of bound states in conventional potential scattering, and in that case, the bound states are orthogonal to the scattering states. A similar situation obtains here. Let $\mathcal{H}_1$ be the orthogonal complement of $\mathcal{H}_0$ in $\mathcal{H}_G$, let P_1 be the orthogonal projection onto $\mathcal{H}_1$, and let $U_1 = P_1 U$. It is easily seen that $|w_k\rangle$ and all of its images under U_1 are orthogonal to $\mathcal{H}_0$. We now have that $|\Phi(z)\rangle$ can be expressed as

$$|\Phi(z)\rangle = \sum_{n=0}^{\infty} z^{n+1} U_1^n|w_k\rangle, \tag{17}$$

takes its values in $\mathcal{H}_1$, is unique, and is analytic for $|z| < 1$. The solution can be extended beyond the disc $|z| < 1$ by making use of the fact that the operator $(I_{\mathcal{H}_1} - zU_1)$ on $\mathcal{H}_1$ has no eigenstates in the closed disc $|z| \leqslant 1$. Because this is an operator on a finite-dimensional space, it has a finite number of eigenvalues, one of which is closest to $z = 0$. Let the magnitude of this eigenvalue be r. For $|z| < r$, the inverse of $(I_{\mathcal{H}_1} - zU_1)$ on $\mathcal{H}_1$ exists and is analytic [17], and therefore, for $|z| < r$ we have that $|\Phi(z)\rangle$ exists and is analytic.

Summarizing, we have that equation (15) has a unique solution, $|\Phi(z)\rangle = |\psi_{G,k}\rangle$, with values in $\mathcal{H}_1$, which is analytic on a domain $|z| < 1 + \epsilon$, for some $\epsilon > 0$. Furthermore, we have that

$$t_j^{(k)}(z) = {}_j\langle 0, 1|U(|\psi_{G,k}(z)\rangle + |1, 0\rangle_k), \tag{18}$$

so that $t_j^{(k)}(z)$ is analytic for $|z| < 1 + \epsilon$, because $|\psi_{G,k}(z)\rangle$ is. We also note that $t_j^{(k)}(0) = 0$.

3. Spectral results

Let $\mathcal{H}_k$ be the closed, linear, U-invariant subspace of $\mathcal{H} = L^2(E)$ spanned by the states $U^l|j, j-1\rangle_k$, for $j = 1, 2 \ldots$ and l an integer. This is just the space of states generated by incoming states on the kth tail. We want to construct the spectral representation of U on $\mathcal{H}_k$. We have that

(1) $U|\psi_k(\mathrm{e}^{\mathrm{i}\theta})\rangle = \mathrm{e}^{-\mathrm{i}\theta}|\psi_k(\mathrm{e}^{\mathrm{i}\theta})\rangle$
(2) $\langle\psi_k(\mathrm{e}^{\mathrm{i}\theta})|1, 0\rangle_k = 1$
(3) $\langle\psi_k(\mathrm{e}^{\mathrm{i}\theta})|v\rangle = 0$ for any $|v\rangle \in \mathcal{H}_0$.

If $|v\rangle \in L^1(E)$, then $\langle\psi_k(\mathrm{e}^{\mathrm{i}\theta})|v\rangle$ is a continuous function of θ, so

$$\frac{1}{2\pi} \int_0^{2\pi} \mathrm{d}\theta|\psi_k(\mathrm{e}^{\mathrm{i}\theta})\rangle\langle\psi_k(\mathrm{e}^{\mathrm{i}\theta})|v\rangle \in L^\infty(E). \tag{19}$$

The arguments in [15] then show that for any $|y\rangle \in \mathcal{H}_k$ and for f any complex-valued continuous function on the unit circle (which we shall denote by C), that

$$\langle y|f(U)|y\rangle = \frac{1}{2\pi} \int_0^{2\pi} \mathrm{d}\theta f(\mathrm{e}^{-\mathrm{i}\theta})|\langle\psi_k(\theta)|y\rangle|^2. \tag{20}$$

Therefore, by the Riesz–Markov theorem, there exists a unique measure, μ_y, a Borel measure on C, called the spectral measure associated with $|y\rangle$, such that

$$\langle y|f(U)|y\rangle = \int_0^{2\pi} \mathrm{d}\mu_y(\theta)f(\mathrm{e}^{-\mathrm{i}\theta}), \tag{21}$$

and hence

$$\mathrm{d}\mu_y = \frac{|\langle\psi_k(\theta)|y\rangle|^2}{2\pi}\mathrm{d}\theta. \tag{22}$$

Now define the operator $V_k : \mathcal{H}_k \to L^2(C)$ by

$$V_k|v\rangle = \frac{1}{\sqrt{2\pi}}\langle\psi(\mathrm{e}^{\mathrm{i}\theta})|v\rangle. \tag{23}$$

We then have the following theorem [15]: V_k is a unitary operator from $\mathcal{H}_k$ to $L^2(C)$ such that for any $g(\theta) \in L^2(C)$, we have that

$$V_k U V_k^{-1} g(\theta) = \mathrm{e}^{-\mathrm{i}\theta} g(\theta). \tag{24}$$

Hence, we have constructed part of the spectral decomposition of U. The U-invariant subspaces $\mathcal{H}_k$ are orthogonal for different values of k, and they are all orthogonal to $\mathcal{H}_0$. We have, in fact, that $L^2(E) = \mathcal{H}_0 \bigoplus_{k=1}^K \mathcal{H}_k$ [15]. This, then, completes the spectral decomposition of U.

4. Properties of the transmission coefficients

The transmission coefficients, $t_j^{(k)}(\theta)$ describe the behavior of a particle that starts on the kth tail and scatters into the jth tail. Many properties of a quantum walk can be found directly from these functions.

Suppose we start a walk in the state $|0, 1\rangle_k$, and after each time step we measure the edge $|0, 1\rangle_j$ in order to see if the particle has arrived there. The probability that we find the particle there after n steps, but did not find it there for any of the previous $n-1$ steps, which we shall denote by $q_j^{(k)}(n)$, is [15]

$$q_j^{(k)}(n) = |{}_k\langle 0, 1|U^n|1, 0\rangle_j|^2. \tag{25}$$

This probability can be expressed in terms of $t_j^{(k)}(\theta)$ as follows. We have already seen that $|\psi_k(z)\rangle$ is analytic in a region including the unit disc, and an examination of equation (11) shows that it vanishes when $z = 0$. This implies that the functions $t_j^{(k)}(z)$ and $\psi_{G,k}(z)\rangle$ are also analytic and vanish at $z = 0$. This implies that

$$|1, 0\rangle_k = \frac{1}{2\pi i} \int_C dz \frac{1}{z} |\psi_k(z)\rangle = \frac{1}{2\pi} \int_0^{2\pi} d\theta |\psi_k(\theta)\rangle. \tag{26}$$

We then have

$$_k\langle 0, 1|U^n|1, 0\rangle_j = \frac{1}{2\pi} \int_0^{2\pi} d\theta e^{-in\theta} t_j^{(k)}(\theta), \tag{27}$$

so that

$$q_j^{(k)}(n) = \left| \frac{1}{2\pi} \int_0^{2\pi} d\theta \, e^{-in\theta} t_j^{(k)}(\theta) \right|^2. \tag{28}$$

This also gives us that the probability of finding the particle on the jth tail at some step is given by

$$P_{j,out}^{(k)} = \sum_{n=1}^{\infty} q_j^{(k)}(n) = \frac{1}{2\pi} \int_0^{2\pi} d\theta \left| t_j^{(k)}(\theta) \right|^2. \tag{29}$$

This probability, and other probabilities of interest, can also be expressed in terms of $t_j^{(k)}(z)$ by means of contour integrals [15].

The transmission coefficients also satisfy an orthogonality relation. In order to derive it, first define

$$|\phi_k(\theta)\rangle = |\psi_{G,k}(\theta)\rangle + |1, 0\rangle_k. \tag{30}$$

We then have that

$$\langle \phi_l(\theta)|\phi_k(\theta)\rangle = \langle \psi_{G,l}(\theta)|\psi_{G,k}(\theta)\rangle + \delta_{k,l}. \tag{31}$$

If we apply U to $|\phi_k(\theta)\rangle$, we find

$$U|\phi_k(\theta)\rangle = e^{-i\theta} \left[|\psi_{G,k}(\theta)\rangle + \sum_{j=1}^{K} t_j^{(k)}(\theta)|0, 1\rangle_j \right], \tag{32}$$

from which it follows that

$$\langle \phi_l(\theta)|\phi_k(\theta)\rangle = \langle \psi_{G,l}(\theta)|\psi_{G,k}(\theta)\rangle + \sum_{j=1}^{K} t_j^{(l)}(\theta)^* t_j^{(k)}(\theta). \tag{33}$$

Comparing equations (31) and (33), we see that

$$\sum_{j=1}^{K} t_j^{(l)}(\theta)^* t_j^{(k)}(\theta) = \delta_{k,l}. \tag{34}$$

Let $\tau(\partial G) = (|0, 1\rangle_l, 1 \leqslant l \leqslant K)$ and $\omega(\partial G) = (|1, 0\rangle_k, 1 \leqslant k \leqslant K)$ be the edges pointing out of G and the edges pointing into G, respectively. Note that by ∂G, we mean the boundary of G, that is the set of vertices to which tails are attached. Let $T(\partial G)$ and $\Omega(\partial G)$ be the corresponding subspaces of L^2 spanned by these edges. If we now define our scattering matrices

$$S(\theta) : \Omega(\partial G) \rightarrow T(\partial G) \tag{35}$$

by

$$S(|1, 0\rangle_k) = \sum_{l=1}^{K} t_l^{(k)}(\theta)|0, 1\rangle_l, \tag{36}$$

our calculation shows that for each value of θ, $S(\theta)$ is an isometry. We also see that

$$\frac{1}{2\pi} \int_0^{2\pi} \left| t_j^{(k)}(\theta) \right|^2 \mathrm{d}\theta \tag{37}$$

is equal to the probability that a particle which starts at $|1, 0\rangle_k$ exits G at $|0, 1\rangle_j$ into the jth outgoing tail Y_j.

We will now investigate how this scattering matrix behaves when we subject Γ to an automorphism, and how it behaves under reversal. Let $\Phi = (f, F)$ be a quantum automorphism on Γ which induces a permutation π_ω on the edges in $\omega(\partial G)$ and a permutation π_τ on the edges of $\tau(\partial G)$. These permutations actually permute the corresponding tails. It is easy to see that

$$S \circ \pi_\omega = \pi_\tau \circ S, \tag{38}$$

if we extend π_ω and π_τ to be linear isometries on $\Omega(\partial G)$ and $T(\partial G)$, respectively. If we write $\pi_\omega|1, 0\rangle_k = |1, 0\rangle_{\pi_\omega(k)}$ and $\pi_\tau|0, 1\rangle_j = |0, 1\rangle_{\pi_\tau(j)}$ we see that

$$t_j^{(k)}(\theta) = t_{\pi_\tau(j)}^{(\pi_\omega(k))}(\theta). \tag{39}$$

The discussion of the effect of reversing the graph is somewhat more complicated. First we have to extend the reversing construction to graphs with a free quantum structure. Let Γ be a given Eulerian graph with incoming (outgoing) tails $X_1, \ldots, X_K (Y_1, \ldots, Y_K)$ attached to G at vertices $v_1, \ldots, v_K (u_1, \ldots, u_K)$, respectively. Let Γ^R be the reverse of Γ. We essentially reverse the orientation on all the oriented edges on Γ which means that we swap the incoming edges for outgoing ones and vice versa. More specifically let R be the reversing map we defined in section 2 which reverses the orientation of each edge. Then $Y_k^R(X_j^R)$ is the kth (j th) outgoing (incoming) tail of Γ^R, which has the same vertices as $X_k(Y_j)$ but with the orientation on the edges reversed. If (l_k), where $l = 1, 2, \ldots$ ((m_j), where $m = 1, 2 \ldots$) are the vertices $X_k(Y_j)$ then the edges of $Y_k^{(R)}(X_j^{(R)})$ are $|(l)_k, (l + 1)_k\rangle = |l, l + 1\rangle_k^{(R)} = R^{-1}(|l + 1, l\rangle_k)(|(m + 1)_j, (m)_j\rangle = |m + 1, m\rangle_j^{(R)} = R^{-1}(|m, m + 1\rangle_j)$. Let $U^{(R)} = R^{-1}U^{-1}R$ be the induced quantum structure on $\Gamma^{(R)}$. Then

$$U^{(R)}|l - 1, l\rangle_k^{(R)} = R^{-1}U^{-1}|l, l - 1\rangle_k = R^{-1}|l + 1, l\rangle_k = |l, l + 1\rangle_k^{(R)}. \tag{40}$$

Similarly we can show that

$$U^{(R)}|m + 1, m\rangle_j^{(R)} = |m, m - 1\rangle_j^{(R)}. \tag{41}$$

Therefore the induced quantum structure on $\Gamma^{(R)}$ is free.

Let $\mathcal{H}_G$ and $\mathcal{H}_G^{(R)}$ be the Hilbert spaces generated by the interior edges of G and $G^{(R)}$, respectively . Let P_G and $P_G^{(R)}$ be the orthogonal projections onto $\mathcal{H}_G$ and $\mathcal{H}_G^{(R)}$, respectively. It is easy to see that

$$P_G \circ R = R \circ P_G^{(R)} \qquad R^{-1} \circ P_G = P_G^{(R)} \circ R^{-1}. \tag{42}$$

Let $U_G^{(R)} = P_G^{(R)} \circ U^{(R)}$. We will now explicitly construct

$$\left| \psi_j^{(R)}(z) \right\rangle = \left| \sigma_{j^-}^{(R)}(z) \right\rangle + \left| \psi_{G,j}^{(R)}(z) \right\rangle + \sum_{l=1}^{K} (t^{(R)})_l^{(j)}(z) \left| \sigma_{l^+}^{(R)}(z) \right\rangle, \tag{43}$$

where

$$\left|\psi_{G,j}^{(R)}(z)\right\rangle = \sum_{n=1}^{\infty} z^n \left(U_G^{(R)}\right)^n |1,0\rangle_j^{(R)}. \tag{44}$$

Formula (18) shows that

$$\begin{aligned}
(t^{(R)})_k^{(j)}(z) &= \left\langle (0,1)_k^{(R)} \middle| U^{(R)} \left[\left|\psi_{G,j}^{(R)}(z)\right\rangle + |1,0\rangle_j^{(R)} \right] \right\rangle \\
&= \left\langle R(0,1)_k^{(R)} \middle| RU^{(R)} \left[\left|\psi_{G,j}^{(R)}(z)\right\rangle + |1,0\rangle_j^{(R)} \right] \right\rangle^* \\
&= \left\langle U(1,0)_k \middle| R \left[\left|\psi_{G,j}^{(R)}(z)\right\rangle \right] + |0,1\rangle_j \right\rangle^*.
\end{aligned} \tag{45}$$

Now

$$\begin{aligned}
\left\langle U(1,0)_k \middle| R\left(z^n \left(U_G^{(R)}\right)^n (1,0)_j^{(R)}\right)\right\rangle &= \left\langle z^n (U P_G)^n U(1,0)_k \middle| (0,1)_j \right\rangle \\
&= \left\langle z^n U(U_G)^n (0,1)_k \middle| (0,1)_j \right\rangle.
\end{aligned} \tag{46}$$

This implies

$$\left\langle U(0,1)_k \middle| R\left[\psi_{G,j}^{(R)}(z)\right]\right\rangle = \left\langle U\psi_{G,k}(z) \middle| (0,1)_j \right\rangle, \tag{47}$$

which gives us the desired formula

$$(t^{(R)})_k^{(j)}(z) = \left\langle U(|\psi_{G,g}(z)\rangle + (1,0)_k) \middle| (0,1)_j \right\rangle^* = t_j^{(k)}(z). \tag{48}$$

This enables us to compute the transmission amplitudes for $\Gamma^{(R)}$ from those of our original graph Γ. If $S(\theta)$ is the scattering matrix for Γ then $S^{\text{tr}}(\theta)$ is the scattering matrix $S^{(R)}(\theta)$ for $\Gamma^{(R)}$. Furthermore we see that

$$R \circ S^{(R)}(\theta) \circ R^{-1} |0,1\rangle_k = \sum_{l=1}^{K} t_k^{(l)}(\theta)^* |0,1\rangle_l. \tag{49}$$

It is because of equation (47) that we need to choose R to be conjugate linear. The right-hand side is clearly a conjugate analytic function of z, so the fact that R interchanges the complex structures forces the left-hand side to be conjugate analytic too. When we defined the reverse graph G_R, we defined the mapping $R : L^2(E_R) \to L^2(E)$ to be a conjugate linear isometry. If instead we replace $L^2(E_R)$ with $L^2(E_R)_c$, the space with the conjugate complex structure and Hermitian inner product, R becomes a complex linear isometry from $L^2(E_R)_c$ onto $L^2(E)$. If we follow the argument above with these changes we get the formula

$$(t^{(R)})_k^{(j)}(z) = t_j^{(k)}(z)^*, \tag{50}$$

which seems to contradict analyticity until we recall that we are dealing with $L^2(E_R)_c$. So the 'z' on the left-hand side refers to the complex structure which is the conjugate of the original one on $L^2(E)$. Hence, the more functorial formula above is as it should be. If we followed through in this vein we would finally arrive at equation (48). We chose to avoid this additional complication because our concern was to give formulae to compute the transition amplitudes.

5. Add a handle

We now want to begin our study of how changing a graph modifies its transmission amplitudes. Let us first consider what happens when we replace a pair of tails, one incoming and one outgoing with a single edge going from the attaching vertex of the outgoing edge to the attaching vertex of the incoming edge. This new graph Γ' will still be Eulerian. It will also inherit a free quantum structure U' from the original free quantum structure U on Γ.

Let us be more specific. Let $\Gamma = (G, (v_1, \ldots, v_K), (u_1, \ldots, u_K))$ be an Eulerian graph with tails. Let $X_1, \ldots, X_K$ be the incoming tails attached at the vertices $v_1, \ldots, v_K$ respectively and let $Y_1, \ldots, Y_K$ be the outgoing tails attached at the vertices $u_1, \ldots, u_K$ respectively. Let $\Gamma' = (G', (v_2, \ldots, v_K), (u_2, \ldots, u_K))$ be the new Eulerian graph with tails. The graph G' has the same vertices as G. Its edges are those of G plus a new one $|u_1, v_1\rangle$, which is an oriented edge from u_1 to v_1. Its incoming (outgoing) tails are $X_2, \ldots, X_K$ ($Y_2, \ldots, Y_K$) with the same attaching vertices as in Γ. We see that $\tau'_v = \tau_v$ and $\omega'_v = \omega_v$ for vertices v not equal to u_1 or v_1. The prime refers to Γ'. The edges of ω'_{v_1} are the same as those of ω_{v_1} with $|1, 0\rangle_1 = |1_1, v_1\rangle$ replaced by $|u_1, v_1\rangle$. The edges τ'_{u_1} are the same as those of τ_{u_1} with $|0, 1\rangle_1 = |u_1, 1_1\rangle$ replaced by $|u_1, v_1\rangle$. We can now see how the original free quantum structure U on Γ induces a new one, U', on Γ'. If a vertex v is unequal to u_1 or v_1 then $U'_v = U_v$. If the vertex is v_1 or u_1 this is still the rule if we consistently replace $|1, 0\rangle_1$ in ω_{v_1} with $|u_1, v_1\rangle$ and $|0, 1\rangle_1$ in τ_{u_1} with $|u_1, v_1\rangle$. So

$$U'_{v_1}|u_1, v_1\rangle = U_v|1, 0\rangle_1, \tag{51}$$

which is unambiguous unless $u_1 = v_1$. In that case $U_v|1, 0\rangle_1$ may contain a term proportional to $|u_1, (1)_1\rangle$. In defining $U'_{v_1}|u_1, v_1\rangle$, we simply take the expression for $U_v|1, 0\rangle_1$ and replace $|u_1, (1)_1\rangle$ by $|u_1, v_1\rangle$ wherever it occurs.

Our aim, now, is to show how to simply compute the transmission amplitudes $\tau_j^{(k)}(z)$ of the new configuration Γ' from the transmission amplitudes $t_j^{(k)}(z)$ of the original Γ. We will adopt the notation of section 2. Let

$$|\psi'_k(z)\rangle = |\sigma_{k^-}(z)\rangle + |\psi_{G',k}(z)\rangle + \Sigma_{j=2}^K \tau_j^{(k)}(z)|\sigma_{j^+}(z)\rangle \tag{52}$$

be the generalized eigenstate of U' which satisfies the equation

$$zU'|\psi'_k(z)\rangle = |\psi'_k(z)\rangle. \tag{53}$$

We want to represent $|\psi_{G',k}(z)\rangle$ in the form

$$|\psi_{G',k}(z)\rangle = |\psi_{G,k}(z)\rangle + a_k(z)(|u_1, v_1\rangle + |\psi_{G,1}(z)\rangle), \tag{54}$$

where $|\psi_{G,k}(z)\rangle$ is the part of the generalized eigenstate of Γ that is supported in G, and $a_k(z)$ is a function to be determined. We have that

$$zU'(|u_1, v_1\rangle + |\psi_{G,1}(z)\rangle) = |\psi_{G,1}(z)\rangle + t_1^{(1)}(z)|u_1, v_1\rangle + \sum_{j=2}^K t_j^{(1)}(z)|0, 1\rangle_j, \tag{55}$$

and

$$zU'(|1, 0\rangle_k + |\psi_{G',k}(z)\rangle) = |\psi_{G',k}(z)\rangle + \sum_{j=2}^K \tau_j^{(k)}(z)|0, 1\rangle_j, \tag{56}$$

where, as previously mentioned, $\tau_j^{(k)}(z)$ denote the transmission amplitudes for Γ'. If we represent $|\psi_{G',k}(z)\rangle$ as in equation (54), we see that

$$zU'(|1, 0\rangle_k + |\psi_{G,k}(z)\rangle + a_k(z)(|u_1, v_1\rangle + |\psi_{G,1}(z)\rangle))$$

$$= |\psi_{G,k}(z)\rangle + \sum_2^K t_j^{(k)}(z)|0, 1\rangle_j + t_1^{(k)}(z)|(u_1, v_1)\rangle$$

$$+ a_k\left(|\psi_{G,1}(z)\rangle + t_1^{(1)}(z)|u_1, v_1\rangle + \sum_{j=2}^K t_j^{(1)}(z)|0, 1\rangle_j\right). \tag{57}$$

Comparing this result with equation (56), we can see that

$$\tau_j^k(z) = t_j^{(k)}(z) + a_k(z)t_j^{(1)}(z) \qquad a_k(z) = t_1^{(k)}(z) + a_k(z)t_1^{(1)}(z), \tag{58}$$

so that, finally,

$$\tau_j^{(k)}(z) = t_j^{(k)}(z) + \frac{t_j^{(1)}(z)t_1^{(k)}(z)}{1 - t_1^{(1)}(z)}, \tag{59}$$

all of which hold in a neighborhood of the unit disc by the discussion in section 2.

We can iterate this procedure by connecting an outgoing tail to an incoming tail as we did above, one pair at a time, thereby adding several 'handles'. We can also use this method to accomplish this in a single step in the following way. Let us try to add L handles by splicing Y_j to $X_j 1 \leqslant j \leqslant L$ respectively and form new edges (handles), $e_1 = (u_1, v_1) e_2 = (u_2, v_2) \ldots e_L = (u_L, v_L)$. The new generalized eigenstate coming from an incoming wave traveling along one of the remaining incoming tails Y_k is

$$|\psi_k'(z)\rangle = \sigma_{k^-}(z) + |\psi_{G',k}(z)\rangle + \sum_{j=L+1}^{K} \tau_j^{(k)}(z)|\sigma_{j^+}(z)\rangle, \tag{60}$$

where $\psi_{G',k}(z)\rangle$ is of the form

$$|\psi_{G',k}(z)\rangle = |\psi_{G,k}(z)\rangle + \sum_{l=1}^{L} a_{k,l}(z)[|u_l, v_l\rangle + |\psi_{G,l}(z)\rangle], \tag{61}$$

where the functions $a_{k,l}(z)$ are to be determined. Exactly as before, we have that

$$zU'(|1,0\rangle_k + |\psi_{G',k}(z)\rangle) = |\psi_{G',k}(z)\rangle + \sum_{j=L+1}^{K} \tau_j^{(k)}(z)|0,1\rangle_j, \tag{62}$$

where $\tau_j^{(k)}(z)$ denotes the appropriate transmission amplitude for Γ' the new Eulerian graph with tails where we replaced the first L pairs of tails with the corresponding handles. As before

$$zU'(|1,0\rangle_k + |\psi_{G,k}(z)\rangle + \sum_{l=1}^{L} a_{k,l}[|1,0\rangle_l + |\psi_{G,l}(z)\rangle])$$

$$= |\psi_{G,k}\rangle + \sum_{j=L+1}^{K} t_j^{(k)}|0,1\rangle_j + \sum_{j=1}^{L} t_j^{(k)}(z)|(u_j, v_j)\rangle$$

$$+ \sum_{l=1}^{L} a_{k,l}(z)\left[|\psi_{G,l}(z)\rangle + \sum_{j=L+1}^{K} t_j^{(l)}(z)|0,1\rangle_j + \sum_{j=1}^{L} t_j^{(l)}(z)|(u_j, v_j)\rangle \right]. \tag{63}$$

These equations lead to two sets of equations. The first set, L in number, is

$$a_{k,l}(z) = t_l^{(k)}(z) + \sum_{j=1}^{L} a_{k,j}(z)t_l^{(j)}(z), \tag{64}$$

where $1 \leqslant l \leqslant L$. This set of equations can be solved by Cramer's rule to give expressions for $a_{k,l}$ as rational functions of $t_l^{(k)}(z)$ and $t_l^{(j)}(z)$ in some neighborhood of the origin in the complex plane, because, the transmission amplitudes of Γ vanish at the origin. The second set of equations is

$$\tau_j^{(k)} = t_j^{(k)} + \sum_{l=1}^{L} a_{k,l}(z)t_j^{(l)}(z), \tag{65}$$

for $L+1 \leqslant j \leqslant K$. If we substitute the solutions to the first set of equations into the second set we get our desired result, which expresses the transition amplitudes of Γ' as rational functions of the transition amplitudes of Γ. The formula holds on a neighborhood of the unit disc in the complex plane. The rational functions themselves only depend upon the numbers K and L.

6. Cut a handle

Let us start with Γ an Eulerian graph with tails. Let $X_2, \ldots, X_K$ $(Y_2, \ldots, Y_K)$ be $K-1$ incoming (outgoing) tails attached at the vertices $v_2, \ldots, v_K$ $(u_2, \ldots, u_K)$, respectively. Let $e = (u_1, v_1)$ be an oriented edge in G. We wish to replace the edge e with a pair of tails, an incoming tail X_1 attached at v_1 and an outgoing tail Y_1 attached at u_1. The new vertices on X_1 the incoming tail will be denoted $1_x, 2_x, \ldots$ and the corresponding edges will be denoted $|k, k-1\rangle_x = |k_x, (k-1)_x\rangle$. The new vertices on Y_1 the outgoing tail will be $1_y, 2_y \ldots$ and the corresponding edges will be $|k, k+1\rangle_y = |k_y, (k+1)_y\rangle k = 1, 2, \ldots$. We will sometimes denote u_1 as 0_y and denote v_1 as 0_x respectively. Let G' be the graph with the same vertices as G and the same edges as G with the edge (u_1, v_1) removed. The new graph with tails $\Gamma' = (G', (v_1, v_2, \ldots, v_K), (u_1, u_2, \ldots, u_K))$ has all the vertices of Γ as well as the new vertices k_x and k_y for the two new tails. The edges of Γ' are those of Γ with (u_1, v_1) removed and the tail edges $|k, k+1\rangle_y$ and $|k+1, k\rangle_x k = 1, 2, \ldots$ added. The original free quantum structure U on Γ induces a new free quantum structure U' on Γ' as follows. First $U'_{k_y}|k-1, k\rangle_y = |k, k+1\rangle_y$ and $U'_{k_x}|k+1, k\rangle_x = |k, k-1\rangle_x$ must hold in order that U' be free. If v is a vertex of G' which is not equal to u_1 or v_1 then $U'_v = U_v$. In order to deal with v_1 and u_1 we note as in the last section that the edges of $\omega'_{v1}(\tau'_{u_1})$ are the same as those of $\omega_{v_1}(\tau_{u_1})$ with the edge (u_1, v_1) of Γ replaced by $|1, 0\rangle_x = |1_x, v_1\rangle(|0, 1\rangle_y = |u_1, 1_y\rangle)$. Thus the rule $U'_v = U_v$ still holds for vertices v_1 and u_1 if we consistently replace $|u_1, v_1\rangle$ in $\omega_{v_1}(\tau_{u_1})$ by $|1, 0\rangle_x(|0, 1\rangle_y)$ so

$$U'_{v_1}|1, 0\rangle_x = U_{v_1}|u_1, v_1\rangle. \tag{66}$$

This is unambiguous unless $u_1 = v_1$ where we replace $|u_1, v_1\rangle$ by $|0, 1\rangle_y$ in the formula.

This operation is clearly the inverse of our add-a-handle procedure. If we create a pair of tails X_1 and Y_1 from an edge (u_1, v_1) as above and the splice the new tails together to reform the edge (u_1, v_1) according to our add-a-handle prescription we end up with the same free quantum structure on the same graph with tails. Similarly if we start by first adding a handle by splicing a pair of tails, and then cut this new handle by the rules above we again arrive back where we started from.

Let $t_j^{(k)}(z), 2 \leqslant j, k \leqslant K$, be the transmission amplitudes for Γ, our original graph with tails, and let $T_j^{(k)}(z), 1 \leqslant k, j \leqslant K$, be the transmission amplitudes for the new configuration Γ'. We wish to compute the functions $T_j^{(k)}(z)$ from the attributes of Γ, which include the functions $t_j^{(k)}(z)$, as simply as possible. We begin by applying the results of the previous section to the graph Γ', as Γ is obtained from Γ' by adding a handle. This immediately gives us that

$$t_j^{(k)}(z) = T_j^{(k)}(z) + \frac{T_1^{(k)}(z)T_j^{(1)}(z)}{1 - T_1^{(1)}(z)}, \tag{67}$$

for $2 \leqslant j, k \leqslant K$. If we could find the functions $T_j^{(1)}(z)$ and $T_1^{(j)}(z)$, for $1 \leqslant j \leqslant K$, then we could solve these equations for the remaining $T_j^{(k)}(z)$. Note that these are the transmission amplitudes associated with the new tails, X_1 and Y_1.

In order to describe how to calculate these transmission amplitudes from Γ, we define the generalized eigenstate on Γ'

$$|\psi_1'(z)\rangle = |\sigma_{1^-}(z)\rangle + |\psi_{G',1}\rangle + \sum_{j=1}^{K} T_j^{(1)}(z)|\sigma_{j^+}(z)\rangle. \tag{68}$$

This is the formula for the generalized eigenstate generated by an incoming wave along X_1, where $|\psi_{G',1}\rangle$ is the part of this eigenstate that is supported on $\mathcal{H}_{G'}$. Let us note that $\mathcal{H}_G$ is the direct sum of $\mathcal{H}_{G'}$ and the one-dimensional subspace consisting of multiples of $|u_1, v_1\rangle$. Let $P_{G'}$ denote the orthogonal projection operator onto $\mathcal{H}_{G'}$, and let $U_{G'} = P_{G'}U$. Considered as a state on Γ', $|\psi_{G',1}\rangle$ satisfies the equation

$$z P_{G'} U'(|\psi_{G',1}(z)\rangle + |1, 0\rangle_x) = |\psi_{G',1}(z)\rangle, \tag{69}$$

and this implies that considered as a state on Γ it satisfies

$$z P_{G'} U(|\psi_{G',1}(z)\rangle + |u_1, v_1\rangle_x) = |\psi_{G',1}(z)\rangle. \tag{70}$$

The solution to this equation is

$$|\psi_{G',1}(z)\rangle = \sum_{n=1}^{\infty} z^n U_{G'}^{(n)} |u_1, v_1\rangle. \tag{71}$$

Note that this equation contains only quantities defined on the original graph, Γ, so that it implies that $|\psi_{G',1}(z)\rangle$ can be calculated from the initial graph. Once we have found $|\psi_{G',1}(z)\rangle$ we can substitute it into the equation

$$T_j^{(1)}(z) = {}_j\langle 0, 1||U'(\psi_{G',1}(z) + |1, 0\rangle_x), \tag{72}$$

defined on Γ', to find $T_j^{(1)}(z)$.

Our remaining task is to find $T_1^{(j)}(z)$, for $2 \leqslant j \leqslant K$. This can be done by looking at the reverse graph Γ^R and its induced quantum structure and following a procedure analogous to the one we followed for Γ. We first find

$$\left|\psi_{G',1}^R(z)\right\rangle = \sum_{n=1}^{\infty} z^n \left(P_{G'}^R U^{(R)}\right)^n |v_1, u_1\rangle, \tag{73}$$

where $P_{G'}^R$ projects onto the subspace spanned by the states corresponding to all of the edges of $G^{(R)}$ except $|v_1, u_1\rangle$. Once we have $\left|\psi_{G',1}^R(z)\right\rangle$, we can use it to find $T_j^{(R)(1)}(z)$ in the same way we used $|\psi_{G',1}(z)\rangle$ to find $T_j^{(1)}(z)$. Finally, we can make use of the relation

$$T_j^{(R)(1)}(z) = T_1^{(j)}(z), \tag{74}$$

to find $T_1^{(j)}(z)$. This means that all of the quantities in equation (67) except $T_j^{(k)}(z)$ for $2 \leqslant j, k \leqslant K$ are then, in principle, known so that they can be used to find the transmission amplitudes for the cut graph.

7. The splice

We can use the results of section 5 to find the transmission amplitudes of a graph that is the result of splicing two other graphs together. Let us assume that the graph G, with entering tails $X_1, \ldots, X_K$ attached to G at the vertices $v_1, \ldots, v_K$, and exiting tails $Y_1, \ldots, Y_K$ attached to G at the vertices $u_1, \ldots, u_K$, can be broken into two disjoint pieces, G_1 and G_2. G_1 contains the vertices $v_1, \ldots, v_{L-1}$, to which the tails $X_1, \ldots, X_{L-1}$ are attached and the
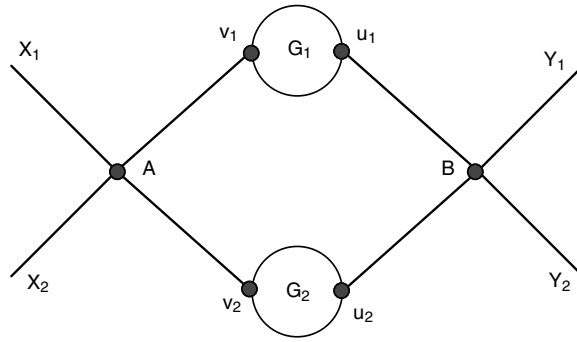
Figure 1. An arrangement for comparing the graphs G_1 and G_2. A particle starting a walk on the tail X_1 will never exit on the tail Y_2 if the graphs G_1 and G_2 are identical.

vertices $u_1 \ldots u_{L-1}$ to which the tails $Y_1 \ldots Y_{L-1}$ are attached. Similarly, G_2 contains the vertices $v_L, \ldots, v_K$, to which the tails $X_L, \ldots, X_K$ are attached and the vertices $u_L \ldots u_K$ to which the tails $Y_L, \ldots, Y_K$ are attached. We now remove the tails Y_1 and X_L and replace them by one directed edge from u_1 to v_L. This is simply a specific example of the adding-a-handle construction.

Let us now apply the results of the previous section. We first note that in the original graph, a particle entering G_1 would never exit from G_2, so $t_j^{(k)} = 0$ if $v_k \in G_1$ and $u_j \in G_2$. Similarly, a particle entering G_2 would never exit from G_1, which implies that $t_j^{(k)} = 0$ if $v_k \in G_2$ and $u_j \in G_1$. Making use of this result, we have from section 5 that

$$
\tau_j^{(k)}(z) = \begin{cases} t_j^{(L)}(z) t_1^{(k)}(z) & L \leqslant j \leqslant K, 1 \leqslant k \leqslant L-1 \\ t_j^{(k)}(z) & \text{otherwise} \end{cases} \tag{75}
$$

Therefore, we can use the add-a-handle construction to construct a quantum walk on a larger graph from walks on smaller ones.

8. Comparing graphs

We can use the techniques developed here to compare two graphs by doing a kind of interferometry with them. Suppose that G_1 has only two tails, an incoming tail X_1 attached to vertex v_1 and an outgoing tail Y_1 attached to u_1. Similarly, G_2 also has only two tails, an incoming tail X_2 attached to v_2 and an outgoing tail Y_2 attached to u_2. We would like to determine whether G_1 and G_2 are the same or different, with the additional constraint that if they are the same, v_1 in G_1 should correspond to v_2 in G_2, and u_1 in G_1 should correspond to u_2 in G_2.

One way of attacking this problem is to put the two graphs into an arrangement like that shown in figure 1. First, we remove the tails from the graphs. We now consider a vertex, A, with two incoming and two outgoing edges. The incoming edges are the initial edges of two incoming tails, X_{1A} and X_{2A}. One outgoing edge is attached to v_1 and the other is attached to v_2. Similarly, we consider a second vertex, B, with two incoming and two outgoing edges. The outgoing edges are the initial edges of two outgoing tails, Y_{1B} and Y_{2B}, and one incoming edge is attached to u_1 and the other is attached to u_2. We shall denote by Γ the graph with tails that we get when we connect G_1 and G_2 to the vertices A and B with the tails X_{1A}, X_{2A}, Y_{1B} and Y_{2B}, and by U the free quantum structure on Γ.

What we have done is to create a larger graph from G_1 and G_2 in which the two graphs are in parallel. We shall choose the unitary operators corresponding to the vertices A and B in such a way that if we start the walk on the incoming tail X_{1A}, and if the graphs G_1 and G_2 are identical, with v_1 in G_1 corresponding to v_2 in G_2, and u_1 in G_1 corresponding to u_2 in G_2, then the transmission amplitude corresponding to the outgoing tail Y_{2B} will be zero. Therefore, if we start a walk on the tail X_{1A}, and eventually find the particle on the tail Y_{2B}, we can conclude that the two graphs are not identical.

We now want to find the transmission amplitudes of the combined graph in terms of the transmission amplitudes of G_1 and G_2. In order to do this, we need to specify what happens at the vertices A and B. The states corresponding to the edges entering vertex A are $|1_1, A\rangle$, which is the initial edge of X_{1A}, and $|1_2, A\rangle$, which is the initial edge of X_{2A}. The states corresponding to the edges leaving vertex A are $|A, v_1\rangle$ and $|A, v_2\rangle$. The local isometry at vertex A mapping incoming to outgoing states has the following action

$$|1_1, A\rangle \rightarrow \tfrac{1}{\sqrt{2}}(|A, v_1\rangle + |A, v_2\rangle) \qquad |1_2, A\rangle \rightarrow \tfrac{1}{\sqrt{2}}(|A, v_1\rangle - |A, v_2\rangle). \qquad (76)$$

The local isometry at vertex B is essentially identical. The states corresponding to the edges entering vertex B are $|u_1, B\rangle$ and $|u_2, B\rangle$. The states corresponding to the edges leaving vertex B are $|B, 1_1\rangle$, which is the initial edge of Y_{1B}, and $|B, v_2\rangle$, which is the initial edge of Y_{2B}. The local isometry at vertex B mapping incoming to outgoing states is given by

$$|u_1, B\rangle \rightarrow \tfrac{1}{\sqrt{2}}(|B, 1_1\rangle + |B, 1_2\rangle) \qquad |u_2, B\rangle \rightarrow \tfrac{1}{\sqrt{2}}(|B, 1_1\rangle - |B, 1_2\rangle). \qquad (77)$$

The generalized eigenstate corresponding to the entering particle being on the tail X_{1A} is

$$|\psi_1(z)\rangle = |\sigma_{1-}(z)\rangle + |\psi_{A,B}(z)\rangle + \sum_{j=1}^{2} \tau_j^{(1)}(z)|\sigma_{j+}(z)\rangle, \qquad (78)$$

where $|\psi_{A,B}(z)\rangle$ is the part between vertices A and B. The transmission amplitude $\tau_1^{(1)}(z)$ corresponds to the tail Y_{1B}, and the transmission amplitude $\tau_2^{(1)}(z)$ corresponds to the tail Y_{2B}. We would like to find these transmission amplitudes in terms of the transmission amplitudes for G_1 and G_2, which we shall denote by $t_{1,1}^{(1)}(z)$ and $t_{1,2}^{(1)}(z)$, respectively. We can find the transmission amplitudes for Γ, and the state $|\psi_{A,B}(z)\rangle$ by making use of the equations

$$zU(|1_1, A\rangle + |\psi_{A,B}(z)\rangle) = |\psi_{A,B}(z)\rangle + \sum_{j=1}^{2} \tau_j^{(1)}(z)|B, 1_j\rangle$$
$$zU(|A, v_k\rangle + |\psi_k(z)\rangle) = |\psi_k(z)\rangle + t_{1,k}^{(1)}(z)|u_k, B\rangle, \qquad (79)$$

where $k = 1, 2$ in the second equation. The states $|\psi_k(z)\rangle$, for $k = 1, 2$ are the internal parts of the generalized eigenfunctions of the graphs G_1 and G_2, respectively. We find that

$$|\psi_{A,B}\rangle = \frac{z}{\sqrt{2}} \sum_{j=1}^{2} \left(|A, v_k\rangle + |\psi_k\rangle + t_{1,k}^{(1)}|u_k, B\rangle \right)$$
$$\tau_1^{(1)}(z) = \frac{z^2}{\sqrt{2}} \left(t_{1,1}^{(1)}(z) + t_{1,2}^{(1)}(z) \right) \qquad (80)$$
$$\tau_2^{(1)}(z) = \frac{z^2}{\sqrt{2}} \left(t_{1,1}^{(1)}(z) - t_{1,2}^{(1)}(z) \right).$$

We can now clearly see that if the graphs G_1 and G_2 are the same, which implies that $t_{1,1}^{(1)}(z) = t_{1,2}^{(1)}(z)$, then $\tau_2^{(1)}(z) = 0$. Therefore, in this case the particle will never enter the tail Y_{2B}.

We have shown that we can compute the transmission amplitudes for the combined graph, Γ, in terms of those of G_1 and G_2, and that one of these amplitudes vanishes if G_1 and G_2 are the same. Therefore, a quantum walk on the combined graph can be used to compare G_1 and G_2. An important issue is how efficient this procedure is. In particular, we would like to know how many steps the walk needs to make to determine whether the graphs are the same or different, and how the number of steps is related to the number of edges in G_1 and G_2. This will remain for future work.

9. Conclusion

We have presented a formalism that describes quantum walks on directed, Eulerian graphs. These graphs have incoming and outgoing tails, and we define a free quantum structure on them that determines the motion of a particle on the graph. We found that the transmission amplitudes of such a graph are very useful in determining the behavior of a quantum walk on that graph. We have shown how the transmission amplitudes of altered graphs, i.e. graphs that are formed from an original one by adding or cutting an edge, can be found from the transmission amplitudes of the original graph. This allowed us, in some cases to find the transmission amplitudes of a graph in terms of those of its subgraphs. Finally, we showed how these constructions can be used to compare two graphs by constructing a larger graph from two smaller ones, which acts as a kind of interferometer. If the two smaller graphs are identical, a particle making a quantum walk on the larger graph can only emerge onto one of the two exit tails, but not onto the other.

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