Some Applications of Quantum Walks to a General Class of Searches and the Computation of Boolean Functions

by

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Abstract

In previous papers about searches on star graphs several patterns have been made apparent; the speed up only occurs when graphs are "tuned" so that their time step operators have degenerate eigenvalues, and only certain initial states are effective. More than that, the searches are never faster than $O\left(\sqrt{N}\right)$ time. In this thesis the problem is defined rigorously, the causes for all of these patterns are identified, sufficient and necessary conditions for quadratic-speed searches for any connected subgraph are demonstrated, the tolerance of these conditions is investigated, and it is shown that (unfortunately) we can do no better than $O\left(\sqrt{N}\right)$ time. Along the way, a useful formalism is established that may be useful in future work involving highly symmetric graphs. For a much shorter, abridged version of the first half of this thesis, see [1].

The tools and techniques so derived are then used to demonstrate that tree graphs can be used for the computation of Boolean functions. The philosophy of Farhi's work [2] on the continuous-time NAND tree is applied to a discrete-time walk with any (AND, OR, NAND, or NOR) gate at each vertex. Tentative results show that the vast majority of possible Boolean functions on N bits can be calculated in $O\left(\sqrt{N}\right)$ time.

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1 Introduction and Review of Quantum Walks

A graph is a structure composed of vertices connected to each other by edges. If we imagine a particle that can sit on on a vertex and move randomly to connected vertices, then we describe where it may be at a given time or the path that it takes using the study of random walks. The particle "randomly walks" from one vertex to the next to the next, with the probability of moving between any pair of vertices described by a transition matrix. Random walks fall broadly into two categories: continuous-time walks and discrete-time walks (the second of which is the focus of this thesis).

Through the study of random walks we can learn remarkable facts about the behavior of some large structures with simple components. For example, if we take an infinite set of vertices indexed by the integers and connect them sequentially (so that vertex jis connected to both vertices j - 1 and j + 1, $\forall j$), then we can talk about a "random walk on a line". In particular, if the probability of a particle jumping to either of the adjacent vertices is equal and time-invariant, then we find that we have a useful model of one-dimensional Brownian motion. We can describing the probability of a particle being at vertex j at time step t as P(j;t). If we place the particle at the origin at time zero, we find that the probability distribution of the particle some time later is roughly Gaussian. More precisely, if P(0;0) = 1, then $P(j;t) = \frac{1}{2^t} \left(\frac{t+j}{2}\right) \approx \sqrt{\frac{2}{\pi t}} e^{-\frac{2j^2}{t}}$, for $\frac{t+j}{2} \in \mathbb{Z}$. With even this trivial example we can model, for example, the diffusion of silt in pipes, and can already see the $O(\sqrt{t})$ rate of that diffusion. A "quantum walk" is a quantum version of a random walk [3]. In a quantum walk, a particle's motion is governed by probability *amplitudes*, whereas in a classical random walk it is governed by probabilities. Importantly, this means that the time-step operator of a classical walk is stochastic while the operator for a quantum walk is unitary. While not immediately obvious, this distinction leads to wildly different (and useful) behaviors. This difference can be clearly seen by comparing the random walk just discussed with the "Hadamard walk", which is arguably the closest quantum analog.

Unitarity implies that the process of the walk must necessarily be reversible. This requires that, at each step, the particle "remember" where it previously was. One method of resolving this issue is to include an ancillary "coin" to each vertex which can be in either of two states: $|\uparrow\rangle$ or $|\downarrow\rangle$. In the Hadamard walk the time step operator performs the following:

$$\mathbf{U}|j\rangle|\uparrow\rangle = \frac{|j+1\rangle|\uparrow\rangle + |j-1\rangle|\downarrow\rangle}{\sqrt{2}} \tag{1}$$

$$\mathbf{U}|j\rangle|\downarrow\rangle = \frac{|j+1\rangle|\uparrow\rangle - |j-1\rangle|\downarrow\rangle}{\sqrt{2}} \tag{2}$$

The probability of finding a particle with state $|\psi(x;m)\rangle$ on a given vertex is $P(x;m) = |\langle\langle j|\langle\uparrow|\rangle|\psi(x;m)\rangle|^2 + |\langle\langle j|\langle\downarrow|\rangle|\psi(x;m)\rangle|^2$. The state of a particle after m time-steps is $|\psi(x;m)\rangle = \mathbf{U}^m |\psi(x;0)\rangle$, where $|\psi(x;0)\rangle$ is the initial state. So, for example, if $|\psi(x;0)\rangle = |0\rangle|\uparrow\rangle$, then $\mathbf{U}|\psi(x;0)\rangle = \frac{1}{\sqrt{2}}(|-1\rangle|\downarrow\rangle + |1\rangle|\uparrow\rangle)$ and $P(1;1) = P(-1;1) = \frac{1}{2}$. After only one step the Hadamard walk yields the same results as the classical random

walk. However, after a few more time-steps we can begin to see the effect of interference. $|\psi(x;3)\rangle = \mathbf{U}^3 |\psi(x;0)\rangle = \frac{1}{\sqrt{8}} (|-3\rangle|\downarrow\rangle - |-1\rangle|\uparrow\rangle + |1\rangle(|\downarrow\rangle + 2|\uparrow\rangle)\rangle + |3\rangle|\uparrow\rangle)$ and therefore $P(-3;3) = P(-1;3) = P(3;3) = \frac{1}{8}$ and $P(1;3) = \frac{5}{8}$. Clearly this is a departure from the behavior of the classical walk, where $P(-1;3) = P(1;3) = \frac{3}{8}$. Advancing time rapidly shows that these differences are profound.



Figure 1: Probability vs. position at t = 100 for the classical and Hadamard walks described above.

While the classical walk diffuses and has a variance of $O(\sqrt{t})$, the quantum walk propagates and has a variance of O(t). Rather than approaching a Gaussian curve, the Hadamard walk oscillates around $P(x;m) = \frac{2m}{\pi(m-x)\sqrt{m^2-2x^2}}$ [3]. Just as bizarre, the probability of a random walk crossing to the left of the initial position is 1 for the classical walk and $\frac{2}{\pi}$ for the Hadamard walk [6].

Of course, the novel behavior of quantum walks is not limited to the line, and the applications are not limited to abstract math. Like classical walks, the time can be either continuous [4] or advance in discrete steps [5, 7]. Within the discrete- time walks, there are another two types. In the coined walk, the particle sits on the vertices and an extra degree of freedom, a quantum coin, is needed to make the dynamics of the walk unitary. In a "scattering walk" the particle sits on the edges and the two-state coin is replaced [8] by the two directions on that edge. There have been a number of experimental implementations of quantum walks, some using trapped ions [9, 10] and others using photons in optical networks [11]-[14].

Quantum walks have already proven useful in finding new quantum algorithms and expanding the applicability of previously known algorithms. The notion of a quantum walk was introduced in 1993 [5] and an analysis of the Hadamard walk had to wait until 2001 [6].

In [7] the notion of the quantum walk was placed on a more rigorous footing. For example, because quantum walks are always quasi-periodic (this is a property of unitary Markov processes) there's nothing directly analogous to a steady state, so a new notion was defined by using time-averaging. This time-average steady state was then used to define new notions for mixing, filling, and dispersion times. More importantly, they demonstrated that quantum walks provide at most a "polynomially faster" speed up over classical walks. Only more recently has interest started to take off as new applications are found. In particular, quantum walks have been shown to be useful for searches: finding marked structures, such as cliques [21], or structures that break the symmetry of a graph [22, 23]. In most cases there is a distinguished vertex, one whose behavior is different from the others, and the object is to find this vertex [16]-[20]. The first such algorithm was found in 2003 and described a search on the vertices of a hypercube [16]. In that case, a database search on 2^N items was reformulated as a walk on an N-dimensional hypercube and a quadratic speed up was the result, which typically seems to be the case with quantum searches.

While it is certainly true that quantum walks, and walks in general, can be used to study the behavior of things that are literally connected to each other (networks, fiber optic bundles, etc.), the graphs we study may be substantially more abstract but none the less useful. The "element distinctness problem" asks whether or not all of the elements in a set are distinct from each other. Classically, this can be solved for a set of size N in $O(N \log N)$ time, but using quantum walks this problem can be solved in $O\left(N^{\frac{2}{3}}\right)$ time [15]. This algorithm relies on reducing the problem to a search on the Johnson graph of the set in question. For a set S, the Johnson graph J(S,k) has one vertex for every kelement subset of S, and two vertices are connected by an edge if they share k-1 elements. With the introduction of a repeated element comes the introduction of new edges into the Johnson graph of the set. So, this set theory problem becomes a graph, and the quantum walk provides an algorithm that functions faster than any known classical algorithm. In the scattering model of quantum walks [8] the states are defined on edges, with two states on every edge; one for each of the two possible directions. So, if two vertices connected by some edge are labeled a and b, then $|a,b\rangle$ is the state on the edge that points from a to b, and $|b,a\rangle$ is the state on the edge pointing from b to a. If the vertices are labeled $1, \dots, m$, then a state of the system is written $|\Psi\rangle = \sum_{j,k=1}^{m} \alpha_{j,k} |j,k\rangle$, where $\alpha_{j,k} \in \mathbb{C}, 0 \leq |\alpha_{j,k}| \leq 1$, and $\sum_{j,k=1}^{m} |\alpha_{j,k}|^2 = 1$. These α 's are probability amplitudes, and $|\alpha_{j,k}|^2$ is the probability of measuring $|\Psi\rangle$ and detecting the particle in the state $|j,k\rangle$.

Each vertex hosts a local unitary operator that maps all of the incoming states to outgoing states. That is, if v is a vertex, and $\{a_j\}$ is the set of connected vertices, then the unitary operator defined on v, denoted \mathbf{U}_v , performs a mapping $\mathbf{U}_v : \{|a_j, v\rangle\} \rightarrow \{|v, a_j\rangle\}$. Notice that the notation used to describe the states indicates which vertex operator to apply. The only operator that will act on the state $|s, t\rangle$ is \mathbf{U}_t , and the vertex operator most recently applied to $|s, t\rangle$ was \mathbf{U}_s . The time step operator, \mathbf{U} , is defined as all of the \mathbf{U}_v taken together; $\mathbf{U} = \bigoplus_v \mathbf{U}_v$, where this direct sum is taken over all vertices. Like each \mathbf{U}_v , \mathbf{U} is unitary, but unlike each of the vertex-specific operators, \mathbf{U} is an endomorphism. As such, we can talk about the eigenvalues and eigenvectors (equivalently, "eigenstates") of \mathbf{U} . Because the edge state implies immediately which of the vertex-specific notation. For example, $\mathbf{U}|s,t\rangle = \oplus_v \mathbf{U}_v|s,t\rangle = \mathbf{U}_t|s,t\rangle$, but it is unnecessary on the right hand side to indicate which vertex operator is being used, since it is already announced by the state, " $|s,t\rangle$ ".

The eigenvalues of **U** all have modulus 1, and there is no "steady state". In an intuitive, not-rigorous sense, because **U** must be unitary (it is a quantum mechanical time evolution operator) it must conserve information. That is, for any given state there is a unique preimage. But a particle on a vertex at time t could have been on any adjacent vertex at time t - 1. In the earliest attempts to define a quantum analog to discrete random walks the states were again defined on the vertices, but it was quickly found that an ancillary "coin space" needed to be attached to each vertex to maintain unitarity and keep track of the state's previous vertex. The edge state formalism (e.g., $|a, b\rangle$) is an equivalent formalism that eliminates the need for ancillary spaces, while still carrying the additional information required.

Definition For the purposes of this thesis a "search" is defined to be a process used to distinguish between N-1 identical elements, and one marked element that a priori can be *any* of the N total elements. Under this definition the Shor algorithm, for example, is not a search because it is used to find numbers with certain properties that set them apart. The set of numbers being considered are not all equally likely to be "marked". Part of the reasoning behind this definition is that it leads naturally to graphs with very high symmetry, which substantially reduces the dimension and difficulty of the problem.

Define a mapping $\phi : E \to E$, where E is the set of edges, to be some rearrangement of edges such that $\mathbf{U} = \phi^{-1} \circ \mathbf{U} \circ \phi$, or equivalently $\phi \circ \mathbf{U} = \mathbf{U} \circ \phi$. ϕ is called a quantum graph automorphism [24], and it is a rearrangement of edges and vertices that leaves the effect of \mathbf{U} invariant. If there is a set of edges that can be mapped into each other by some quantum graph automorphism, then we say that these edges belong to the same equivalence class, and a uniform superposition of states on these edges is seen as a single edge on the "collapsed graph".

For example, consider the complete graph K_3 with vertices labeled A, B, C. Define A to be a strictly reflecting vertex (i.e., $\mathbf{U}|B, A\rangle = |A, B\rangle$) and B and C as strictly transmitting (i.e., $\mathbf{U}|B, C\rangle = |C, A\rangle$). We find that the only non-trivial quantum graph automorphism is the one that exchanges B and C. That is, ϕ makes the following exchanges: $|A, B\rangle \leftrightarrow$ $|A, C\rangle, |B, A\rangle \leftrightarrow |C, A\rangle$, and $|B, C\rangle \leftrightarrow |C, B\rangle$.



Figure 2: Collapsing a graph.

Whereas the original graph consisted of six states,

 $G = \{ |A, B\rangle, |B, A\rangle, |A, C\rangle, |C, A\rangle, |B, C\rangle, |C, B\rangle \}, \text{ the collapsed graph consists of only three states, } G_A = \{ \frac{1}{\sqrt{2}} \left(|A, B\rangle + |A, C\rangle \right), \frac{1}{\sqrt{2}} \left(|B, A\rangle + |C, A\rangle \right), \frac{1}{\sqrt{2}} \left(|B, C\rangle + |C, B\rangle \right) \}.$

There are two things to notice here. First, this set is closed under the action of U, and

second, each state in G_A is mapped to itself under ϕ . Indeed, the states on any collapsed quantum graph are composed of exactly those states that are left invariant under the action of every ϕ .

Definition For any graph G with a time step operator \mathbf{U} we define the "collapsed graph" or "automorphism graph" as $G_A \equiv \{|\psi\rangle : \phi|\psi\rangle = |\psi\rangle, \forall \phi$ where $\mathbf{U} = \phi^{-1}\mathbf{U}\phi\}$. That is, the collapsed graph is composed only of those states that are left invariant under the mapping of every automorphism that commutes with \mathbf{U} .

It is straightforward to demonstrate that G_A is closed under U. If $|\psi\rangle$ is a state on G_A , then

$$\begin{split} |\psi\rangle \in G_A \\ \Rightarrow \phi |\psi\rangle &= |\psi\rangle \\ \Rightarrow \mathbf{U}\phi |\psi\rangle &= \mathbf{U}|\psi\rangle \\ \Rightarrow \phi \mathbf{U}|\psi\rangle &= \mathbf{U}|\psi\rangle \\ \Rightarrow \mathbf{U}|\psi\rangle \in G_A \end{split}$$

By using collapsed quantum graphs we can decrease the dimension of the state space substantially. In the example above the number of dimensions was cut in half, but the greater the symmetry the greater the decrease in dimensions.

In this thesis, the high dimensionality of a large star graph is replaced with a variable and then the behavior of the graph in response to changes in that variable are analyzed. It will be shown that searches on star graphs with N edges can be executed in $O\left(\sqrt{N}\right)$ time, and that the subgraph used to "mark" an edge can be *any* known graph (this is a great generalization over the Grover algorithm). It will be shown that the algorithm is tolerant of some noise, with a bound dictated by the size of the star graph.

Some of the tools used will be applied toward the question of what structures can be detected through the use of signals reflected off of a graph. A technique will be described for finding the proportion of differently marked edges in a star graph. Finally, it will be shown that tree graphs can be used to calculate most Boolean functions in $O\left(\sqrt{N}\right)$ time, where N is the number of inputs, by using a discrete time quantum walk that reflects a signal off of the tree graph. This is also a generalization over previous results [2].

In section 2 a motivating example, the "Grover Graph", is introduced and the search algorithm is stated explicitly.

In section 3 some of the necessary mathematical machinery is constructed.

In section 4 the central idea behind the algorithm, "pairing", is established and several important theorems governing the behavior of pairing are proven.

In section 5 we investigate how much the graph can be changed before a the algorithm breaks down.

In section 6 the results regarding searches on the star graph are summarized and some methods of generalization are described.

In section 7 the tools and philosophies used in the first half of the paper are applied to the problem of determining the structure of a given graph through the interpretation of signals "reflected" off of the graph.

In section 8 those techniques are applied to star graphs and tree graphs. It is shown that tree graphs, properly prepared, can be used to calculate any given Boolean function.

2 Star Graphs With an Arbitrary Subgraph



Figure 3: A star graph with an unspecified subgraph, G.

This section describes the model that will be used throughout this thesis.

In figure 3 the 0 vertex is the "hub vertex". A hub vertex is a vertex with N connections, where N is allowed to vary. It is generally assumed that the reflection and transmission coefficients at a hub are the same for each of the N edges, so any incoming state, $|j, 0\rangle$ will be mapped to

$$\mathbf{U}|j,0\rangle = r|0,j\rangle + t\sum_{k\neq j}|0,k\rangle \tag{3}$$

Unitarity at the hub requires that $|r|^2 + (N-1)|t|^2 = 1$ and $2Re(r^*t) + (N-2)|t|^2 = 0$. We will assume that the hub is a standard "diffusive vertex" which means that $r = -1 + \frac{2}{N}$ and $t = \frac{2}{N}$, although it is easy to generalize away from this (section 6).

The subgraph, G, is attached to any one of the N edges radiating from vertex 0. We assume throughout this thesis that the structure of G is known, but not the vertex to which

it is attached. We can, without loss of generality, assume that it is attached to vertex 1, and in this way, vertex 1 is "marked".

Vertices 2 through N "reflect with a phase of ϕ ", which means that $\mathbf{U}|0, j\rangle = e^{i\phi}|j, 0\rangle$. ϕ is left with an unspecified value, so that it can be used to "dial in" certain eigenvalues of **U** (how this is done will be shown momentarily).

Vertices 0 and 1, the states between them, and everything in G make up the Right side of the graph.

Vertices 0 and 2 through N, as well as the edges connecting them, are called the Left side of the graph.

Throughout this thesis I will be referring to Right or Left eigenvalues or vectors. This will always indicate that the thing in question is native to that side of the graph, as opposed to the traditional meaning (e.g., normally a "left eigenvector" is one such that $\langle v | \mathbf{M} = \lambda \langle v | \rangle$.

The goal of a quantum search on a star graph is to somehow get the probability amplitude on the states $|0,1\rangle$ and $|1,0\rangle$ as high as possible, so that when a measurement is made the result is likely to be the marked edge. In this way the marked edge is found, and the search completed. Typically it is assumed that measurements cannot be made on G itself since, in some sense, if we had access to G we wouldn't be looking for it. So if a particle would have been measured on an edge in G, the measurement is assumed to be a null result. This turns out to be a smaller problem than it might seem at first and so a better, less-specific goal is to get the state supported mostly on the Right side. The effect of **U** on $|0,1\rangle$, as well as on any of the states in *G*, is different for different graphs, and will be left as a "black box".

For every value of $N \ge 2$ we have another, different graph, and a new problem to solve. However, by taking advantage of the obvious symmetries on the Left side, this graph can be collapsed substantially. For ease of notation define the following:

$$|in\rangle \equiv \frac{1}{\sqrt{N-1}} \sum_{j=2}^{N} |j,0\rangle \tag{4}$$

$$|out\rangle \equiv \frac{1}{\sqrt{N-1}} \sum_{j=2}^{N} |0,j\rangle \tag{5}$$

This is the collapsing discussed in the previous section. While there may be additional collapsing/simplification taking place inside of the subgraph, G, that will not be directly addressed in this thesis. At the hub vertex we find that **U** does this:

$$\mathbf{U}|in\rangle = [r + (N-2)t]|out\rangle + t\sqrt{N-1}|0,1\rangle$$
(6)

$$\mathbf{U}|1,0\rangle = r|0,1\rangle + t\sqrt{N-1}|out\rangle \tag{7}$$

Rewriting this in terms of a new perturbation variable, $\epsilon \equiv \frac{1}{N}$, we find:

$$\mathbf{U}|in\rangle = (1 - 2\epsilon)|out\rangle + 2\sqrt{\epsilon - \epsilon^2}|0,1\rangle \tag{8}$$

$$\mathbf{U}|1,0\rangle = (-1+2\epsilon)|0,1\rangle + 2\sqrt{\epsilon - \epsilon^2}|out\rangle \tag{9}$$

Note that **U** is a function of ϵ , and define $\mathbf{U}_0 \equiv \mathbf{U}|_{\epsilon=0}$. The number of edges, N, connected to the hub vertex is the only variable in the graph, and studying the dependence of the eigenvalues and eigenvectors on $\epsilon = \frac{1}{N}$ will be the focus of most of this thesis. Unless otherwise noted, assume that every variable (eigenvalues, eigenvectors, etc.) is a function of ϵ . In general, denote $f_0 \equiv f(\epsilon)|_{\epsilon=0}$. For example, suppose $|w\rangle$ is an eigenvector of **U**. It may depend on ϵ , because **U** depends on ϵ . $|w_0\rangle$ is the corresponding eigenvector of \mathbf{U}_0 , defined as $|w_0\rangle \equiv |w\rangle|_{\epsilon=0}$, and it is constant.

When $\epsilon = 0$, which is the $N \to \infty$ limit, the states of the two sides of the graph, Left $\equiv \{|in\rangle, |out\rangle\}$ and Right $\equiv \{G, |0,1\rangle, |1,0\rangle\}$, are kept separate by \mathbf{U}_0 . The eigenvalues and vectors of both the Left and Right sides are changed relatively little by ϵ (this will be proven), so once they have been found they can be used without modification. Clearly, $\epsilon = 0$ is the easiest case to work with, and dealing with very large values of N (where search algorithms are useful) corresponds to very small values of ϵ . Phrased in this way, the problem lends itself naturally to a perturbative approach.

It is worth taking a moment to repeat that, and to point out how profound it is. The original problem involved an infinite family of graphs indexed by the number of edges in the star graph, N, each of which had a Hilbert space of dimension 2N + |G|, where |G| is the number of edge states in G. But by using the symmetry of vertices 2 through N to

collapse the graph, the problem now only considers a *single* graph with a Hilbert space of no more than dimension 4 + |G| and a single non-constant vertex (the "hub") that behaves like a value between the Left and Right sides in a simple and predictable way.

Because the location of vertex 1 is unknown, the initial states we have access to are of the form,

$$|\psi\rangle = \frac{\alpha}{\sqrt{N}} \sum_{j=1}^{N} |j,0\rangle + \frac{\beta}{\sqrt{N}} \sum_{j=1}^{N} |0,j\rangle$$
(10)

Which can also be written,

$$|\psi\rangle = \alpha |in\rangle + \beta |out\rangle + O\left(\frac{1}{\sqrt{N}}\right) \tag{11}$$

In other words, the initial state is (to within a small error) just a superposition of $|in\rangle$ and $|out\rangle$.

There's absolutely nothing stoping us from starting with a state like $\frac{1}{\sqrt{N}} \sum_{j=1}^{N} (-1)^{j} |0, j\rangle$. However, this state breaks the graph's symmetry a bit, since we now have to treat the odd and even vertices separately, and the graph becomes that much more unwieldy.

A cursory look at \mathbf{U}_0 reveals that the eigenvalues from the Left side of the graph are $\lambda = \pm e^{i\frac{\phi}{2}}$, and that the corresponding eigenvectors are $\frac{1}{\sqrt{2}} \left(|out\rangle \pm e^{i\frac{\phi}{2}} |in\rangle \right)$. It will be shown that if the Right side of the graph shares one or both of these eigenvalues, then a "rotation" (as described in section 4) may occur, and an initial state of the form $|\ell_0\rangle = \frac{1}{\sqrt{2}} \left(|out\rangle \pm e^{i\frac{\phi}{2}} |in\rangle \right)$ will move into another eigenstate with the same eigenvalue, $|\mathfrak{r}_0\rangle$, in the Right side in $O\left(\sqrt{N}\right)$ time.

So, finding G boils down to finding one of the eigenvalues and eigenvectors of the Right side, and this can be done by "dialing in" ϕ so that the Left side shares an eigenvalue with the Right. This, by the way, is the great advantage of star graphs; any eigenvalue can be easily attained, and there are only two dimensions ($|in\rangle$ and $|out\rangle$). That said, the results and techniques of this thesis can be applied far more generally.

The "paired" eigenvalues of **U** that are involved in searches with a quadratic speed up take the form $\lambda(\epsilon) = \sum_{j=0}^{\infty} a_j (\pm \sqrt{\epsilon})^j$ (this will be proven). In what follows, it will often be advantageous to write this as $\lambda = \lambda_0 e^{\pm ic\sqrt{\epsilon}} + O(\epsilon)$. It will be shown that finding a known graph merely requires matching Left and Right eigenvalues of **U**₀.

2.1 Grover Graph Example

For the Grover graph, G is simply a vertex that reflects with a phase of π . The Grover graph is named for the Grover algorithm, which it exactly emulates. This example is simple enough that it can be completed by hand. The pairing of eigenvectors, the $\sqrt{\epsilon}$ dependences and errors, as well as the $O(\sqrt{N})$ time required to execute the search are all evident here.

The Grover graph is a motivating example, but in the appendix a more complicated graph, the "bolo graph", is used to demonstrate how the various theorems and techniques of this thesis can be quickly applied.

The basis states of the (collapsed) Grover graph are:

$$\begin{aligned} |\psi_1\rangle &= |out\rangle \\ |\psi_2\rangle &= |in\rangle \\ |\psi_3\rangle &= |0,1\rangle \\ |\psi_4\rangle &= |1,0\rangle \end{aligned}$$

The time step matrix, **U**, is defined as before with the addition that $\mathbf{U}|0,1\rangle = -|1,0\rangle$. So, using the basis states as listed above,

$$\mathbf{U} = \begin{pmatrix} 0 & 1 - 2\epsilon & 0 & 2\sqrt{\epsilon - \epsilon^2} \\ e^{i\phi} & 0 & 0 & 0 \\ 0 & 2\sqrt{\epsilon - \epsilon^2} & 0 & 2\epsilon - 1 \\ 0 & 0 & -1 & 0 \end{pmatrix} \text{ and } \mathbf{U}_0 = \begin{pmatrix} 0 & 1 & 0 & 0 \\ e^{i\phi} & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \end{pmatrix}$$

The characteristic polynomial for \mathbf{U}_0 is $C_0(\lambda) = \lambda^4 - (e^{i\phi} + 1)\lambda^2 + e^{i\phi} = (\lambda^2 - e^{i\phi})(\lambda^2 - 1)$. This clean factoring is symptomatic of the separation of the Right and Left sides when $\epsilon = 0$. Clearly, double roots can be found when $\phi = 0$, so in what follows ϕ will be set to 0. The eigenvectors on the Left are $|\ell^{(1)}\rangle = \frac{1}{\sqrt{2}}(|out\rangle + |in\rangle)$ and $|\ell^{(-1)}\rangle = \frac{1}{\sqrt{2}}(|out\rangle - |in\rangle)$, for $\lambda = \pm 1$, and the eigenvectors on the Right are $|\mathbf{r}^{(1)}\rangle = \frac{1}{\sqrt{2}}(|0,1\rangle - |1,0\rangle)$ and $|\mathbf{r}^{(-1)}\rangle = \frac{1}{\sqrt{2}}(|0,1\rangle + |1,0\rangle)$, for $\lambda = 1$ and $\lambda = -1$ respectively.

The characteristic polynomial for **U** (with $\phi = 0$) is $C(\lambda) = \lambda^4 - 2(1 - 2\epsilon)\lambda^2 + 1$. The solutions of this equation are $\lambda(\epsilon) = \pm \sqrt{1 - 2\epsilon \pm 2i\sqrt{\epsilon - \epsilon^2}}$, where the \pm 's are independent of each other. The four eigenvalues and their associated eigenvectors are:

$$\begin{split} \lambda^{(1)}(\epsilon) &= \sqrt{1 - 2\epsilon + 2i\sqrt{\epsilon - \epsilon^2}}, \\ \lambda^{(2)}(\epsilon) &= \sqrt{1 - 2\epsilon - 2i\sqrt{\epsilon - \epsilon^2}}, \\ \lambda^{(3)}(\epsilon) &= -\sqrt{1 - 2\epsilon + 2i\sqrt{\epsilon - \epsilon^2}}, \\ \lambda^{(4)}(\epsilon) &= -\sqrt{1 - 2\epsilon - 2i\sqrt{\epsilon - \epsilon^2}}, \\ |V^{(1)}(\epsilon)\rangle &= \frac{1}{2} \begin{pmatrix} \sqrt{1 - 2\epsilon + 2i\sqrt{\epsilon - \epsilon^2}} \\ 1 \\ -i\sqrt{1 - 2\epsilon + 2i\sqrt{\epsilon - \epsilon^2}} \\ i \end{pmatrix}, |V^{(2)}(\epsilon)\rangle &= \frac{1}{2} \begin{pmatrix} \sqrt{1 - 2\epsilon - 2i\sqrt{\epsilon - \epsilon^2}} \\ 1 \\ i\sqrt{1 - 2\epsilon - 2i\sqrt{\epsilon - \epsilon^2}} \\ -i \end{pmatrix}, \\ |V^{(3)}(\epsilon)\rangle &= \frac{1}{2} \begin{pmatrix} \sqrt{1 - 2\epsilon + 2i\sqrt{\epsilon - \epsilon^2}} \\ -1 \\ -i\sqrt{1 - 2\epsilon + 2i\sqrt{\epsilon - \epsilon^2}} \\ -1 \\ -i\sqrt{1 - 2\epsilon + 2i\sqrt{\epsilon - \epsilon^2}} \\ -i \end{pmatrix}, |V^{(4)}(\epsilon)\rangle &= \frac{1}{2} \begin{pmatrix} \sqrt{1 - 2\epsilon - 2i\sqrt{\epsilon - \epsilon^2}} \\ -1 \\ i\sqrt{1 - 2\epsilon - 2i\sqrt{\epsilon - \epsilon^2}} \\ -1 \\ i\sqrt{1 - 2\epsilon - 2i\sqrt{\epsilon - \epsilon^2}} \\ i \end{pmatrix}. \end{split}$$

Notice that looping ϵ around 0 permutes $\{\lambda^{(1)}(\epsilon), \lambda^{(2)}(\epsilon)\}\$ and $\{\lambda^{(3)}(\epsilon), \lambda^{(4)}(\epsilon)\}\$. This property is important later. Written more simply,

$$\begin{split} \lambda^{(1)}(\epsilon) &= e^{i\sqrt{\epsilon}} + O(\epsilon), \\ \lambda^{(2)}(\epsilon) &= e^{-i\sqrt{\epsilon}} + O(\epsilon), \\ \lambda^{(3)}(\epsilon) &= -e^{i\sqrt{\epsilon}} + O(\epsilon), \\ \lambda^{(4)}(\epsilon) &= -e^{-i\sqrt{\epsilon}} + O(\epsilon), \end{split}$$

$$\begin{split} |V^{(1)}(\epsilon)\rangle &= \frac{1}{2} \begin{pmatrix} 1\\ 1\\ -i\\ -i\\ i \end{pmatrix} + O(\sqrt{\epsilon}) &= \frac{1}{\sqrt{2}} \left(|\ell^{(1)}\rangle - i|\mathfrak{r}^{(1)}\rangle \right) + O(\sqrt{\epsilon}), \\ |V^{(2)}(\epsilon)\rangle &= \frac{1}{2} \begin{pmatrix} 1\\ 1\\ i\\ -i\\ -i \end{pmatrix} + O(\sqrt{\epsilon}) &= \frac{1}{\sqrt{2}} \left(|\ell^{(1)}\rangle + i|\mathfrak{r}^{(1)}\rangle \right) + O(\sqrt{\epsilon}), \\ |V^{(3)}(\epsilon)\rangle &= \frac{1}{2} \begin{pmatrix} 1\\ -1\\ -i\\ -i\\ -i \end{pmatrix} + O(\sqrt{\epsilon}) &= \frac{1}{\sqrt{2}} \left(|\ell^{(-1)}\rangle - i|\mathfrak{r}^{(-1)}\rangle \right) + O(\sqrt{\epsilon}), \\ |V^{(4)}(\epsilon)\rangle &= \frac{1}{2} \begin{pmatrix} 1\\ -1\\ i\\ i\\ i \end{pmatrix} + O(\sqrt{\epsilon}) &= \frac{1}{\sqrt{2}} \left(|\ell^{(-1)}\rangle + i|\mathfrak{r}^{(-1)}\rangle \right) + O(\sqrt{\epsilon}). \end{split}$$

Notice that the two eigenspaces of \mathbf{U}_0 are both two dimensional, and are spanned differently. For example, the 1-eigenspace is spanned by $\{|\ell^{(1)}\rangle, |\mathbf{r}^{(1)}\rangle\}$ as well as by $\{|V^{(1)}(0)\rangle, |V^{(2)}(0)\rangle\}$. Moreover, the space spanned by $\{|V^{(1)}(\epsilon)\rangle, |V^{(2)}(\epsilon)\rangle\}$ for $0 < \epsilon \ll 1$ is nearly the same. Using the eigenvectors of \mathbf{U}_0 , instead of the "true" eigenvectors of \mathbf{U} does introduce errors, but they are small (this will be proven). The only reasonable initial states we have access to, under the assumption that the target vertex, 1, is unknown, are even superpositions of the form $\frac{1}{\sqrt{N}} \sum_{j=1}^{N} |0, j\rangle$ and $\frac{1}{\sqrt{N}} \sum_{j=1}^{N} |j, 0\rangle$. These states are located almost completely on the Left side and are nearly equal to $|out\rangle$ and $|in\rangle$, as their inner product reveals:

$$\langle out | \left(\frac{1}{\sqrt{N}} \sum_{j=1}^{N} |0, j\rangle\right) = \frac{1}{\sqrt{N(N-1)}} \sum_{j=2}^{N} \langle 0, j | 0, j\rangle = \sqrt{\frac{N-1}{N}} = 1 - O\left(\frac{1}{N}\right)$$

This means that the initial states will always start on the Left, up to a tiny error. Setting the initial state to be (approximately) in the 1-eigenspace we find: $|\psi\rangle = \frac{1}{\sqrt{2N}} \sum_{j=1}^{N} (|0, j\rangle + |j, 0\rangle) = \frac{1}{\sqrt{2}} (|in\rangle + |out\rangle) + O(\sqrt{\epsilon}) = |\ell^{(1)}\rangle + O(\sqrt{\epsilon}).$

Applying U repeatedly yields:

$$\begin{split} \mathbf{U}^{m} |\psi\rangle \\ &= \mathbf{U}^{m} \left(|\ell^{(1)}\rangle + O(\sqrt{\epsilon}) \right) \\ &= \mathbf{U}^{m} |\ell^{(1)}\rangle + O(\sqrt{\epsilon}) \\ &= \frac{1}{\sqrt{2}} \mathbf{U}^{m} |V^{(1)}\rangle + \frac{1}{\sqrt{2}} \mathbf{U}^{m} |V^{(2)}\rangle + O(\sqrt{\epsilon}) \\ &= \frac{1}{\sqrt{2}} e^{im\sqrt{\epsilon}} |V^{(1)}\rangle + \frac{1}{\sqrt{2}} e^{-im\sqrt{\epsilon}} |V^{(2)}\rangle + O(\sqrt{\epsilon}) \\ &= \frac{1}{\sqrt{2}} \begin{pmatrix} e^{im\sqrt{\epsilon}} + e^{-im\sqrt{\epsilon}} \\ e^{im\sqrt{\epsilon}} + e^{-im\sqrt{\epsilon}} \\ -ie^{im\sqrt{\epsilon}} + ie^{-im\sqrt{\epsilon}} \\ ie^{im\sqrt{\epsilon}} - ie^{-im\sqrt{\epsilon}} \end{pmatrix} + O(\sqrt{\epsilon}) \\ &= \frac{1}{\sqrt{2}} \begin{pmatrix} \cos(m\sqrt{\epsilon}) \\ \cos(m\sqrt{\epsilon}) \\ \sin(m\sqrt{\epsilon}) \\ -\sin(m\sqrt{\epsilon}) \end{pmatrix} + O(\sqrt{\epsilon}) \end{split}$$

So, if $m = \frac{\pi}{2\sqrt{\epsilon}} = \frac{\pi}{2}\sqrt{N}$, then to within an error of $O\left(\frac{1}{\sqrt{N}}\right)$ the system will be on the Right side, in either the state $|0,1\rangle$ or $|1,0\rangle$. A measurement at this time will complete the search.

It is worth pointing out that if we hadn't set $\phi = 0$ then the "true" eigenvectors $|V^{(k)}(\epsilon)\rangle$ would have been almost entirely constrained to one side or the other. This is because $|V^{(k)}(0)\rangle$ span the same eigenspaces as the Right and Left eigenvectors of \mathbf{U}_0 . If the Right and Left sides share no common eigenvalues, then we have four distinct eigenvalues and four distinct eigenspaces. So, rather than being a rearrangement of the eigenvectors of \mathbf{U}_0 , as was the case above, the $|V^{(k)}(\epsilon)\rangle$ are merely tiny perturbations of each of them individually.

Grover originally described his algorithm with a diffusion operator and an oracle operator. The diffusion operator is here replaced by the hub vertex, and the oracle with the differently-phased reflections from the remaining vertices. The result is exactly the same, and we can see that Grover's proof of optimality is merely a statement about the nature of the hub. That is, there's no way to modify the hub alone to get a better speed up.

2.2 The Search Algorithm on a Star Graph

Why this algorithm works will be derived throughout the next several sections. Details about the errors and tolerances are addressed in sections 5 and 6.

• Step 1) Find the eigenvalues and eigenvectors of the Right side.

Setting $\epsilon = 0$ separates the two sides and we are free to find the eigenvalues and vectors of \mathbf{U}_0 that correspond only to the Right side.

• Step 2) Select a target eigenvalue.

Every eigenspace on the Right side that is in contact with the hub vertex is a viable target. For a given eigenvalue there is only one possible target eigenvector on the Right, $|\mathbf{r}_0\rangle$.

• Step 3) Tune the Left side eigenvalues to match the target eigenvalue.

If the reflection coefficient at the end of edges 2 through N is $e^{i\phi}$, the eigenvectors on the Left are $|\ell_0\rangle = \frac{|out\rangle \pm e^{i\frac{\phi}{2}}|in\rangle}{\sqrt{2}}$ and the eigenvalues are $\lambda = \pm e^{i\frac{\phi}{2}}$.

• Step 4) Initialize the system with the state $|\Psi\rangle = \frac{1}{\sqrt{2N}} \sum_{j=1}^{N} (|0, j\rangle + \lambda |j, 0\rangle).$

It can't be helped that this initial state overlaps the Right side on the edge between vertex 1 and the hub, however this has very little impact on the results since it is such a tiny part of the initial state.

- Step 5) Iterate the time step operator, $\mathbf{U}, m = \lfloor \frac{\pi \sqrt{N}}{2c} \rfloor$ times. Where $c = \sqrt{2} |\langle 1, 0 | \mathfrak{r}_0 \rangle|$. This "rotates" the initial state into the target eigenstate on the Right.
- Step 6) Measure the system.

Being on the Right side means that the probability of measuring any edge other than those in the subgraph G or on the edge connecting G to the hub is very small.

2.3 Important Points

- An important difference between U₀ and U is that U₀ treats the Left and Right sides separately and is therefore block-diagonal, whereas U transmits across the hub with amplitude √ε. That is, ⟨out|U|1,0⟩ ≈ 2√ε.
- A uniform superposition of the edge states is nearly equal $(O(\epsilon))$ to some combination of $|in\rangle = \frac{1}{\sqrt{N-1}} \sum_{j=2}^{N} |j,0\rangle$ and $|out\rangle = \frac{1}{\sqrt{N-1}} \sum_{j=2}^{N} |0,j\rangle$. As such, any symmetric initial state on the edges connected to the hub will be concentrated almost entirely

on the Left side.

• This example shows that a quantum search algorithm can be seen as a "rotation" from the Left to the Right in $O(\sqrt{N})$ time steps.

3 Algebraic Functions and the Behavior of Zeros

In this section we will consider the relationship between the zeros of a polynomial and the coefficients of that polynomial. Later these results will be applied to characteristic polynomials. For more background on the math used in this section see [25] and [26].

Definition A "globally analytic function" is an analytic function that is defined as every possible analytic continuation of an analytic function from a particular point in a domain. Globally analytic functions can be many-valued.

For example, the globally analytic function $f(z) = \sqrt{z}$ has two branches (when $z \neq 0$): $f^{(0)}(re^{i\theta}) = \sqrt{r}e^{i\frac{\theta}{2}}$ and $f^{(1)}(re^{i\theta}) = \sqrt{r}e^{i\frac{\theta}{2}+\pi}$ with the branch cut (arbitrarily) taken at $\theta = 0$.

Just to emphasize the point that globally analytic functions can be many-valued, if $f(z) = \sqrt[4]{z}$, then f(16) = 2, 2i, -2, -2i, that is; f is "4-valued". For the different branches, $f^{(0)}(16) = 2, f^{(1)}(16) = 2i, f^{(2)}(16) = -2$, and $f^{(3)}(16) = -2i$.

Theorem 3.1. If f(z) is globally analytic in an annulus around 0, and is m-valued, then f(z) can be expressed as a Puiseux series (a Laurent series with certain rational powers) of the form $f(z) = \sum_{n=-\infty}^{\infty} A_n z^{\frac{n}{m}}$. Moreover, the m different branches of f, $f^{(k)}$, can be separated by an arbitrary branch cut through the annulus and expressed as $f^{(k)}(z) =$ $\sum_{n=-\infty}^{\infty} A_n \omega^{kn} z^{\frac{n}{m}}$, where ω is a primitive mth root of unity, $\omega = e^{i\frac{2\pi}{m}}$.

Proof The proof of this theorem is included in the appendix.

Define $P(z,\epsilon)$ to be a polynomial in z and ϵ , written $P(z,\epsilon) = \sum_{j=0}^{d} a_j(\epsilon) z^j$, where each $a_j(\epsilon)$ is a polynomial.

Assume that $a_d(0) \neq 0$ and that P(z, 0) has no zeros with a multiplicity higher than 1. That is, P(z, 0) has d independent roots: $\lambda^{(1)}, \dots, \lambda^{(d)}$.

Theorem 3.2. If $P(z, \epsilon)$ is a degree d polynomial in z, then there exists an open disk D, containing 0, and d analytic functions, $f^{(1)}, \dots, f^{(d)}$, such that:

- (i) $P(f^{(k)}(\epsilon), \epsilon) = 0, \epsilon \in D$
- $(ii) \quad f^{(k)}(0) = \lambda^{(k)}$
- $(iii) \quad P(\lambda,\epsilon)=0, \epsilon\in D \Rightarrow \lambda=f^{(k)}(\epsilon), for \; some \; k$

Note that $f^{(k)}$ are indexed functions, and not necessarily branches of the same globally analytic function. It is true that when $P(z, \epsilon)$ is not simultaneously reducible in both zand ϵ the zeros are all branches of a single globally analytic function of ϵ , however it is not necessary to know that here.

Proof In appendix.

Issues can crop up with the theorem above; specifically, if P(z, 0) has a repeated zero. But before dealing with higher order roots we need a few more tools.

Theorem 3.3. If $P(z, \epsilon)$ is an irreducible polynomial in z and ϵ , then all of the double roots of P are isolated in the ϵ -plane. That is, if for some value ϵ_0 , $P(z, \epsilon_0)$ has a double root, then there exists $\delta > 0$ such that when $0 < |\epsilon - \epsilon_0| < \delta$, $P(z, \epsilon)$ does not have a double root in z.

Proof In appendix.

Theorem 3.4. In the neighborhood of a zero of $P(z, \epsilon)$ of multiplicity s > 1, the zeros take the form $f^{(j)}(\epsilon) = \sum_{n=-\infty}^{\infty} A_n \omega^{jn} \epsilon^{\frac{n}{H}}$, where $H \leq s$. Specifically, the zeros are branches of one or more H_i -valued global analytic functions, with the given Puiseux series expansion, such that $\sum H_i = s$.

Proof In appendix

Notice that the only new case that this last theorem applies to are repeated roots. We've continued to assume that $a_d(\epsilon) \neq 0$.

The reason the " H_i 's" have been introduced is to deal with the possibility that a multiple root may not permute *all* of the branches of the function. For example, it may be the case that $\lambda^{(1)}(0) = \lambda^{(2)}(0) = \lambda^{(3)}(0) = \lambda^{(4)}(0)$, but that looping around $\epsilon = 0$ only permutes $\lambda^{(1)}(\epsilon)$ and $\lambda^{(2)}(\epsilon)$, in which case $H_1 = 2$, $H_2 = 1$, and $H_3 = 1$.

3.1 A Note on the Analyticity of the Characteristic Polynomial

In the section above it was assumed that the polynomial $P(z, \epsilon)$ is a polynomial with respect to both z and ϵ . Yet a quick look at **U** reveals that this may not necessarily be the case for the characteristic polynomial, since **U** contains entries of $O(\sqrt{\epsilon})$.

However, it can be shown that for the situation being considered in this thesis $C(z, \epsilon) =$
$|\mathbf{U}(\epsilon) - z\mathbf{I}|$ is always a polynomial with respect to ϵ . In fact, it is affine with respect to ϵ .

Theorem 3.5. Assume that **U** is a time step matrix as described so far. That is, there is a Left and Right side and these are connected only through a hub vertex with N edges where the reflection and transmission coefficients are $r = -1 + \frac{2}{N}$ and $t = \frac{2}{N}$. Then $C(z, \epsilon) =$ $|\mathbf{U} - z\mathbf{I}|$ is an affine polynomial of $\epsilon = \frac{1}{N}$, and can be written $C(z, \epsilon) = C_0(z) + \epsilon f(z)$.

Proof The proof of this is in the appendix.

Clearly, $C(z, \epsilon) = C_0(z) + \epsilon f(z)$ can never be factored into two polynomials in z and ϵ . The roots of an irreducible polynomial (such as this) can always be expressed as a single globally analytic function. An interesting consequence of this (not essential to this thesis) is that while looping ϵ around zero may not permute all of the zeros, there is always a path through the ϵ -plane which does.

For example, the zeros of the Grover graph are $\lambda(\epsilon) = \pm \sqrt{1 - 2\epsilon \pm 2i\sqrt{\epsilon - \epsilon^2}}$. Looping around $\epsilon = 0$ switches the sign on the inner " \pm " (i.e., $-2i\sqrt{\epsilon - \epsilon^2} \leftrightarrow 2i\sqrt{\epsilon - \epsilon^2}$), thereby permuting the zeros in pairs. So, $H_1 = H_2 = 2$. However, a loop around $\epsilon = \frac{1}{2}$ switches the sign on the outer " \pm ", so each branch of the function is connected to each of the others.

3.2 Important Points

- If $P(z,\epsilon)$ is a polynomial in both z and ϵ and $P(\lambda_0,0) = 0$, then the zeros are functions of the form $\lambda^{(j)}(\epsilon) = \sum_{n=-\infty}^{\infty} A_n \left(e^{i\frac{2\pi}{H}j}\right)^n \epsilon^{\frac{n}{H}}$ where $H \leq deg(\lambda_0, P(z,0))$.
- For a star graph as described in section 2, the characteristic polynomial of the time

step operator is a polynomial in z and an *affine* polynomial in ϵ . That is; it takes the form $C(z, \epsilon) = C_0(z) + \epsilon f(z)$, where $C_0(z)$ is the characteristic polynomial of \mathbf{U}_0 and f(z) is some polynomial in z. $deg(C_0) > deg(f)$.

4 Pairing

In the last section it was seen that the zeros, $\lambda^{(k)}$, of a (characteristic) polynomial with coefficients that are polynomials of ϵ take the form

$$\lambda^{(k)}(\epsilon) = \sum_{j=-\infty}^{\infty} A_j \omega^{jk} \epsilon^{\frac{j}{H}}$$
(12)

and these eigenvalues are grouped together into sets of size H which permute when ϵ loops around zero. For any given eigenvalue of \mathbf{U}_0 there can be more than one of these sets, and they may have different sizes. When the polynomial in question is the characteristic polynomial of the time step operator of a quantum walk, $C(z, \epsilon) = a_0(\epsilon) + a_1(\epsilon)z + \cdots + a_{d-1}(\epsilon)z^{d-1} + z^d$, then some new restrictions are brought into play.

The perturbation is assumed to be set up in such a way that for some path in the ϵ -plane starting at $\epsilon = 0$ **U** is unitary and along this path and therefore $|\lambda^{(k)}(\epsilon)| = 1$, $\forall k$. In a star graph **U** is unitary for all positive integer values of N. Since $\epsilon = \frac{1}{N}$ this path is along the positive real axis in the ϵ -plane.

Theorem 4.1. The eigenvalues, λ , of the matrix for a quantum walk, **U**, with a characteristic polynomial that is a polynomial in both λ and ϵ , can only take the form of $\lambda(\epsilon) = \sum_{j=0}^{\infty} A_j \epsilon^j$ or $\lambda(\epsilon) = \sum_{j=0}^{\infty} (\pm 1)^j A_j (\sqrt{\epsilon})^j$.

Proof Since \mathbf{U}_0 is unitary, $\lim_{\epsilon \to 0} \lambda(\epsilon)$ exists and is finite $(|\lambda^{(k)}(0)| = 1$, for all k). Therefore the Puiseux series for $\lambda^{(k)}(\epsilon)$ has no negative terms. For a particular eigenvalue of \mathbf{U}_0 , λ_0 , with multiplicity at least H, the various branches satisfy $\lambda^{(k)}(\epsilon) - \lambda_0 = \sum_{j=1}^{\infty} A_j \omega^{jk} \epsilon^{\frac{j}{H}}$. We can explore how the *H* branches, $\{\lambda^{(1)}(\epsilon), \dots, \lambda^{(H)}(\epsilon)\}$, separate from λ_0 by looking at the angle (phase difference) between two branches, $\lambda^{(k)}(\epsilon) - \lambda_0$ and $\lambda^{(j)}(\epsilon) - \lambda_0$. If Δ is the angle between two complex numbers, *x* and *y*, then $|x||y|\cos(\Delta) = Re(xy^*)$. So,

$$\begin{split} |\lambda^{(k)}(\epsilon) - \lambda_0| |\lambda^{(j)}(\epsilon) - \lambda_0| \cos{(\Delta)} &= Re\left((\lambda^{(k)}(\epsilon) - \lambda_0)(\lambda^{(j)}(\epsilon) - \lambda_0)^*\right) \\ \Rightarrow |A_1\omega^k \epsilon^{\frac{1}{H}} + O(\epsilon^{\frac{2}{H}})| |A_1\omega^j \epsilon^{\frac{1}{H}} + O(\epsilon^{\frac{2}{H}})| \cos{(\Delta)} &= Re\left((A_1\omega^k \epsilon^{\frac{1}{H}} + O(\epsilon^{\frac{2}{H}}))(A_1\omega^j \epsilon^{\frac{1}{H}} + O(\epsilon^{\frac{2}{H}}))^*\right) \\ \Rightarrow \left(|A_1|^2|\omega|^{k+j}|\epsilon|^{\frac{2}{H}} + O(\epsilon^{\frac{3}{H}})\right) \cos{(\Delta)} &= Re\left(|A_1|^2\omega^k(\omega^*)^j|\epsilon|^{\frac{2}{H}} + O(\epsilon^{\frac{3}{H}}))\right) \\ \Rightarrow \left(|A_1|^2 + O(\epsilon^{\frac{1}{H}})\right) \cos{(\Delta)} &= Re\left(|A_1|^2\omega^{k-j} + O(\epsilon^{\frac{1}{H}}))\right) \\ \Rightarrow \cos{(\Delta)} &= \frac{Re\left(|A_1|^2\omega^{k-j} + O(\epsilon^{\frac{1}{H}})\right)}{|A_1|^2 + O(\epsilon^{\frac{1}{H}})} \\ \Rightarrow \cos{(\Delta)} &= Re\left(\omega^{k-j}\right) + O(\epsilon^{\frac{1}{H}}) \\ \Rightarrow \Delta &= \arccos\left(\cos\left(\frac{2\pi}{H}(k-j)\right) + O(\epsilon^{\frac{1}{H}})\right) \\ \Rightarrow \Delta &= 2\frac{2\pi}{H}(k-j) + O(\epsilon^{\frac{1}{H}}) \end{split}$$

So, the angle between any two branches is at least $\frac{2\pi}{H}$. Indeed, the *H* directions that the different zeros take as they move away from λ_0 are initially evenly spaced. The only effect of ϵ taking different paths from zero is to rotate every $(\lambda^{(k)}(\epsilon) - \lambda_0)$. If there is a path that maintains the unitarity of $\mathbf{U}(\epsilon)$, then for values of ϵ along that path $|\lambda^{(k)}(\epsilon)| = 1$. But for small values of ϵ the unit circle is essentially a line. Specifically, if $\lambda^{(k)}(\epsilon)$ are restricted to the unit circle and $\lambda^{(k)}(\epsilon) - \lambda_0$ are evenly spaced, then either the angle between $\lambda^{(1)}(\epsilon) - \lambda_0$ and $\lambda^{(2)}(\epsilon) - \lambda_0$ must be π , or $\lambda(\epsilon)$ is single-valued. Therefore H = 1 or H = 2.

This theorem does *not* say that the roots of the characteristic polynomial have degree at most two. Indeed, the Bolo graph example (in the appendix) has a degree 3 root at z = -1. This theorem is stating that whatever the degree of the root, looping around $\epsilon = 0$ permutes those roots at most in pairs.

Definition Two eigenvalues are said to be "paired" when a small loop around 0 in the ϵ -plane causes them to switch (H = 2). As seen above, paired eigenvalues vary on the order of $O(\sqrt{\epsilon})$, and non-paired eigenvalues vary by $O(\epsilon)$. In addition, the associated eigenvectors and eigenprojections, **P**, are also said to be paired.

Theorem 4.2. $||\mathbf{P}^{(k)}(\epsilon) - \mathbf{P}^{(k)}(0)|| = O(\sqrt{\epsilon}) \text{ and } |V^{(k)}(\epsilon)\rangle = |V^{(k)}(0)\rangle + O(\sqrt{\epsilon}).$

Proof The proof of this is included in the appendix.

In that proof it was shown that $\mathbf{P}^{(k)}(\epsilon)$ can be expressed as a power series in $\sqrt{\epsilon}$. This means that since we can define $|V^{(k)}\rangle$ using these projections, not only do we find that the eigenvectors can likewise be written as power series in $\sqrt{\epsilon}$, but we automatically gain normalization: $|\langle V^{(k)}|V^{(k)}\rangle| = 1, \forall \epsilon$. What follows barely deserves to be a theorem, but it needs to be emphasized.

Theorem 4.3. If the vector $|W\rangle$ is some combination of eigenvectors of \mathbf{U} , $|W\rangle = \sum_j a_j |V^{(j)}\rangle$ where the a_j are independent of ϵ , then $|W\rangle = |W_0\rangle + O(\sqrt{\epsilon})$, where $|W_0\rangle \equiv \lim_{\epsilon \to 0} |W\rangle$.

Proof Since all eigenprojections can be written as power series in $\sqrt{\epsilon}$, eigenvectors with distinct eigenvalues can as well and it follows that a linear combination of such eigenvectors

can also be written as a power series in $\sqrt{\epsilon}$. $|W\rangle = \sum_{j=0}^{\infty} (\sqrt{\epsilon})^j |W_j\rangle = |W_0\rangle + O(\sqrt{\epsilon}).$

An extremely useful consequence of these theorems is that eigenvectors of \mathbf{U}_0 , which are easy to find, can be used as approximations of the exact eigenvectors of \mathbf{U} , which are difficult to find, are variable, and needlessly complex.

Theorem 4.4. $\mathbf{U}|V^{(k)}(\epsilon)\rangle = \lambda^{(k)}(\epsilon)|V^{(k)}(\epsilon)\rangle$ for all k. Define $\mathcal{S} = span\{|V^{(1)}(0)\rangle, \cdots, |V^{(j)}(0)\rangle\}$ to be some subset of eigenvectors of \mathbf{U}_0 , and $\mathbf{P}_{\mathcal{S}}$ as the projection operator onto \mathcal{S} .

- If $|u\rangle \in \mathcal{S}$, then $\forall m$
- $i) \quad \mathbf{P}_{\mathcal{S}^{\perp}} \mathbf{U}_0^m | u \rangle = 0$
- *ii*) $\mathbf{P}_{\mathcal{S}^{\perp}}\mathbf{U}^{m}|u\rangle = O(\sqrt{\epsilon})$

That is, if $|u\rangle \in S$, then $\mathbf{U}_0^m |u\rangle$ is also in S, and $\mathbf{U}^m |u\rangle$ is almost entirely in S.

Proof The proof of this theorem is trivial, but takes up a lot of space. It can be found in the appendix.

The essential idea behind this theorem is that if an initial state starts in an eigenstate or collection of eigenstates of \mathbf{U}_0 , then it will approximately stay there under arbitrarily many applications of \mathbf{U} . This means that, when setting up a search, only one eigenspace/eigenvalue of \mathbf{U}_0 needs to be considered. This keeps the situation much simpler.

4.1 Necessary and Sufficient Conditions for Pairing

In this section it will be shown that the eigenvectors of \mathbf{U}_0 can be disjointly divided up into "constant eigenvectors" and "active eigenvectors".

Theorem 4.5 (the three-case theorem). If λ_0 is a root of $C_0(z)$ with multiplicity s, then one and only one of the following cases applies to the " λ_0 family" of roots of $C(z, \epsilon)$, $\{\lambda^{(1)}(\epsilon), \dots, \lambda^{(s)}(\epsilon)\}$, where $\lambda^{(k)}(0) = \lambda_0$, $\forall k$.

i) $\lambda^{(k)}(\epsilon) = \lambda_0$, $\forall k$. That is, all of the roots are constant.

ii) $\lambda^{(k)}(\epsilon) = \lambda_0$, for all but one value of k. This root takes the form $\lambda^{(k)}(\epsilon) = \lambda_0 e^{ib\epsilon} + O(\epsilon^2)$.

iii) $\lambda^{(k)}(\epsilon) = \lambda_0$, for all but two values of k. These two are paired and take the form $\lambda^{\pm} = \lambda_0 e^{\pm ic\sqrt{\epsilon}} + O(\epsilon).$

Proof From theorem 3.5, the characteristic equation can be written $C(z, \epsilon) = C_0(z) + \epsilon f(z)$. Making the substitution $z = \lambda_0 + \delta$ this becomes $0 = C(\lambda_0 + \delta, \epsilon) = \sum_{j=s} a_j \delta^j + \epsilon \sum_{j=t} b_j \delta^j$, where $t = deg(\lambda_0, f)$. If $s \ge t$, then

$$0 = \sum_{j=s} a_j \delta^j + \epsilon \sum_{j=t} b_j \delta^j$$

$$\Rightarrow \epsilon \sum_{j=t} b_j \delta^j = -\sum_{j=s} a_j \delta^j$$

$$\Rightarrow \epsilon \left(b_t \delta^t + O(\delta^{t+1}) \right) = -a_s \delta^s + O(\delta^{s+1})$$

$$\Rightarrow \epsilon = -\frac{a_s}{b_t} \delta^{s-t} + O(\delta^{s-t+1})$$

$$\Rightarrow \delta = O\left(\epsilon^{\frac{1}{s-t}}\right)$$

However, by theorem 4.1 we know that unitarity implies $s - t \leq 2$. Therefore, if λ_0 is

a zero of $C_0(z)$ with multiplicity s, then it must also be a zero of f(z) with a multiplicity of at least s - 2. This leads to three cases:

i) If
$$deg(\lambda_0, f) \ge s$$
, then $0 = C(z, \epsilon) = (z - \lambda_0)^s (g(z) + \epsilon h(z))$, where $g(\lambda_0) \ne 0$. Here
the entire λ_0 family is identically equal to λ_0 , and has no ϵ dependence.

ii) If $deg(\lambda_0, f) = s - 1$, then $0 = C(z, \epsilon) = (z - \lambda_0)^{s-1}((z - \lambda_0)g(z) + \epsilon h(z))$, where $g(\lambda_0), h(\lambda_0) \neq 0$. In this case s - 1 of the members of the λ_0 family are constant, and the last root is a solution of $0 = (z - \lambda_0)g(z) + \epsilon h(z) = (g(\lambda_0)\delta + O(\delta^2)) + \epsilon(h(\lambda_0) + O(\delta))$. But this implies that $\delta = O(\epsilon)$.

iii) If $deg(\lambda_0, f) = s - 2$, then $0 = C(z, \epsilon) = (z - \lambda_0)^{s-2}((z - \lambda_0)^2 g(z) + \epsilon h(z))$, where $g(\lambda_0), h(\lambda_0) \neq 0$. Therefore, all but two members of the λ_0 family are constant, and the remaining two are of the form $\lambda_0 + O(\sqrt{\epsilon})$. But by theorem 3.4, and the definition of pairing, an eigenvalue of this form can only show up with another eigenvalue to which it is paired. It follows that, since there are no other possible eigenvalues to pair with, the two non-constant members of the λ_0 family must be paired with each other.

•	-	-	-	

Since there is only one paired set of eigenvectors for a given λ_0 , we can label them $|V^+\rangle$ and $|V^-\rangle$, where $\mathbf{U}|V^{\pm}\rangle = \lambda_0 e^{\pm ic\sqrt{\epsilon}+O(\epsilon)}|V^{\pm}\rangle = \lambda_0 e^{\pm ic\sqrt{\epsilon}}|V^{\pm}\rangle + O(\epsilon)$.

In the next few theorems the following properties will be important.

Theorem 4.6. Assume that $|V\rangle \equiv |V_0\rangle + \sqrt{\epsilon}|V_1\rangle + O(\epsilon)$, $|W\rangle \equiv |W_0\rangle + \sqrt{\epsilon}|W_1\rangle + O(\epsilon)$, $\langle V|V\rangle = \langle W|W\rangle = 1 \ \forall \epsilon$, and $\langle V|W\rangle = 0 \ \forall \epsilon$, then $i) \langle V_0 | V_0 \rangle = 1$ $ii) \langle V_0 | V_1 \rangle + \langle V_1 | V_0 \rangle = 0$ $iii) \langle V_0 | W_1 \rangle + \langle V_1 | W_0 \rangle = 0$

Proof These three results are immediate, upon inspection.

Theorem 4.7. Paired eigenvectors "straddle the hub". That is, if $|V\rangle$ is a paired eigenvector, then $|V_0\rangle$ has both a Left and Right side component.

Proof Paired eigenvectors have eigenvalues that always take the form
$$\lambda = \lambda_0 e^{ic\sqrt{\epsilon}} + O(\epsilon)$$
.
 $\langle V | \mathbf{U} | V \rangle = \lambda \langle V | V \rangle = \lambda$
 $\Rightarrow (\langle V_0 | + \sqrt{\epsilon} \langle V_1 |) (\mathbf{U}_0 + \sqrt{\epsilon} \mathbf{U}_1) (|V_0 \rangle + \sqrt{\epsilon} |V_1 \rangle) + O(\epsilon) = \lambda_0 + ic\lambda_0 \sqrt{\epsilon} + O(\epsilon)$
 $\Rightarrow \langle V_0 | \mathbf{U}_0 | V_0 \rangle + \sqrt{\epsilon} (\langle V_1 | \mathbf{U}_0 | V_0 \rangle + \langle V_0 | \mathbf{U}_0 | V_1 \rangle + \langle V_0 | \mathbf{U}_1 | V_0 \rangle) = \lambda_0 + ic\lambda_0 \sqrt{\epsilon}$
 $\Rightarrow \lambda_0 + \sqrt{\epsilon} (\lambda_0 \langle V_1 | V_0 \rangle + \lambda_0 \langle V_0 | V_1 \rangle + \langle V_0 | \mathbf{U}_1 | V_0 \rangle) = \lambda_0 + ic\lambda_0 \sqrt{\epsilon}$
 $\Rightarrow \sqrt{\epsilon} (\lambda_0 [\langle V_1 | V_0 \rangle + \langle V_0 | V_1 \rangle] + \langle V_0 | \mathbf{U}_1 | V_0 \rangle) = ic\lambda_0 \sqrt{\epsilon}$
 $\Rightarrow \lambda_0 [0] + \langle V_0 | \mathbf{U}_1 | V_0 \rangle = ic\lambda_0$
Since \mathbf{U}_i the $O(\sqrt{\epsilon})$ terms of \mathbf{U}_i is only involved in the transmission between the Leff

Since \mathbf{U}_1 , the $O(\sqrt{\epsilon})$ terms of \mathbf{U} , is only involved in the transmission between the Left and Right sides, in order for $\langle V_0 | \mathbf{U}_1 | V_0 \rangle$ to be non-zero, $|V_0\rangle$ must show up on both sides. That is; if $|V_0\rangle$ was entirely supported on the Right side, then $\mathbf{U}_1 | V_0 \rangle$ would be entirely supported on the Left side.

Theorem 4.8. Assume that the Right side λ_0 -eigenspace of \mathbf{U}_0 is D dimensional.

1) If the λ_0 -eigenspace of \mathbf{U}_0 is bound in G, then the λ_0 -eigenspace of \mathbf{U} is D dimensional and all of the associated eigenvectors are constant. This is case i) of the Three Case Theorem.

2) If the λ_0 -eigenspace of \mathbf{U}_0 is in contact with the hub vertex, then the Right sided λ_0 -eigenspace of \mathbf{U} is D-1 dimensional and the D-1 associated eigenvectors are constant and bound in G. This leaves one eigenvector which is non-constant in ϵ , and is in contact with the hub vertex. This is either case ii) or case iii) of the Three Case Theorem.

Proof The first result is trivial. If an eigenvector is bound in G, then varying ϵ (which only affects reflection and transmission across the hub vertex) can't have any impact on it. So, for eigenvectors bound in G, $\mathbf{U}|V\rangle = \mathbf{U}_0|V\rangle = \lambda_0|V\rangle$. The contra-positive is likewise clear; if an eigenvector is non-constant, then it must be in contact with the hub vertex.

The second result is far more hard won, and is included in the appendix.

In the proof of the above theorem (in the appendix), the Left side was given a particular form; it consisted of the states $|in\rangle$ and $|out\rangle$, with $\mathbf{U}|out\rangle = e^{i\phi}|in\rangle$. It may seem strange that a particular form for the Left side can be used to say such general things about the Right side. But keep in mind that what's been shown is that a certain number of the Right side λ_0 eigenvectors are bound in G. Once we know that an eigenvector on the Right is definitely not in contact with the hub vertex, then it doesn't matter what the Left side is doing. This last theorem can be stated far more succinctly as,

Theorem 4.9. Excluding a special case, a Right side eigenvector is constant and has a constant eigenvalue if and only if it is not in contact with the hub vertex.

That special case is $\lambda_0^2 + e^{i\phi} = 0$. When this happens the eigenvectors on each side are "balanced", and there is no net flow of probability across the hub. In the Grover graph example, this happens when $e^{i\phi} = -1$, which means that all of the edges become identical to the marked edge. As a result, the quantum graph can be collapsed to just two states: $|A\rangle = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} |0, j\rangle$ and $|B\rangle = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} |j, 0\rangle$. Without two sides, there is no net flow. In general, even though there may not be a further collapsing of the graph, when $\lambda_0^2 + e^{i\phi} = 0$ there is no net flow of probability across the hub.

Definition This unique non-constant member of the λ_0 family of eigenvectors, $|w\rangle$, depends on the Left side. But while $|w\rangle$ may depend on ϕ and ϵ , $|w_0\rangle \equiv \lim_{\epsilon \to 0} |w\rangle$ does not. It is unique so long as $\lambda_0^2 \neq e^{i\phi}$ (so long as there is no pairing). $|w_0\rangle$ is precisely the λ_0 eigenvector of \mathbf{U}_0 lost when moving from the $\epsilon = 0$ case to the $\epsilon \neq 0$ case. This $|w_0\rangle$ is a uniquely defined Right side λ_0 eigenvector of \mathbf{U}_0 , and it is called the "Right side active λ_0 eigenvector". An essentially identical proof demonstrates the existence of "Left side active λ_0 eigenvectors".

Definition All of the other λ_0 eigenvectors are bound in G, and so are called "bound λ_0 eigenvectors". Bound eigenvectors are independent of ϵ , or any structure on the far side

of the hub. If the λ_0 -eigenspace of \mathbf{U}_0 is *D*-dimensional overall, then the space of bound λ_0 eigenvectors of \mathbf{U} will be *D*, *D*-1, or *D*-2 dimensional depending on whether the Left and Right sides have active eigenvectors.

Definition The "active subspace" is the span of all of the active eigenvectors of \mathbf{U}_0 , for all eigenvalues. Since it is the compliment of the span of all of the bound eigenvectors, and each non-constant eigenvector is perpendicular to every bound eigenvector, every nonconstant eigenvector is contained in the active subspace.

Theorem 4.10 (The fundamental pairing theorem). The λ_0 -eigenspace is in contact with both the Left and Right sides of the hub vertex if and only if there exists paired vectors $|V^{\pm}\rangle$ with eigenvalues of the form $\lambda_0 e^{\pm ic\sqrt{\epsilon}} + O(\epsilon)$.

Proof The proof of this is somewhat involved and so is included in the appendix. Among the useful results of the Fundamental Pairing Theorem is the fact that \mathbf{U} can be expressed in the following form:

$$\mathbf{U}\left(\begin{array}{c}|\ell_{0}\rangle\\|\mathfrak{r}_{0}\rangle\end{array}\right) = \lambda_{0}\left(\begin{array}{c}\cos(c\sqrt{\epsilon}) & i\sin(c\sqrt{\epsilon})\\i\sin(c\sqrt{\epsilon}) & \cos(c\sqrt{\epsilon})\end{array}\right)\left(\begin{array}{c}|\ell_{0}\rangle\\|\mathfrak{r}_{0}\rangle\end{array}\right) + O(\epsilon)$$
(13)

And, with correctly chosen complex phases, the paired eigenvectors take the form:

$$|V^{\pm}\rangle = \frac{|\ell_0\rangle \pm |\mathfrak{r}_0\rangle}{\sqrt{2}} + O\left(\sqrt{\epsilon}\right) \tag{14}$$

So, on each side of the hub vertex we have a unique active eigenvector and paired eigenvectors are just combinations of the active eigenvectors from both sides, up to an error of $O(\sqrt{\epsilon})$. This makes the situation pretty simple, and we can ignore the bound states entirely.

4.2 The Efficiency of Searches Using Paired Eigenvectors

In order to execute a search in $O(\sqrt{N})$ it is necessary to use paired eigenspaces, since this is where changes of $O(\sqrt{\epsilon})$ can take place. The question addressed in this section is: given an initial state on one side of the hub vertex, how much of it can be transferred to the other? That is, what is the lower bound on the probability of a successful measurement under ideal conditions? Happily, the answer is $1 - |O(\sqrt{\epsilon})|$.

In the course of proving the fundamental pairing theorem an important additional fact was also proven, and is worth noting separately.

Theorem 4.11. Paired eigenvectors are always evenly divided across the hub vertex. That is, if **P** is a projection onto either the Left or Right side and $|V^{\pm}\rangle$ is a paired eigenvector, then $|\langle V_0^{\pm} | \mathbf{P} | V_0^{\pm} \rangle| = \frac{1}{2}$.

Proof As established in the fundamental pairing theorem, $|V_0^{\pm}\rangle = \frac{1}{\sqrt{2}} (|\ell_0\rangle \pm |\mathfrak{r}_0\rangle)$. For the Left side projector,

$$\begin{split} |\langle V_0^{\pm} | \mathbf{P}_L | V_0^{\pm} \rangle| \\ &= \frac{1}{2} | \left(\langle \ell_0 | \pm \langle \mathfrak{r}_0 | \right) \mathbf{P}_L \left(| \ell_0 \rangle \pm | \mathfrak{r}_0 \rangle \right) | \\ &= \frac{1}{2} | \left(\langle \ell_0 | \pm \langle \mathfrak{r}_0 | \right) | \ell_0 \rangle | \\ &= \frac{1}{2} | \langle \ell_0 | \ell_0 \rangle + 0 | \\ &= \frac{1}{2} \end{split}$$

The same holds for the Right side projector.

Theorem 4.12. If the paired eigenvalues are of the form $\lambda^{\pm} = \lambda_0 e^{\pm ic\sqrt{\epsilon}} + O(\epsilon)$, then $c = |\langle \ell_0 | \mathbf{U}_1 | \mathbf{\mathfrak{r}}_0 \rangle| = 2 \, |\langle out | \ell_0 \rangle| \, |\langle 1, 0 | \mathbf{\mathfrak{r}}_0 \rangle|.$

Proof In the last subsection it was established that (

Proof In the last subsection it was established that

$$\mathbf{U}\begin{pmatrix} |\ell_0\rangle \\ |\mathfrak{r}_0\rangle \end{pmatrix} = \lambda_0 \begin{pmatrix} \cos(c\sqrt{\epsilon}) & i\sin(c\sqrt{\epsilon}) \\ i\sin(c\sqrt{\epsilon}) & \cos(c\sqrt{\epsilon}) \end{pmatrix} \begin{pmatrix} |\ell_0\rangle \\ |\mathfrak{r}_0\rangle \end{pmatrix} + O(\epsilon).$$

From which it follows that,

$$\begin{aligned} \langle \ell_0 | \mathbf{U} | \mathbf{\mathfrak{r}}_0 \rangle \\ &= \langle \ell_0 | \mathbf{U}_0 | \mathbf{\mathfrak{r}}_0 \rangle + \langle \ell_0 | \mathbf{U}_1 | \mathbf{\mathfrak{r}}_0 \rangle \sqrt{\epsilon} + O(\epsilon) \\ &= \lambda_0 \langle \ell_0 | \mathbf{\mathfrak{r}}_0 \rangle + \langle \ell_0 | \mathbf{U}_1 | \mathbf{\mathfrak{r}}_0 \rangle \sqrt{\epsilon} + O(\epsilon) \\ &= 0 + \langle \ell_0 | \mathbf{U}_1 | \mathbf{\mathfrak{r}}_0 \rangle \sqrt{\epsilon} + O(\epsilon) \\ &= \langle \ell_0 | \mathbf{U}_1 | \mathbf{\mathfrak{r}}_0 \rangle \sqrt{\epsilon} + O(\epsilon) \\ &\Rightarrow i \, \lambda_0 \sin(c\sqrt{\epsilon}) + O(\epsilon) = \langle \ell_0 | \mathbf{U}_1 | \mathbf{\mathfrak{r}}_0 \rangle \sqrt{\epsilon} + O(\epsilon) \\ &\Rightarrow i \, \lambda_0 c \sqrt{\epsilon} + O(\epsilon) = \langle \ell_0 | \mathbf{U}_1 | \mathbf{\mathfrak{r}}_0 \rangle \sqrt{\epsilon} + O(\epsilon) \\ &\Rightarrow c = -i \, \lambda_0^* \langle \ell_0 | \mathbf{U}_1 | \mathbf{\mathfrak{r}}_0 \rangle \end{aligned}$$

Because $1 = |\lambda^{\pm}|$ we can infer that c is real, and we can therefore use the somewhat

simpler expression $c = |\langle \ell_0 | \mathbf{U}_1 | \mathbf{\mathfrak{r}}_0 \rangle|$. Finally,

$$c = |\langle \ell_0 | \mathbf{U}_1 | \mathbf{r}_0 \rangle|$$

= $|\langle \ell_0 | out \rangle \langle out | \mathbf{U}_1 | 1, 0 \rangle \langle 1, 0 | \mathbf{r}_0 \rangle|$
= $2 |\langle \ell_0 | out \rangle| |\langle 1, 0 | \mathbf{r}_0 \rangle|$
= $2 |\langle out | \ell_0 \rangle| |\langle 1, 0 | \mathbf{r}_0 \rangle|$

Theorem 4.13. \mathbf{U}^m , where $m = \left\lfloor \frac{\pi \sqrt{N}}{2|\langle \mathbf{r}_0 | \mathbf{U}_1 | \ell_0 \rangle|} \right\rfloor$, exchanges the Left and Right λ_0 active eigenvectors, $|\ell_0\rangle$ and $|\mathbf{r}_0\rangle$, almost completely (to within $O(\sqrt{\epsilon})$).

Proof To show that **U** interchanges $|\ell_0\rangle$ and $|\mathfrak{r}_0\rangle$ it suffices to show that $|\langle \mathfrak{r}_0 | \mathbf{U}^m | \ell_0 \rangle| =$

 $1 + O(\sqrt{\epsilon})$. Note that $m = \left\lfloor \frac{\pi}{2c\sqrt{\epsilon}} \right\rfloor = \frac{\pi}{2c\sqrt{\epsilon}} + O(1)$, since the floor function rounds down by at most 1.

$$\begin{aligned} |\langle \mathbf{r}_{0} | \mathbf{U}^{m} | \ell_{0} \rangle| \\ &= \frac{1}{2} \left| \left(\langle V_{0}^{+} | - \langle V_{0}^{-} | \right) \mathbf{U}^{m} \left(| V_{0}^{+} \rangle + | V_{0}^{-} \rangle \right) \right| \\ &= \frac{1}{2} \left| \left(\langle V^{+} | - \langle V^{-} | \right) \mathbf{U}^{m} \left(| V^{+} \rangle + | V^{-} \rangle \right) \right| + O(\sqrt{\epsilon}) \\ &= \frac{1}{2} \left| \left(\langle V^{+} | - \langle V^{-} | \right) \left((\lambda_{0} e^{ic\sqrt{\epsilon} + O(\epsilon)})^{m} | V^{+} \rangle + (\lambda_{0} e^{-ic\sqrt{\epsilon} + O(\epsilon)})^{m} | V^{-} \rangle \right) \right| + O(\sqrt{\epsilon}) \\ &= \frac{1}{2} \left| \lambda_{0}^{m} \right| \left| \left(\langle V^{+} | - \langle V^{-} | \right) \left(e^{ic\sqrt{\epsilon} + O(\epsilon)} \right)^{m} | V^{+} \rangle + (e^{-ic\sqrt{\epsilon} + O(\epsilon)})^{m} | V^{-} \rangle \right) \right| + O(\sqrt{\epsilon}) \\ &= \frac{1}{2} \left| \left(e^{ic\sqrt{\epsilon} + O(\epsilon)} \right)^{\frac{\pi}{2c\sqrt{\epsilon}} + O(1)} - \left(e^{-ic\sqrt{\epsilon} + O(\epsilon)} \right)^{\frac{\pi}{2c\sqrt{\epsilon}} + O(1)} \right| + O(\sqrt{\epsilon}) \\ &= \frac{1}{2} \left| e^{i\frac{\pi}{2} + O(\sqrt{\epsilon})} - e^{-i\frac{\pi}{2} + O(\sqrt{\epsilon})} \right| + O(\sqrt{\epsilon}) \\ &= \frac{1}{2} \left| e^{i\frac{\pi}{2}} - e^{-i\frac{\pi}{2}} + O(\sqrt{\epsilon}) \right| + O(\sqrt{\epsilon}) \\ &= \left| \sin\left(\frac{\pi}{2} \right) \right| + O(\sqrt{\epsilon}) \\ &= 1 + O(\sqrt{\epsilon}) \\ \Box \end{aligned}$$

So, when $m = \left\lfloor \frac{\pi \sqrt{N}}{2|\langle \mathfrak{r}_0 | \mathbf{U}^n | \ell_0 \rangle|} \right\rfloor$, $|\langle \mathfrak{r}_0 | \mathbf{U}^m | \ell_0 \rangle| = 1 + O(\sqrt{\epsilon})$. This means that searches with $|\ell_0 \rangle$ as the initial state are almost guaranteed to succeed, and all of the work that goes into setting up the search: choosing an initial state, knowing what to look for afterward, and figuring out how many times to iterate \mathbf{U} , has now been pushed back to finding the active eigenvectors $|\ell_0 \rangle$ and $|\mathfrak{r}_0 \rangle$.

Even this is relatively straightforward. $|\mathfrak{r}_0\rangle$ can be found be looking for the one eigen-

vector of $\mathbf{P}_R \mathbf{U}_0$ with eigenvalue λ_0 that is in contact with the hub vertex. This can be done in a few ways. For example, by removing each bound λ_0 eigenvector, or by comparing the λ_0 -eigenspaces of \mathbf{U}_0 and a quantum graph with the hub vertex's behavior replaced with something simple, like $\mathbf{U}|1,0\rangle = 0$. Trivially, if the Right side λ_0 -eigenspace is one dimensional and in contact with the hub, then the λ_0 eigenvector *is* the active eigenvector.

The value of N or ϵ , and the entire Left side, are unimportant to determining the active eigenvectors.

4.3 Best Choice Selection and the Best Time Bound

The bigger c is the faster a search will proceed. So, when the eigenvalue can be selected (when the Left side is such that it can be tuned to any given eigenvalue), the best choice is that eigenvalue with the largest value of c. The question remains: how good will the best choice be?

The specificity of the star graph described in section 2 allows us to be more precise about the value of c. Regardless of the value of ϕ , $|\langle out|\ell_0\rangle| = \frac{1}{\sqrt{2}}$. Therefore, $c = 2|\langle out|\ell_0\rangle| |\langle 1,0|\mathfrak{r}_0\rangle| = \sqrt{2}|\langle 1,0|\mathfrak{r}_0\rangle|.$

So for a star graph, $0 \le c \le \sqrt{2}$. Since $m = \left\lfloor \frac{\pi}{2c} \sqrt{N} \right\rfloor$, not being able to bound c from below means not being able to bound m from above. While we can't bound c from below in general, we find that we can bound the *largest* value from below.

Define d to be the number of Right side active eigenvectors, denoted $|\mathbf{r}_{0}^{(j)}\rangle$ for $j = 1, \dots, d$. These eigenvectors have eigenvalues $\lambda_{0}e^{ic^{(j)}\sqrt{\epsilon}}$. While there is no lower bound for

all of these, we can construct a lower bound for at least some of them.

Theorem 4.14. For Left side eigenvectors of the form $|\ell_0\rangle = \frac{1}{\sqrt{2}} \left(|out\rangle + e^{i\frac{\phi}{2}}|in\rangle \right)$, if d is the number of Right side active eigenvectors, then $\sum_{j=1}^d (c^{(j)})^2 = 2$ and there exists at least one j such that $c^{(j)} \ge \sqrt{\frac{2}{d}}$.

Proof $|1,0\rangle$ is adjacent to the hub vertex and therefore $|1,0\rangle$ is entirely contained in the active subspace. It follows that $1 = \sum_{j=1}^{d} |\langle 1,0|\mathfrak{r}_{0}^{(j)}\rangle|^{2} = \frac{1}{2} \sum_{j=1}^{d} (c^{(j)})^{2}$. Since $E\left[\left(c^{(j)}\right)^{2}\right] = \frac{2}{d}$, we know that there is at least one j such that $\left(c^{(j)}\right)^{2} \geq \frac{2}{d}$, which implies that $c^{(j)} \geq \sqrt{\frac{2}{d}}$.

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Definition The last theorem shows that there is at least one eigenvalue such that $m \leq \frac{\pi}{2\sqrt{2}}\sqrt{dN}$. This is the "best time bound" on the star graph. If the eigenvalue with the highest value of c is used, then the search will require this many time steps *at most*.

best time bound
$$= \frac{\pi\sqrt{dN}}{2\sqrt{2}} \le \frac{\pi\sqrt{(|G|+2)N}}{2\sqrt{2}}$$
 (15)

Where |G| is the number of states in G. Examples can be constructed where there is an arbitrarily small value of $c^{(j)} = \sqrt{2} |\langle 1, 0 | \mathfrak{r}_0 \rangle|$ for some values of j, but not for all. So long as there is a bound on the size of G, there is at least one eigenvalue where $c^{(j)}$ can be bound from below, and the corresponding number of required time steps is bound from above.

4.4 Important Points

For a star graph, with $\epsilon = \frac{1}{N}$:

- For a given eigenspace of \mathbf{U}_0 on either side, there is a unique vector called the "active eigenvector" that is dependent on ϵ and is in contact with the hub. All other eigenvectors in the same eigenspace are bound (not in contact with the hub) and are constant.
- The restriction to the unit circle requires that the roots of the characteristic polynomial take the form $\lambda(\epsilon) = \sum_{j=0}^{\infty} A_j \epsilon^j$ or $\lambda^{\pm}(\epsilon) = \sum_{j=0}^{\infty} (\pm 1)^j A_j (\sqrt{\epsilon})^j$. In the latter case the roots are said to be "paired".
- There is a pairing if and only if the Right and Left side both have an active eigenvector with the same eigenvalue. In the case that the eigenvalues of either side of the graph can be controlled, then a matching eigenvalue needs to be "dialed in".
- The eigenvalues and eigenvectors of U vary from those of U₀ by O(√ε). There might have been issues when an eigenspace of U₀ is degenerate, but we can uniquely specify eigenvectors of U₀ in these degenerate spaces by taking the limit of the non-degenerate eigenvectors of U as ε → 0.
- When there is no pairing these "constructed by limit" eigenvectors of U₀ are the active eigenvectors. In the case that there is a pairing we find that the paired eigenvectors, |V[±]>, of U are equal to a very specific combination of the Right and Left

active eigenvectors: $\frac{1}{\sqrt{2}} \left(|\ell_0\rangle \pm |\mathfrak{r}_0\rangle \right) + O(\sqrt{\epsilon}).$

- Paired eigenvalues can be expressed as $\lambda^{\pm} = \lambda_0 e^{\pm i c \sqrt{\epsilon}} + O(\epsilon)$, where $c = |\langle \ell_0 | \mathbf{U}_1 | \mathbf{\mathfrak{r}}_0 \rangle| = \lim_{\epsilon \to 0} \frac{1}{\sqrt{\epsilon}} |\langle \ell_0 | \mathbf{U} | \mathbf{\mathfrak{r}}_0 \rangle|$.
- The optimal number of time steps for a search is $m = \lfloor \frac{\pi}{2c} \sqrt{N} \rfloor$.
- For $|\ell_0\rangle = |out\rangle + e^{i\frac{\phi}{2}}|in\rangle$, we find that there is always a value of ϕ such that the paired eigenvalues produced will have $c > \sqrt{\frac{2}{d}}$, where d is the number of Right side active eigenvectors. For this value of $c, m < \frac{\pi}{2}\sqrt{\frac{dN}{2}}$.
- After *m* time steps the probability of the state being either in *G* or on the edge between *G* and the hub is $1 O(\sqrt{\epsilon})$.

5 Tolerances

For any number of reasons the Left and Right eigenvalues may not exactly match. However, the pairing doesn't break immediately, but instead fades away quickly as the disagreement between the eigenvalues increases. The eigenvalues don't have to be exactly equal in order for a $O(\sqrt{N})$ search, but they do have to be *nearly* equal by an amount dictated by ϵ .

This section will make heavy use of the math introduced in section 3.

5.1 Grover Graph example revisited

This is exactly the same situation previously seen in section 2.1, but now we are allowing $e^{i\phi}$ to take values other than 1. The advantage of the Grover graph is that it is simple enough that it is exactly solvable, even with this generalization.

The characteristic polynomial is $C(z) = z^4 - (1 - 2\epsilon)(1 + e^{i\phi})z^2 + e^{i\phi}$.

The four eigenvalues, expressed as one global function, is

$$\lambda = \pm \sqrt{\frac{1}{2}(1 - 2\epsilon)(e^{i\phi} + 1)} \pm \sqrt{\left(\frac{e^{i\phi} - 1}{2}\right)^2 - (e^{i\phi} + 1)^2(\epsilon - \epsilon^2)}$$

Where the ±'s are independent. In the original example, $\phi = 0$, so $\left(\frac{e^{i\phi}-1}{2}\right)^2 = 0$ and looping ϵ around zero permutes pairs of eigenvalues. When $\phi = 0$, then to lowest order $\lambda = \pm 1 \pm i\sqrt{\epsilon} + O(\epsilon) = \pm e^{\pm i\sqrt{\epsilon}} + O(\epsilon).$

When $\phi \neq 0$ the characteristic polynomial no longer has a double zero when $\epsilon = 0$. We can still expand around $\epsilon = 0$, but we find that the power series is in ϵ , not $\sqrt{\epsilon}$.

$$\lambda = \begin{cases} \pm e^{i\frac{\phi}{2}} \left(1 + i\cot\left(\frac{\phi}{2}\right)\epsilon\right) + O\left(\epsilon^{2}\right) \\ \pm \left(1 - i\cot\left(\frac{\phi}{2}\right)\epsilon\right) + O\left(\epsilon^{2}\right) \end{cases} = \begin{cases} \pm e^{i\frac{\phi}{2}}e^{i\cot\left(\frac{\phi}{2}\right)\epsilon} + O\left(\epsilon^{2}\right) \\ \pm e^{-i\cot\left(\frac{\phi}{2}\right)\epsilon} + O\left(\epsilon^{2}\right) \end{cases}$$
(16)

Clearly the pairing has been lost. However, the double zero required for pairing hasn't vanished, merely moved. This new location is ϵ_0 . To find it we set the discriminant equal to zero and solve for ϵ . In this particular case the discriminant is exactly what's found under the inner radical, $\mathcal{D} = (e^{i\phi} - 1)^2 - 4(e^{i\phi} + 1)^2\epsilon + 4(e^{i\phi} + 1)^2\epsilon^2$. We find immediately that $\epsilon_0 = \frac{1}{2} \pm \frac{1}{e^{i\phi} + 1}e^{i\frac{\phi}{2}} = \frac{1}{2} \pm \frac{1}{2\cos(\frac{\phi}{2})}$. We're interested in the zero that corresponds to $\epsilon_0|_{\phi=0} = 0$, and find that $\epsilon_0 = \frac{1}{2} - \frac{1}{2\cos(\frac{\phi}{2})} = -\frac{1}{16}\phi^2 + O(\phi^4)$. Expanding λ as a power series in $\sqrt{\epsilon - \epsilon_0} = \sqrt{\epsilon - \frac{1}{2} + \frac{1}{2\cos(\frac{\phi}{2})}}$, which we find can be done, the eigenvalues can now be written,

$$\lambda = \pm e^{i\frac{\phi}{4}} \pm ie^{i\frac{\phi}{4}} \sqrt{\cos\left(\frac{\phi}{2}\right)} \sqrt{\epsilon - \epsilon_0} + O(\epsilon - \epsilon_0) = \pm e^{i\frac{\phi}{4}} e^{\pm i\sqrt{\epsilon - \epsilon_0}} + O(\phi^2 \sqrt{\epsilon - \epsilon_0}, \epsilon - \epsilon_0)$$
(17)

Notice that if $|\epsilon| \gg |\epsilon_0|$, then the quadratic behavior is recovered. This will be discussed in substantially more detail below.

There's something subtle that happens with the eigenvectors here as well. When $\phi = 0$, all four of the eigenvectors of **U** are evenly divided between the Left and Right sides, to within $O(\sqrt{\epsilon})$. That is, **U** has four eigenvectors and when $\phi = 0$ the limit of all of them, as $\epsilon \to 0$, are evenly divided between the two sides since all four are paired.

When $\phi \neq 0$, \mathbf{U}_0 has four distinct eigenvalues: $\{1, e^{i\frac{\phi}{2}}, -1, -e^{i\frac{\phi}{2}}\}$. Therefore, the four

eigenvectors of **U**, in the limit as $\epsilon \to 0$, converge to two couples of vectors. Two on the Left for $\lambda_0 = e^{i\frac{\phi}{2}}, -e^{i\frac{\phi}{2}}$, and two on the Right for $\lambda_0 = 1, -1$.

Clearly there is a dramatic difference between these limits. This is a "twisting" of the eigenvectors of **U** that occurs around a double zero. A careful reading of theorem 4.2 reveals that it says that eigenvectors are continuous when they have distinct eigenvalues. When an eigenvalue is degenerate this "continuity of eigenvectors" becomes a "continuity of eigenspaces". There are two degenerate eigenspaces when $\epsilon = \frac{1}{2} - \frac{1}{2\cos(\frac{\phi}{2})}$ (when $\phi = 0$ these are the $\lambda = \pm 1$ eigenspaces of the original graph). Picking either, the degenerate space turns into two paired eigenvectors as ϵ moves away from this point, and it turns into two non-paired and single sided eigenvectors as ϕ moves away from this point.

From either direction the two eigenvectors of \mathbf{U} converge to the same degenerate eigen*space*. The fact that the vectors they converge to are different is unimportant.

5.2 Altering the Graph

We know that eigenvalues can pair, and that their values vary on the order of $\sqrt{\epsilon} = \frac{1}{\sqrt{N}}$, when \mathbf{U}_0 has an identical eigenvalue on both the Left and Right sides. However, we can hope that there should be some leeway, and that there will be pairing for *nearly* equal eigenvalues. The concern here is that changing the graph will turn a double root of C(z, 0)into a closely-spaced pair of <u>distinct</u> roots of C(z, 0). Since pairing and quadratic speed searches depend on the existence of double roots, these may be lost along with the double root. Define a new parameter, ξ , which describes a change in the graph, such as a change in the reflection and transmission coefficients of some of the vertices. Further, define ξ such that $C(z, \epsilon, \xi)$ is a polynomial in all of its arguments, and so that C(z, 0, 0) has a double root in z. $\xi = e^{i\phi} - 1 \approx i\phi$, from section 5.1, is the motivating example.

Theorem 5.1. If **U** has entries that are analytic functions of a given variable, ξ , then the eigenvectors of **U**, and by extension the eigenvalues, vary by $O(\xi)$.

Proof Using the same argument seen in the proof of theorem 4.2 (which is in the appendix) we can show that the resolvent, $\mathbf{R}(\zeta, \epsilon, \xi) = (\mathbf{U} - \zeta \mathbf{I})^{-1}$, can be expressed as a power series in ζ , $\sqrt{\epsilon}$, and ξ . Since $\mathbf{R}(\zeta, \epsilon, \xi)$ is a power series in ξ , it follows that the eigenprojections, $\mathbf{P}^{(k)}(\epsilon, \xi) = -\frac{1}{2\pi i} \oint_{\lambda^{(k)}} \mathbf{R}(\zeta, \epsilon, \xi) d\zeta$, and the eigenvectors, $|V^{(k)}\rangle$, are also expressible as power series in ξ .

Because each eigenvector can be written as $|V\rangle = |V_0\rangle + \xi |V_1\rangle + \xi^2 |V_2\rangle + \cdots$, and because by definition $\mathbf{U} = \mathbf{U}_0 + \xi \mathbf{U}_1 + \xi^2 \mathbf{U}_2 + \cdots$ it follows that the eigenvalues cannot have fractional exponents in ξ .

$$\begin{aligned} \mathbf{U}|V\rangle &= \lambda|V\rangle \\ \Rightarrow (\mathbf{U}_0 + O(\xi))(|V_0\rangle + O(\xi)) &= (\lambda_0 + O(\xi^s))(|V_0\rangle + O(\xi)) \\ \Rightarrow \mathbf{U}_0|V_0\rangle + O(\xi) &= \lambda_0|V_0\rangle + O(\xi^s) + O(\xi) \\ \Rightarrow O(\xi) &= O(\xi^s) + O(\xi) \\ \Rightarrow s \geq 1 \\ \Box \end{aligned}$$

Notice that this theorem does not rule out ordinary pairing of $O(\sqrt{\epsilon})$, since **U** has entries of the form $2\sqrt{\epsilon - \epsilon^2} = 2\sqrt{\epsilon} + O\left(\epsilon^{\frac{3}{2}}\right)$.

 ξ has been defined so that C(z, 0, 0) has a double root. By applying the arguments of section 3 to isolated roots of $C(z, \epsilon, \xi)$ we find that those roots, $\lambda^{(k)}(\epsilon, \xi)$, are analytic with respect to both ϵ and ξ .

Theorem 5.2. Changing ξ causes the location of double-zeros to drift. That is, a new value of ϵ that depends on ξ , labeled ϵ_0 , may be found such that $C(z, \epsilon_0(\xi), \xi)$ has a double root in z, and $\epsilon_0(\xi)$ is a continuous function of ξ .

Proof Consider the discriminant of C, defined as $\mathcal{D} = \prod_{j>k} (\lambda^{(j)} - \lambda^{(k)})^2$, where $\{\lambda^{(k)}\}$ are the roots of C in the variable z. The well-known and relevant properties of $\mathcal{D}(\epsilon, \xi)$ are 1) $\mathcal{D}(\epsilon, \xi) = 0$ if and only if $C(z, \epsilon, \xi)$ has a double root in z, and 2) if $C(z, \epsilon, \xi)$ is a polynomial in its arguments, then $\mathcal{D}(\epsilon, \xi)$ is also a polynomial in its arguments.

Because C(z, 0, 0) has a double root, we know that $\mathcal{D}(0, 0) = 0$. Using the same trick that was used to describe the behavior of λ with respect to ϵ (theorem 3.2), we can describe the new location of the double root in ϵ space with respect to ξ as $\epsilon_0(\xi) = \frac{1}{2\pi i} \oint t \frac{\partial_t \mathcal{D}(t,\xi)}{\mathcal{D}(t,\xi)} dt =$ $\sum_j b_j (\sqrt[s]{\xi})^j$ where s is less than or equal to the multiplicity of the root in $\mathcal{D}(\epsilon, \xi)$ in the variable ϵ . The important thing to notice here is that $\epsilon_0(\xi)$ is continuous with respect to ξ .

Note that since we're assuming that C(z, 0, 0) has a double root, $\epsilon_0(0) = 0$.

As shown in thm. 3.4, the only time that the Puiseux series of $\lambda^{(k)}(\epsilon)$ can have noninteger powers is when the expansion is taken about the location in the ϵ -plane of a double root of $C(z,\epsilon)$. With the introduction of ξ , as shown in the last theorem, the location of the double root is a function, $\epsilon_0(\xi)$. In order for the Puiseux series of $\lambda^{(k)}(\epsilon)$ to have half-integer powers in ϵ it must be expanded about ϵ_0 and so it takes the form $\lambda^{(k)}(\epsilon,\xi) =$ $\sum_{n=0}^{\infty} a_n(\xi) \left(\sqrt{\epsilon - \epsilon_0(\xi)}\right)^n$.

There are no new issues with expanding around $\epsilon = \epsilon_0$ as opposed to $\epsilon = 0$, and the above series can certainly be constructed.

5.3 Nearly-Paired Eigenvalues

Assume that the graph is altered in the manner described in the last subsection. Define the Left and Right eigenvalues when $\epsilon = 0$ as λ_{ℓ} and λ_r respectively. These are both analytic functions of ξ , and thus the phase difference between them can also be described as an analytic function of ξ . Define this phase difference as δ .

$$e^{i\delta} = \lambda_\ell \lambda_r^* \tag{18}$$

So long as $\lambda_{\ell}\lambda_{r}^{*}$ is invertible as a function of ξ , we can express ξ as a power series in δ and $\delta \propto \xi + O(\xi^{2})$. This is a fairly reasonable assumption. In the Grover Graph example provided at the beginning of this section $\delta = \frac{\phi}{2}$.

So, we can reasonably assume that \mathbf{U} , the eigenvectors, and the eigenvalues are all

analytic functions of $\delta = \lambda_{\ell} \lambda_r^*$. In addition the point in the ϵ -plane about which the eigenvalues permute, ϵ_0 , is a continuous function of δ .

We can now write λ as a power series in δ and $\sqrt{\epsilon - \epsilon_0}$.

$$\lambda^{\pm} = \sum_{j=0}^{\infty} (\pm 1)^j a_j(\delta) \left(\sqrt{\epsilon - \epsilon_0(\delta)}\right)^j \tag{19}$$

Since e^x is an analytic function, we can express this in a somewhat more convenient form:

$$\lambda^{\pm} = e^{i\sum_{j=0}^{\infty} (\pm 1)^j b_j(\delta) \left(\sqrt{\epsilon - \epsilon_0(\delta)}\right)^j} \tag{20}$$

Already we can make a few observations. Since these eigenvalues must have modulus 1 over a range of values of ϵ and δ , it follows that $b_j(\delta)$ is real for all j. This is important for the following proof.

Theorem 5.3. If the Left and Right eigenvalues have a phase difference of δ , then the location of the double root, ϵ_0 , is given by $\epsilon_0 = -\left(\frac{\delta}{2c}\right)^2 + O\left(\delta^4\right)$.

Proof Since λ is a power series is $\sqrt{\epsilon}$ and δ , it follows that

 $\lambda(0,\delta) = e^{ib_0(\delta) + ib_1(\delta)} \sqrt{-\epsilon_0(\delta)} + ib_2(\delta)(-\epsilon_0(\delta)) + \cdots \text{ is a power series in } \delta.$ Therefore, either $\epsilon_0(\delta)$ is a power series in δ^2 , or all of the odd terms (b_1, b_3, \ldots) are zero. However this can't be the case, since $b_1(0) = c$ (this is the same c used throughout the rest of this thesis). So, ϵ_0 is a power series in δ^2 .

From the definition of δ , $e^{i\delta} = \lambda_{\ell}\lambda_{r}^{*}$, we find that:

$$\begin{split} e^{i\delta} &= \lambda_{\ell} \lambda_{r}^{*} \\ &= \left[e^{i \sum_{j=0}^{\infty} b_{j}(\delta) \left(\sqrt{-\epsilon_{0}} \right)^{j}} \right] \left[e^{i \sum_{j=0}^{\infty} (-1)^{j} b_{j}(\delta) \left(\sqrt{-\epsilon_{0}} \right)^{j}} \right]^{*} \\ &= \left[e^{i \sum_{j=0}^{\infty} b_{j}(\delta) \left(\sqrt{-\epsilon_{0}} \right)^{j}} \right] \left[e^{-i \sum_{j=0}^{\infty} (-1)^{j} b_{j}(\delta) \left(\sqrt{-\epsilon_{0}} \right)^{j}} \right] \\ &= e^{i \sum_{j=0}^{\infty} (1 - (-1)^{j}) b_{j}(\delta) \left(\sqrt{-\epsilon_{0}} \right)^{j}} \\ &\Rightarrow \delta = \sum_{j=0}^{\infty} \left(1 - (-1)^{j} \right) b_{j}(\delta) \left(\sqrt{-\epsilon_{0}} \right)^{j} \\ &= 2b_{1}(\delta) \sqrt{-\epsilon_{0}} + 2b_{3}(\delta) \left(\sqrt{-\epsilon_{0}} \right)^{3} + \cdots \\ &= 2b_{1}(\delta) \sqrt{-\epsilon_{0}} + O\left(\delta^{3} \right) \\ &= 2 \left(b_{1}(0) + O(\delta) \right) \sqrt{-\epsilon_{0}} + O\left(\delta^{3} \right) \\ &= 2 c \sqrt{-\epsilon_{0}} + O\left(\delta^{2} \right) \\ &\Rightarrow 2 c \sqrt{-\epsilon_{0}} = \delta + O\left(\delta^{2} \right) \\ &\Rightarrow \epsilon_{0} = - \left(\frac{\delta}{2c} \right)^{2} + O\left(\delta^{3} \right) \\ \text{Finally, since } \epsilon_{0} \text{ is a power series in } \delta^{2}, \ \epsilon_{0} = - \left(\frac{\delta}{2c} \right)^{2} + O\left(\delta^{4} \right). \end{split}$$

Notice also that

$$\begin{split} \lambda_{\ell} \lambda_{r} \\ &= \left(e^{i \sum_{j=0}^{\infty} b_{j}(\delta) \left(\sqrt{0 - \epsilon_{0}(\delta)} \right)^{j}} \right) \left(e^{i \sum_{j=0}^{\infty} (-1)^{j} b_{j}(\delta) \left(\sqrt{0 - \epsilon_{0}(\delta)} \right)^{j}} \right) \\ &= e^{i 2 \sum_{j=0}^{\infty} b_{2j}(\delta) (-\epsilon_{0}(\delta))^{j}} \\ &= e^{i 2 b_{0}(\delta)} e^{i 2 \sum_{j=1}^{\infty} b_{2j}(\delta) (-\epsilon_{0}(\delta))^{j}} \\ &= e^{i 2 b_{0}(\delta)} e^{O\left(\delta^{2}\right)} \\ &= e^{i 2 b_{0}(\delta)} + O\left(\delta^{2}\right) \\ &\Rightarrow e^{i b_{0}(\delta)} = \sqrt{\lambda_{\ell} \lambda_{r}} + O\left(\delta^{2}\right) \end{split}$$

We can now write,

$$\lambda^{\pm} = e^{i\sum_{j=0}^{\infty} (\pm 1)^{j} b_{j}(\delta) \left(\sqrt{\epsilon - \epsilon_{0}(\delta)}\right)^{j}}$$

$$= e^{ib_{0}(\delta)} e^{\pm ib_{1}(\delta)\sqrt{\epsilon - \epsilon_{0}(\delta)} + i\sum_{j=2}^{\infty} (-1)^{jk} b_{j}(\delta) \left(\sqrt{\epsilon - \epsilon_{0}(\delta)}\right)^{j}}$$

$$= \left(\sqrt{\lambda_{\ell}\lambda_{r}} + O\left(\delta^{2}\right)\right) e^{\pm i(c + O(\delta))\sqrt{\epsilon - \epsilon_{0}(\delta)} + O(\epsilon - \epsilon_{0})}$$

$$= \sqrt{\lambda_{\ell}\lambda_{r}} e^{\pm ic\sqrt{\epsilon - \epsilon_{0}(\delta)} + O\left(\delta\sqrt{\epsilon - \epsilon_{0}(\delta)}, \epsilon - \epsilon_{0}\right)} + O\left(\delta^{2}\right)$$

$$= \sqrt{\lambda_{\ell}\lambda_{r}} e^{\pm ic\sqrt{\epsilon - \epsilon_{0}}} + O\left(\delta^{2}, \delta\sqrt{\epsilon - \epsilon_{0}}, \epsilon - \epsilon_{0}\right)$$

So, the double zeros of the characteristic polynomial and the pairing of the eigenvectors and eigenvalues aren't lost. The new double zero is halfway between λ_{ℓ} and λ_r . The pairing still exists, however it is in terms of $\sqrt{\epsilon + (\frac{\delta}{2c})^2 + O(\delta^4)}$, not $\sqrt{\epsilon}$.

5.4 Nearly-Paired Eigenvectors

Eigenvalues and eigen*spaces* vary by $O(\delta, \sqrt{\epsilon})$. This is an important distinction to make. The fundamental pairing theorem is essentially the statement that when $\delta = 0$, then $|V_0^{\pm}\rangle \equiv \lim_{\epsilon \to 0} |V^{\pm}\rangle = \frac{1}{\sqrt{2}} (|\ell_0\rangle \pm |\mathfrak{r}_0\rangle)$. However, when $\delta \neq 0$ we find that $|V_0^{\pm}\rangle$ must each converge independently to $|\ell_0\rangle$ and $|\mathfrak{r}_0\rangle$. $|V_0^{\pm}\rangle$ is defined as a limit of eigenvectors of \mathbf{U} , and must itself be an eigenvector of \mathbf{U}_0 . But if $\lambda_{\ell} \neq \lambda_r$, then no combination of the Left and Right active eigenvectors can be eigenvectors of \mathbf{U}_0 .

Therefore, $\lim_{\delta,\epsilon\to 0} |V^{\pm}(\delta,\epsilon)\rangle$ doesn't exist. Clearly, the "angle" between $|V^{\pm}(\delta,\epsilon)\rangle$ and the active eigenvectors, $|\ell_0\rangle$ and $|\mathfrak{r}_0\rangle$, is somehow dependent on δ and possibly some relationship between δ and ϵ .

With some foresight, define:

$$|V^{+}(\delta,\epsilon)\rangle = \cos\left(\omega\right)|\ell_{0}\rangle + \sin\left(\omega\right)|\mathfrak{r}_{0}\rangle + O(\delta,\sqrt{\epsilon})$$
(21)

$$|V^{-}(\delta,\epsilon)\rangle = -\sin(\omega) |\ell_{0}\rangle + \cos(\omega) |\mathfrak{r}_{0}\rangle + O(\delta,\sqrt{\epsilon})$$
(22)

That is, we can define ω using $\cos(\omega) \equiv \langle \ell_0 | V^+(\delta, \epsilon) \rangle + O(\delta, \sqrt{\epsilon}).$

Theorem 5.4. The angle between the paired eigenvectors and the active eigenvectors, ω , is to lowest order a function of $\frac{\delta^2}{4c^2\epsilon}$.

Proof The proof of this is included in the appendix.

This relationship (as derived in the proof of the above theorem) is

$$\sin^2(2\omega) = \left(1 + \frac{\delta^2}{4c^2\epsilon} + O\left(\frac{\delta^3}{\epsilon}, \delta, \epsilon\right)\right)^{-1}$$
(23)

In the first version of this proof, when dealing with exactly-matched eigenvalues, there was no issue with taking the limit $\epsilon \to 0$ to find the value of ω . However, in this case we have terms involving $\frac{\delta^2}{\epsilon}$ making that difficult.

5.5 Tuning

We now make the declarations that $\frac{\delta^2}{4c^2\epsilon} \equiv t = O(1)$ and that $O(\delta, \epsilon)$ is still small. In this way we can take the limit as both ϵ and δ go to zero, but fix a relationship between them. Then,

$$\sin^{2}(2\omega) = (1 + t + O(t\delta, \delta, \epsilon))^{-1}$$

$$\Rightarrow \sin^{2}(2\omega) = (1 + t + O(\delta, \epsilon))^{-1}$$

$$\Rightarrow \sin^{2}(2\omega) = \frac{1}{1+t}$$

$$\Rightarrow t \sin^{2}(2\omega) = 1 - \sin^{2}(2\omega)$$

$$\Rightarrow t = \frac{\cos^{2}(2\omega)}{\sin^{2}(2\omega)}$$

$$\Rightarrow t = \cot^{2}(2\omega)$$

When $t \approx 0$, $N \ll \left(\frac{2c}{\delta}\right)^2$ and $\omega \approx \frac{\pi}{4}$. In this case the graph behaves like a normal, paired system. That is, the mis-matching of the eigenvalues is not large enough to affect

the algorithm. The paired eigenvectors are each equal combinations of both the Right and Left active eigenvectors (to within $O(\sqrt{\epsilon}, \delta)$), and quadratic speed searches can be executed using the vectors $|\ell_0\rangle$ and $|\mathfrak{r}_0\rangle$.

For $t \approx 0$, in the $\{|\ell\rangle, |\mathfrak{r}\rangle\}$ basis,

$$\mathbf{U} = \lambda_0 \begin{pmatrix} \cos(c\sqrt{(1+t)\epsilon}) & -i\sin\left(c\sqrt{(1+t)\epsilon}\right) \\ -i\sin\left(c\sqrt{(1+t)\epsilon}\right) & \cos(c\sqrt{(1+t)\epsilon}) \end{pmatrix} + O(\epsilon)$$

When $t \gg 1$, $N \gg \left(\frac{2c}{\delta}\right)^2$ and $\omega \approx 0$. The system does not behave like a paired system, but instead behaves as though there are no matched eigenvalues at all. So, for large values of t the initial state stays where it is. The Left and Right eigenstates are decoupled, and are no longer useful for a search.

For
$$t \gg 1$$
, in the $\{|\ell\rangle, |\mathfrak{r}\rangle\}$ basis,

$$\mathbf{U} = \lambda_0 \begin{pmatrix} e^{ic\sqrt{(1+t)\epsilon}} & 0\\ 0 & e^{-ic\sqrt{(1+t)\epsilon}} \end{pmatrix} + O(t\epsilon)$$

"t" describes how "well tuned" a pair of active eigenvectors are for given values of ϵ and δ . It also provides an easy way to move back and forth between ϵ and $\epsilon - \epsilon_0$, since $\epsilon - \epsilon_0 = \epsilon + \left(\frac{\delta}{2c}\right)^2 + O\left(\delta^4\right) = \epsilon(1+t) + O\left(\delta^4\right)$. Graphs with a large value of t are "poorly tuned", and graphs with a small value of t are "well tuned".

We now wish to calculate $P(m) = |\langle \mathbf{r}_0 | \mathbf{U}^m | \ell_0 \rangle|^2$, which is the probability of a successful search, using $|\ell_0\rangle$ as an initial state and $|\mathbf{r}_0\rangle$ as a target state, after *m* time steps. How this depends on *t* will be considered in the following theorem.

Theorem 5.5. There is a better than 50% chance of a successful search of the N edges of the hub vertex using the states $|\ell_0\rangle$ and $|\mathfrak{r}_0\rangle$ after $m = \left\lfloor \frac{\pi}{2c}\sqrt{N} \right\rfloor$ iterations of the time step operator, whenever

$$\delta < c\sqrt{\frac{2}{N}} \tag{24}$$

where δ is the difference in phase between the Left and Right eigenvalues, and $c = |\langle \mathfrak{r}_{\mathfrak{o}} | \mathbf{U} | \ell_0 \rangle|.$

Proof The proof of this theorem will be included in the appendix.

So, when the error between the Left and Right eigenvalues is less than $c\sqrt{\frac{2}{N}}$, then we can ignore that error, and the algorithm will continue to work normally more than half of the time. We can do slightly better. A careful reading of the proof reveals that the lower bound on the probability is actually closer to $\approx 58.7\%$. The usual " $O(\sqrt{\epsilon}, \delta)$ " error does appear here, because that extra 8% can be used to ignore these terms for sufficiently large values on N ($N \ge O(100)$) and sufficiently small values of δ ($\delta \le O(0.1)$).

5.6 Important Points

- Left and Right eigenvalues of \mathbf{U}_0 don't need to match *exactly* for a pairing to exist, merely be very close: $|\lambda - \lambda'| = \delta \ll 1$.
- The double root "drifts left" in the ϵ -plane as a graph is perturbed: $\epsilon_0 = -\left(\frac{\delta}{2c}\right)^2 + O(\delta^4)$.

• If $\delta < c\sqrt{\frac{2}{N}}$, then all concerns over the eigenvalues not matching can be ignored completely, and the algorithm will still work as normal more than half of the time.

6 Summary of Results for Star Graph Searches

Take as given a star graph as described in section 2, with an attached subgraph G and a time step operator **U**. Define $\epsilon = \frac{1}{N}$, where N is the number of edges attached to the hub vertex.

- There are two kinds of eigenvectors of U₀: bound eigenvectors, and active eigenvectors. For a given eigenvalue, λ₀, of U₀ there is at most one active eigenvector, |**r**₀⟩. The "Right side λ₀ active eigenvector" is unique, and will exist if and only if the λ₀ eigenspace of U₀ is in contact with the Right side of the hub.
- Bound eigenvectors are completely isolated inside of G and are independent of ϵ .
- The same statements apply to the Left side (although frequently throughout this thesis we have assumed it to have a fixed, simple structure), and the Left side active λ₀ eigenvector is denoted |ℓ₀⟩.
- There is a pairing if and only if both the Left and Right sides have an active eigenvector with the same eigenvalue. A pairing means that there are eigenvalues of U of the form λ[±] = λ₀e^{±ic√ϵ} + O(ϵ). To first order, these eigenvalues vary by O(√ϵ), instead of by O(ϵ) as non-paired eigenvectors do. Paired eigenvalues are so named because they always appear in pairs.
- The eigenvectors associated with the two eigenvalues λ^{\pm} are $|V^{\pm}\rangle$ which have the property that $|V_0^{\pm}\rangle = \frac{1}{\sqrt{2}} (|\ell_0\rangle \pm |\mathfrak{r}_0\rangle)$, for properly chosen phases.

- There can be no eigenvectors or eigenvalues that vary faster than $O(\sqrt{\epsilon})$.
- $|\ell_0\rangle$ and $|\mathfrak{r}_0\rangle$ are rotated almost entirely into each other in $O\left(\sqrt{N}\right)$ time. That is, there exists m such that $|\langle \mathfrak{r}_0 | \mathbf{U}^m | \ell_0 \rangle| = 1 + O(\sqrt{\epsilon})$.
- That value of m is $m = \left\lfloor \frac{\pi \sqrt{N}}{2c} \right\rfloor$, where c is defined by the paired eigenvalues, $\lambda_0 e^{\pm ic\sqrt{\epsilon}}$. Writing the **U** as $\mathbf{U} = \mathbf{U}_0 + \sqrt{\epsilon}\mathbf{U}_1 + \cdots$, the value of c is $c = |\langle \mathbf{r}_0 | \mathbf{U}_1 | \ell_0 \rangle|$. For a Left side consisting of only the states $|out\rangle$ and $|in\rangle$, we find that $c = \sqrt{2}|\langle 1, 0 | \mathbf{r}_0 \rangle|$.
- We can quickly find a λ_0 , $|\ell_0\rangle$, and $|\mathfrak{r}_0\rangle$ because all of them are determined entirely by \mathbf{U}_0 , which tends to be easy to work with. This is because, in addition to being block-diagonal (the blocks corresponding to the Left and Right sides), \mathbf{U}_0 is often sparse, and unlike \mathbf{U} , it has no dependence on ϵ . With $|\ell_0\rangle$ and $|\mathfrak{r}_0\rangle$ in hand, the values of c and m follow immediately.
- λ₀ doesn't need to be an exact double eigenvalue in order for a quadratic speed up to occur, however the allowable difference in the eigenvalues, δ, is smaller for larger values of N. That is; larger searches require more exact control.
- When $\delta < c\sqrt{\frac{2}{N}}$, the probability of a successful search after $m = \left\lfloor \frac{\pi\sqrt{N}}{2c} \right\rfloor$ iterations of **U** is greater than 50%.

6.1 Sources of Error

In practice, the errors are produced by:
- Approximations of all of the important terms (i.e., $\lambda = \lambda_0 e^{ic\sqrt{\epsilon}} + O(\epsilon)$).
- The initial state is not exactly equal to |l₀>, since it has a small component on the Right side.
- $|\ell_0\rangle$ and $|\mathbf{r}_0\rangle$ are eigenvectors of \mathbf{U}_0 , not \mathbf{U} , but are approximated by linear combinations of $|V^{\pm}\rangle$: the actual eigenvectors of \mathbf{U} with eigenvalues λ_{\pm} .
- Rounding error due to the fact that *m* must be an integer.
- λ_0 may not be an exact double root, but instead a pair such that $|\lambda_0 \lambda'_0| = \delta \ll \sqrt{\epsilon}$.

All of these produce errors of $O(\sqrt{\epsilon}) = O\left(\frac{1}{\sqrt{N}}\right)$ or less in the final state. This is unlikely to be a problem on any individual run of the algorithm, and can be easily dealt with by repetition.

6.2 Generalizations and Future Work for Highly Symmetric Graphs

Generalized Values of r and t

In section 2, r and t were introduced, along with the unitarity conditions:

$$|r|^{2} + (N-1)|t|^{2} = 1$$
(25)

$$2Re(tr^*) + (N-2)|t|^2 = 0$$
(26)

Throughout this thesis the standard solution, $r = -1 + 2\epsilon$, $t = 2\epsilon$, has been used, where $\epsilon = \frac{1}{N}$ as usual. These are found by assuming $\arg(r) = \pi$ and $\arg(t) = 0$. However, by allowing arbitrary phase angles we find a family of solutions:

$$r = \frac{1 - 2\epsilon}{\sqrt{1 - 4\sin^2\left(x - y\right)(\epsilon - \epsilon^2)}} e^{ix} \tag{27}$$

$$t = \frac{-2\cos\left(x - y\right)\epsilon}{\sqrt{1 - 4\sin^2\left(x - y\right)(\epsilon - \epsilon^2)}} e^{iy}$$
(28)

where $\cos(x - y) < 1$. This condition is necessary for the second unitary condition to have solutions. In the collapsed graph we find $R_R = r$ and $R_L = r + (N - 2)t$ to be the reflection coefficients for the hub vertex from the Right and Left sides respectively, and $T = t\sqrt{N-1}$ as the transmission coefficient. By unitarity, $|R_R|^2 + |T|^2 = |R_L|^2 + |T|^2 = 1$ and $R_R^*T + R_LT^* = 0$. We can use this last relation to quickly find $R_L = -R_R^*(\frac{T}{T^*}) = -R_R^*e^{i2y}$.

We can now use this to re-visit theorems 3.5 and 4.2. In the proof of theorem 3.5 we found that $T^2 - R_R R_L = 1$ for the standard r and t, but this generalized solution may put that clean result at risk. Luckily, $T^2 - R_R R_L = |T|^2 e^{i2y} - (R_R)(-R_R^* e^{i2y}) =$ $(|T|^2 + |R_R|^2) e^{i2y} = e^{i2y}.$

In the proof of 3.5 it was shown that $C(z, \epsilon) = p_1(z) + p_2(z)R_R(\epsilon) + p_3(z)R_L(\epsilon)$, where p_1, p_2, p_3 are polynomials. So, while we still have a clean result, $C(z, \epsilon)$ is no longer a polynomial of ϵ . But if a substitution is made, $r = \frac{(1-2\epsilon)e^{ix}}{\sqrt{1-4\sin^2(x-y)(\epsilon-\epsilon^2)}} = e^{ix} - 2\cos^2(x-y)e^{ix}\epsilon + O(\epsilon^2) \equiv e^{ix}(1-2\mu)$, then $C(z,\mu)$ is a polynomial with respect to μ . Notice that

 μ is real when ϵ is real, and when $x = \pi$ and y = 0 we find $\mu = \epsilon$. Using μ instead of ϵ in section 3 we find that paired eigenvalues are of the form $\lambda = \lambda_0 e^{\pm i\sqrt{\mu}} + O(\mu)$. However, because $\mu = O(\epsilon)$, this result is the same as the original: $\lambda = \lambda_0 e^{\pm i\sqrt{\epsilon}} + O(\epsilon)$. Otherwise, since $\sqrt{\mu} = O(\sqrt{\epsilon})$, $\mu = O(\epsilon)$, and so on, all of the other results in this thesis remain the same.

Multiple Copies of G

Assume there are N total edges connected to the hub vertex, as before, but rather than 1 edge connected to G there are M edges connected to M copies of G. These various copies of G can be connected to each other, but (for this generalization) in such a way that in the automorphism graph there is only one remaining edge on the Left and Right sides.

The reflection and transmission coefficients are $R_L = r + (N - M - 1)t$, $R_R = r + (M - 1)t = -1 + 2\frac{M}{N}$, and $T = t\sqrt{M}\sqrt{N - M}$. Plugging in the standard solutions, $r = -1 + \frac{2}{N}$ and $t = \frac{2}{N}$, yields $R_L = 1 - 2\frac{M}{N}$, $R_R = -1 + 2\frac{M}{N}$, and $T = 2\sqrt{\frac{M}{N} - \left(\frac{M}{N}\right)^2}$, where again R_L and R_R are the Left and Right side reflection coefficients respectively. Clearly, by using $\epsilon = \frac{M}{N}$ instead of $\epsilon = \frac{1}{N}$ all of the behavior of a single copy of G is recovered (see section 2). Using the general solution for r and t doesn't provide quite such a clean result. For example, $T = \frac{-2\cos(x-y)\sqrt{\frac{M}{N}-\left(\frac{M}{N}\right)^2}}{\sqrt{1-4\sin^2(x-y)(\frac{1}{N}-\frac{1}{N}^2)}}e^{iy}$. But notice that to first order, like the standard solution, this is proportional to $\sqrt{\frac{M}{N}}$.

The important result to take away from this generalization is that we can expect searches to take a time of $O\left(\sqrt{\frac{N}{M}}\right)$. $\frac{N}{M}$ is the "effective degree" of the hub vertex.

Multiple Subgraphs

If there are multiple subgraphs that share a common eigenvalue but have different forms, then it can be shown that they will behave collectively as though they were a single subgraph. The probability of a particular subgraph being the result of a search increases with increasing c, as one might expect. These results fall immediately out of the fact that if there are S Right side subgraphs, each with a λ_0 active eigenvector, then we can construct S-1 "un-communicating" eigenstates from a linear combinations of those vectors. This leaves one "collective" active eigenvector that is a linear combination of the constituent active eigenvectors, weighted by their values of c.

The un-communicating eigenvectors are in contact with the hub vertex, but are bound in the sense that they are independent of ϵ and destructively interfere in such a way that they never interact with the Left side.

General Highly-Symmetric Graphs

The star graph gives us a way of looking at the behavior of a hub vertex in depth. For highly symmetric graphs with bounded diameter (the maximum distance between any pair of vertices is bound), we will find at least one hub vertex. Using the techniques of this thesis it should be fairly straight forward to generalize to automorphism graphs with multiple hubs. For example, in the investigation of the behavior of finite-depth tree graphs.

7 Quantum Sounding

The situation in question is an arbitrary graph, G, attached to an infinite string of edges. The vertices on this string are labeled 0, 1, 2, ... where 0 is a given vertex of G. We define the unitary time step operator on the edges as the one that passively moves each edge state one step. I.e., $\mathbf{U}|j, j+1\rangle = |j+1, j+2\rangle$ and $\mathbf{U}|j+1, j\rangle = |j, j-1\rangle$. The behavior of \mathbf{U} in the graph G is not specified here.

"Quantum Sounding" is the practice of gaining information from about G by sending signals along the tail, and then "listening" to the response. It is named in analogy to "depth sounding", which is a primitive form of sonar. Like depth sounding we find that we can gain some information, but not a detailed picture.

To simplify the question of how incoming and outgoing states interact with G we will first consider the much simpler (and finite) graph where the infinite tail is cut off at vertex 1 and replaced with a reflection that multiplies by α . That is:

$$\mathbf{U}|0,1\rangle = \alpha|1,0\rangle \tag{29}$$

Each section will conclude with an example where the results of that section will be applied to the Bolo graph.



Figure 4: The Bolo Graph

7.1 The Characteristic Polynomial

Theorem 7.1. $C(z, \alpha) = |z\mathbf{I} - \mathbf{U}| = b(z)(f(z) + \alpha g(z))$, where each of these are polynomials in z, f(z) and g(z) share no common factors, and the roots of b(z) all have modulus 1.

Proof This is easy to verify immediately by inspection of the matrix $\mathbf{U} - z\mathbf{I}$. α appears once, so every term in the characteristic polynomial either contains an α or doesn't. Clearly, the characteristic polynomial is affine in α .

We can collect the terms with and without α 's into two polynomials. Trivially, those polynomials can be labeled b(z)f(z) and $\alpha b(z)g(z)$, where b(z) is the collection of all of the factors common to both polynomials.

Finally, since the roots of b(z) are independent of α , and since U can be unitary (when $|\alpha| = 1$), the roots of b(z) are eigenvalues of a unitary matrix and therefore have modulus 1.

In everything that follows b(z) either doesn't play a roll, is not relevant, or factors out. So, it will be suppressed. A lot can be gained by the simple fact that **U** is unitary when $|\alpha| = 1$.

Theorem 7.2. $C(z, \alpha) = g_0 \alpha z^{d+s} C^* \left(\frac{1}{z}, \frac{1}{\alpha}\right), \quad \forall z, \forall \alpha \neq 0 \text{ where } C^* \text{ indicates the coef$ $ficients are conjugated, or equivalently, <math>f(z) = z^s \prod_{j=1}^d (z - \eta_j), \quad g(z) = g_0 z^{d'} f^* \left(\frac{1}{z}\right) = g_0 \prod_{j=1}^d \left(1 - z\eta_j^*\right), \text{ where } d' = d + s \text{ is the degree of } C(z, \alpha).$

Proof In what follows assume that $|\alpha| = 1$. This means that **U** is unitary, and the roots of the associated characteristic polynomial, $C(z, \alpha)$, all have modulus 1. While this proof will only consider f(z) and g(z), it works in exactly the same way for b(z)f(z) and b(z)g(z).

Define $C(z, \alpha) = \prod_{k=1}^{d'} (z - \lambda_k) = \sum_{k=0}^{d'} f_k z^k + \alpha \sum_{k=0}^{d'} g_k z^k$. Note that $f_{d'} = 1$ and $g_{d'} = g_{d'-1} = 0$, since when the determinant was taken any term with α necessarily did not include 2 diagonal elements (2 powers of z).

 $f(\lambda_k) + \alpha g(\lambda_k) = 0$ $\Leftrightarrow C(\lambda_k, \alpha) = 0$ $\Leftrightarrow (C(\lambda_k, \alpha))^* = 0$ $\Leftrightarrow C^*(\lambda_k^*, \alpha^*) = 0$ $\Leftrightarrow C^*\left(\frac{1}{\lambda_k}, \frac{1}{\alpha}\right) = 0$ $\Leftrightarrow 0 = f^*\left(\frac{1}{\lambda_k}\right) + \frac{1}{\alpha}g^*\left(\frac{1}{\lambda_k}\right)$ Therefore, $C(z, \alpha)$ and $C^*\left(\frac{1}{z}, \frac{1}{\alpha}\right)$ have the same set of zeros. It also follows that $\alpha z^{d'}C^*\left(\frac{1}{z}, \frac{1}{\alpha}\right) = \alpha z^{d'}f^*\left(\frac{1}{z}\right) + z^{d'}g^*\left(\frac{1}{z}\right)$ is a polynomial in z and α which, again, has the same set of zeros. Therefore, $\alpha z^{d'}C^*\left(\frac{1}{z}, \frac{1}{\alpha}\right)$ and $C(z, \alpha)$ are proportional to each other.

$$bC_{\alpha}(z) = \alpha z^{d'} (C^{*})_{\frac{1}{\alpha}} \left(\frac{1}{z}\right)$$

$$= \alpha z^{d'} \left[\sum_{k=0}^{d'} f_{k}^{*} \frac{1}{z^{k}} + \frac{1}{\alpha} \sum_{k=0}^{d} g_{k}^{*} \frac{1}{z^{k}}\right]$$

$$= \alpha \sum_{k=0}^{d'} f_{k}^{*} z^{d'-k} + \sum_{k=0}^{d} g_{k}^{*} z^{d'-k}$$

$$= \alpha \sum_{k=0}^{d'} f_{d'-k}^{*} z^{k} + \sum_{k=0}^{d} g_{d'-k}^{*} z^{k}$$

$$\Rightarrow \begin{cases} bf_{k} = g_{d'-k}^{*} \\ bg_{k} = f_{d'-k}^{*} \\ bg_{k} = f_{d'-k}^{*} \end{cases}$$
Now,
$$\begin{cases} f_{d'} = 1 \implies b = g_{0}^{*} \\ g_{d'-1} = g_{d'} = 0 \implies f_{0} = f_{1} = 0 \end{cases}$$

It follows that, since the constant term in a characteristic equation is equal to the

determinant, $1 = |\alpha g_0| = |g_0|$. We now have that $C(z, \alpha) = g_0 \alpha z^{d'} C^* \left(\frac{1}{z}, \frac{1}{\alpha}\right)$.

This last equation is merely a statement about the polynomial $C(z, \alpha)$. It is true regardless of the value of α .

$$C(z,\alpha) = g_0 \alpha z^{d'} C^* \left(\frac{1}{z}, \frac{1}{\alpha}\right)$$
(30)

in general, $\forall \alpha \neq 0$. Or equivalently,

$$f(z) = g_0 z^{d'} g^* \left(\frac{1}{z}\right) \tag{31}$$

$$g(z) = g_0 z^{d'} f^*\left(\frac{1}{z}\right) \tag{32}$$

We can say even more about the characteristic polynomial. The zeros of f(z) and g(z) have a very particular behavior and relationship.

Theorem 7.3.
$$C(z, \alpha) = \underbrace{z^s \prod_{j=1}^d (z - \eta_j) + \alpha g_0 \prod_{j=1}^d (1 - z\eta_j^*)}_{f(z)} and \ 0 < |\eta_j(\alpha)| < 1, \ \forall j.$$

Proof We know already that $f(z) = g_0 z^{d'} g^* \left(\frac{1}{z}\right)$. It follows that for $\eta_j \neq 0$, $f(\eta_j) = 0 \Leftrightarrow g\left(\frac{1}{\eta_j^*}\right) = 0$. Therefore, if $f(z) = z^s \prod_j (z - \eta_j)$, then $g(z) \propto \prod_j \left(z - \frac{1}{\eta_j^*}\right)$. With g_0 the constant term in g(z), we can write $g(z) = g_0 \prod_j \left(1 - z\eta_j^*\right)$.

Notice that f(z) and g(z) share a root if and only if $\eta_j = \frac{1}{\eta_j^*}$ or $|\eta_j| = 1$. But this is the necessary condition for, and an important property of, the roots of b(z). So, since we are assuming that f and g share no common factors, $|\eta_j| \neq 1$.

When $\alpha = 0$, $\mathbf{U}|0,1\rangle = 0$ and the eigenvalues of \mathbf{U} are the roots of C(z,0) = f(z). If a unit eigenvector, defined by $\mathbf{U}|V_j\rangle = \eta_j|V_j\rangle$, has the form $|V_j\rangle = S_j|0,1\rangle + |G_j\rangle$, then

$$|\eta_j|^2 = \langle V_j | \mathbf{U}^{\dagger} \mathbf{U} | V_j \rangle$$

= $\langle V_j | \mathbf{U}^{\dagger} \mathbf{U} | V_j \rangle$
= $\left(S_j^* \langle 0, 1 | + \langle G_j | \right) \mathbf{U}^{\dagger} \mathbf{U} \left(S_j | 0, 1 \rangle + | G_j \rangle \right)$
= $\langle G_j | \mathbf{U}^{\dagger} \mathbf{U} | G_j \rangle$
= $\langle G_j | G_j \rangle$
 $\Rightarrow 0 \le |\eta_j| \le 1$

 $\langle G_j | \mathbf{U}^{\dagger} \mathbf{U} | G_j \rangle = \langle G_j | G_j \rangle$ is due to the fact that, aside from the 1 vertex, **U** is unitary. Finally, since $|\eta_j| \neq 1$, we have that the roots of f satisfy $0 \leq |\eta_j| < 1$.

Theorem 7.4. When $|\alpha| = 1$, the solutions of $C(z, \alpha)$ are distinct.

Proof When $|\alpha| = 1$ we know that **U** is unitary. An immediate consequence of which is the fact that **U** is diagonalizable and expressible as $\mathbf{U} = \sum_{\lambda} \lambda \mathbf{P}_{\lambda}$, where \mathbf{P}_{λ} is a projection operator onto the λ -eigenspace. Each of these projections can be expressed in terms of the resolvent, which in turn can be written as a power series in $\alpha - \alpha_0$ near α_0 , where α_0 is any arbitrary point on the unit circle.

This implies that the projection operators can likewise be expressed as a power series in $\alpha - \alpha_0$, and since $\mathbf{P}_{\lambda} = |V_{\lambda}\rangle \langle V_{\lambda}|$, it follows that the eigenvectors share the same property. Finally, since **U** and $|V_{\lambda}\rangle$ are power series in $\alpha - \alpha_0$, and $\mathbf{U}|V_{\lambda}\rangle = \lambda |V_{\lambda}\rangle$, we can see that the eigenvalues themselves, λ , are power series in $\alpha - \alpha_0$. Now define $c_0(z)(z - \lambda_0)^t = f(z) + \alpha_0 g(z)$. Note that according to the last theorem $g(z) \neq 0$ when |z| = 1.

$$0 = f(\lambda) + \alpha g(\lambda)$$
$$= f(\lambda) + \alpha_0 g(\lambda) + (\alpha - \alpha_0) g(\lambda)$$
$$= c_0(\lambda)(\lambda - \lambda_0)^t + (\alpha - \alpha_0) g(\lambda)$$
$$\Rightarrow (\lambda - \lambda_0)^t = -\frac{g(\lambda)}{c_0(\lambda)}(\alpha - \alpha_0)$$
$$\Rightarrow \lambda = \lambda_0 + O\left(\sqrt[t]{\alpha - \alpha_0}\right)$$

However, since the eigenvalues are expressible as a power series in $\alpha - \alpha_0$, t = 1. Therefore, because α_0 is arbitrary, the degree of any zero of $f(z) + \alpha g(z)$ is one when $|\alpha| = 1$.

In this proof it was important that $|\alpha| = 1$ because it ensures that **U** is unitary. For a finite set of values of α (off the unit circle) the characteristic polynomial can have higher degree roots, however at those points we find that **U** is no longer diagonalizable and the degenerate eigenvalues correspond to *generalized* eigenvectors.

7.1.1 Example

The states on the Bolo graph are

$$\begin{aligned} |\psi_1\rangle &= |1,0\rangle \\ |\psi_2\rangle &= |A,0\rangle \\ |\psi_3\rangle &= |b\rangle \\ |\psi_4\rangle &= |0,A\rangle \\ |\psi_5\rangle &= |0,1\rangle \end{aligned}$$

and ${\bf U}$ is defined to act on these states as

	0	0	0	0	α
	0	0	0	-1	0
$\mathbf{U} =$	$\frac{2}{3}$	$\frac{2}{3}$	$-\frac{1}{3}$	0	0
	$\frac{2}{3}$	$-\frac{1}{3}$	$\frac{2}{3}$	0	0
	$\left(-\frac{1}{3}\right)$	$\frac{2}{3}$	$\frac{2}{3}$	0	0)

The characteristic polynomial, $|z\mathbf{I} - \mathbf{U}|$, is $z^5 + \frac{1}{3}z^4 + \frac{1}{3}(\alpha - 1)z^3 + \frac{1}{3}(1 - \alpha)z^2 + \frac{1}{3}\alpha z + \alpha$ which can be factored and re-written as

$$|z\mathbf{I} - \mathbf{U}| = \underbrace{(z+1)}_{h(z)} \left[\underbrace{\frac{z^2 \left(z - \frac{1}{3}(1+i\sqrt{2}) \right) \left(z - \frac{1}{3}(1-i\sqrt{2}) \right)}_{f(z)}}_{f(z)} + \alpha \underbrace{\left(1 - z\frac{1}{3}(1+i\sqrt{2}) \right) \left(1 - z\frac{1}{3}(1-i\sqrt{2}) \right)}_{g(z)} \right]$$
(33)
Clearly, $\eta_j = \left\{ \frac{1+i\sqrt{2}}{3}, \frac{1-i\sqrt{2}}{3} \right\}, \ s = 2, \text{ and } g_0 = 1.$

7.2 Imitating the Pure Momentum State

The response to an infinite incoming signal of the form $\sum_{k=0}^{\infty} \lambda^k |k+1,k\rangle$ can be found by finding the eigenstate for λ of the form $|V\rangle = \sum_{k=0}^{\infty} \lambda^k |k+1,k\rangle + R(\lambda) \sum_{k=0}^{\infty} \lambda^{-(k+1)} |k,k+1\rangle + |G\rangle$.

The $R(\lambda)$ in this equation is the effective reflection coefficient for G. This function encapsulates all of the information we can obtain from G from each pure momentum state: the difference in phase between the incoming and outgoing signals. For a given pure momentum state, G can be replaced by a vertex that reflects with phase $R(\lambda)$.

The eigenstate $|V\rangle$ can be imitated by finding the eigenstates of the graph defined by replacing the "runway" with $\mathbf{U}|0,1\rangle = \alpha|1,0\rangle$. The λ_j -eigenstate must take the form $|V_j\rangle = S_j|1,0\rangle + \frac{\lambda_j}{\alpha}S_j|0,1\rangle + |G_j\rangle$. In this way we "feed the output to the input", and the amplitude on the "input edge", $|1,0\rangle$, is multiplied by λ in each time step (exactly as it was in the case with the infinite tail). This method resolves issues with non-normalizable states, but introduces a new variable, α . As we shall see, this method provides remarkable insights.

Upon brief inspection, $R(\lambda_j) = \frac{\lambda_j^2}{\alpha}$. The question now is whether or not there exists an α such that any eigenvalue, λ_j , can be "dialed up".

Theorem 7.5. When α loops once around the unit circle the eigenvalues cyclicly permute one step. That is, looping α changes $\lambda_j \rightarrow \lambda_{j+1}$ and $\lambda_{d'} \rightarrow \lambda_1$, where $\arg(\lambda_1) < \arg(\lambda_2) < \cdots < \arg(\lambda_{d'})$.



Figure 5: Looping α once around the unit circle permutes the eigenvalues as shown.

Proof We know that looping α once (returning it to its original value) can't change the spectrum of the eigenvalues, so the effect must be a permutation. In addition, since the eigenvalues are always distinct for every value of $|\alpha| = 1$, this permutation must be cyclic; the eigenvalues can't "slide past each other" on the unit circle.

So we know that looping α produces a permutation of the eigenvalues of the form $\lambda_j \to \lambda_{j+t}$ (where $\lambda_{d'} \equiv \lambda_0$). The only question that remains is the value of t.

Define $\lambda = e^{i\theta}$. The eigenvalues satisfy

$$0 = f(\lambda) + \alpha g(\lambda)$$

$$\Rightarrow -f(e^{i\theta}) = \alpha g(e^{i\theta})$$

$$\Rightarrow -e^{is\theta} \prod_{j=1}^{d} (e^{i\theta} - \eta_j) = \alpha g_0 \prod_{j=1}^{d} (1 - e^{i\theta} \eta_j^*)$$

$$\Rightarrow -e^{is\theta} \prod_{j=1}^{d} (e^{i\theta} - \eta_j) = \alpha g_0 \prod_{j=1}^{d} e^{i\theta} (e^{i\theta} - \eta_j)^*$$

$$\Rightarrow i\pi + is\theta + \sum_{j=1}^{d} \log (e^{i\theta} - \eta_j) = i \arg (\alpha) + \log (g_0) + id\theta + \sum_{j=1}^{d} \log (e^{-i\theta} - \eta_j^*)$$

$$\Rightarrow i \arg (\alpha) = i\pi - \log (g_0) + i(s - d)\theta + \sum_{j=1}^{d} \left[\log (e^{i\theta} - \eta_j) - \log (e^{-i\theta} - \eta_j^*) \right]$$

$$\Rightarrow i \arg (\alpha) = i\pi - \log (g_0) + i(s - d)\theta + 2i \sum_{j=1}^{d} \arg (e^{i\theta} - \eta_j)$$

$$\Rightarrow \arg (\alpha) = \pi + i \log (g_0) + (s - d)\theta + 2 \sum_{j=1}^{d} \arg (e^{i\theta} - \eta_j)$$

At this point we allow θ to smoothly increase by 2π , then take the difference. Since $|\eta_j| < 1$, the angle between $e^{i\theta}$ and η_j sweeps from 0 to 2π monotonically.

 $\Rightarrow \Delta \arg(\alpha) = (s-d)2\pi + 2\sum_{j=1}^{d} 2\pi$ $\Rightarrow \Delta \arg(\alpha) = (s+d)2\pi$ $\Rightarrow \Delta \arg(\alpha) = 2\pi d'$

Looping a given eigenvalue once around the unit circle, causes α to loop s + d = d'times. Looping an eigenvalue once is a permutation of the form $\lambda_j \to \lambda_{j+d'} = \lambda_j$. It follows that if looping α once produces a permutation of the form $\lambda_j \to \lambda_{j+t}$, then looping λ_j means that α loops $\frac{d'}{t}$ times. But we know that looping an eigenvalue once requires α to loop d' times, and therefore t = 1. **Theorem 7.6.** Any eigenvalue λ , such that $|\lambda| = 1$, can be induced by choosing the correct value of α . Moreover, this value of α is unique.

Proof In the last theorem it was shown that the eigenvalues, which are functions of $\alpha = e^{ia}$, have the property that $\lambda_j|_{a=2\pi} = \lambda_{j+1}|_{a=0}$. These functions are continuous, so every value between these eigenvalues exist as well, by the intermediate value theorem. Moreover, $\arg(\lambda)$ is a strictly monotonic function of $\arg(\alpha)$, and therefore there is only one permissible value of α for a given eigenvalue.

This can be seen by first showing that $\frac{\partial}{\partial \theta} \arg \left(e^{i\theta} - \eta_j \right) > \frac{1}{2}$ when $|\eta_j| < 1$. This can be proven by either using the inscribed angle theorem to establish a lower bound or by direct calculation. It follows that

$$\arg(\alpha) = \pi + (s - d)\theta + i\log(g_0) + 2\sum_{j=1}^d \arg(e^{i\theta} - \eta_j)$$
$$\Rightarrow \frac{\partial}{\partial \theta} \arg(\alpha) = (s - d) + 2\sum_{j=1}^d \frac{\partial}{\partial \theta} \arg(e^{i\theta} - \eta_j) > (s - d) + 2d\left(\frac{1}{2}\right) = s \ge 0$$
$$\Rightarrow \frac{\partial}{\partial \theta} \arg(\alpha) > 0$$

Therefore $\arg(\alpha)$ and $\arg(\lambda)$ are strictly monotonic functions of each other, and $\alpha(\lambda)$ is single-valued.

We now have enough mathematical machinery in place to describe any incoming pure momentum state, $\sum_{k=0}^{\infty} \lambda^k |k+1, k\rangle$, as well as the graph's response, $R(\lambda) \sum_{k=0}^{\infty} \lambda^{-(k+1)} |k, k+1\rangle$. **Theorem 7.7.** The graph attached to vertex zero can be replaced by a single vertex with frequency-dependent reflection coefficient $R(\lambda) = \frac{\lambda^2}{\alpha} = -\lambda^2 \frac{g(\lambda)}{f(\lambda)}$.

Proof By finding an appropriate value of α we can "feed the output to the input" in such a way that at time step n the amplitude of the state $|1,0\rangle$ is λ^n . This happens when we can find a λ -eigenvector of the form $|V\rangle = S|1,0\rangle + \frac{R(\lambda)}{\lambda}S|0,1\rangle + |G\rangle$, where $|G\rangle \equiv \mathbf{P}_G|V\rangle$ (the projection of the eigenvector onto the states in the graph G), and S is a normalizing real constant. We can see this because

$$\begin{split} \mathbf{U} \left[S|1,0\rangle + \frac{R(\lambda)}{\lambda}S|0,1\rangle + |G\rangle \right] &= \lambda \left[S|1,0\rangle + \frac{R(\lambda)}{\lambda}S|0,1\rangle + |G\rangle \right] \\ \Rightarrow \begin{cases} \mathbf{U} \left[S|1,0\rangle + |G\rangle \right] &= R(\lambda)S|0,1\rangle + \lambda|G\rangle \\ \\ \frac{S\alpha}{\lambda}R(\lambda)|1,0\rangle &= S\lambda|1,0\rangle \\ \\ \Rightarrow \begin{cases} \mathbf{U} \left[S|1,0\rangle + |G\rangle \right] &= R(\lambda)S|0,1\rangle + \lambda|G\rangle \\ \\ R(\lambda) &= \frac{\lambda^2}{\alpha} \end{cases} \end{split}$$

As shown above (thm. 7.6), any eigenvalue can be realized for some value of α . We can therefore solve for α using the characteristic equation: $\alpha = -\frac{f(\lambda)}{g(\lambda)}$. Plugging into the second of the above equations we see that

$$R(\lambda) = -\lambda^2 \frac{g(\lambda)}{f(\lambda)} = -\frac{g_0}{\lambda^{s-2}} \prod_j \frac{1 - \lambda \eta_j^*}{\lambda - \eta_j}$$
(34)

where $|\eta| < 1$, by thm. 7.3.

If the graph is sent the signal $x[n] = c\lambda^n$ (that is; at time step n the amplitude of the

state $|1,0\rangle$ is $c\lambda^n$), then it will respond in exactly the same way that a vertex that reflects with phase $e^{i\phi} = R(\lambda)$ at vertex 0 would respond. Theorem 7.6 shows that we can solve for α , and in theorem 7.7 we did exactly that. Now that we have an equation for the reflection coefficient we see that α , and the rest of the machinery needed to make the graph finite, are no longer necessary and can be left to work "in the background".

Knowing the roots of f(z) is helpful for understanding the behavior of the reflection coefficient, but those roots are not necessary for a direct calculation since we can express $R(\lambda) = -\lambda^2 \frac{g(\lambda)}{f(\lambda)}.$

7.2.1 Example

The characteristic equation for the Bolo graph is $C(z, \alpha) =$

$$(z+1)\left[z^{2}\left(z-\frac{1}{3}(1+i\sqrt{2})\right)\left(z-\frac{1}{3}(1-i\sqrt{2})\right)+\alpha\left(1-z\frac{1}{3}(1+i\sqrt{2})\right)\left(1-z\frac{1}{3}(1-i\sqrt{2})\right)\right]$$

This has five roots and when $|\alpha| = 1$ all five have modulus 1.

The frequency response is

$$R(e^{i\theta}) = -\frac{\left(1 - e^{i\theta}\frac{1 - i\sqrt{2}}{3}\right)\left(1 - e^{i\theta}\frac{1 + i\sqrt{2}}{3}\right)}{\left(e^{i\theta} - \frac{1 + i\sqrt{2}}{3}\right)\left(e^{i\theta} - \frac{1 - i\sqrt{2}}{3}\right)}$$
(35)

Graphing the magnitude of the relevant part of the polynomial (ignoring the "b(z) = z + 1") demonstrates the theorems in this section.



Figure 6: The graph of the magnitude of the characteristic polynomial, $|C(z, \alpha)|$, where $\alpha = e^{ix}$ and $z = e^{iy}$. The troughs are the locations of the roots.

7.3 Arbitrary Inputs

In the language of signal analysis, the last section was a derivation of the "frequency response" of the graph G. We can define the input x[n] (output y[n]) as the amplitude on the state $|1,0\rangle$ (state $|0,1\rangle$) at time step n. The input can be encoded onto the tail in an initial state of the form $|input\rangle = \sum_{k=0}^{\infty} x[k]|k+1,k\rangle$.

At time step n, the overall state of the graph and tail will be:

$$\sum_{k=0}^{\infty} x[k+n]|k+1,k\rangle + \sum_{k=0}^{\infty} y[n-k]|k,k+1\rangle + |G\rangle$$
(36)

In general we can assume that y[k] = 0, $\forall k \leq 0$ since only positive values of k can be a reaction to the input.

Using the frequency response we can derive an expression for the "impulse response", h[n], which is the response y[n] produced from the input $x[n] = \delta[n]$, the Kronecker delta function. The response of any signal can be found using the fact that $y[n] = (x * h)[n] = \sum_k h[k]x[n-k]$. So rather than being a single example, the impulse response is the key to finding the response to *any* input.

Theorem 7.8. The impulse response, h[n], is given by $h[n] = -\frac{1}{2\pi i} \oint_{|z|=1} z^n \frac{g(z)}{f(z)} dz$

Proof For a single frequency, $x[n] = \lambda^n$, we find that

$$y[n] = \sum_{k} h[k]x[n-k]$$
$$= \sum_{k} h[k]\lambda^{n-k}$$
$$= \sum_{k} h[k]\lambda^{-k}\lambda^{n}$$
$$= \left(\sum_{k} h[k]\lambda^{-k}\right)x[n]$$

We already have a way of writing this from the previous section. Setting $\sum_{k=0}^{\infty} \lambda^k |k + 1, k\rangle + R(\lambda) \sum_{k=0}^{\infty} \lambda^{-(k+1)} |k, k+1\rangle + |G\rangle$ equal to $\sum_{k=0}^{\infty} x[k+n]|k+1, k\rangle + \sum_{k=0}^{\infty} y[n-k]|k, k+1\rangle + |G\rangle$ we find that $\sum_k h[k]\lambda^{-k} = \frac{R(\lambda)}{\lambda} = -\lambda \frac{g(\lambda)}{f(\lambda)}$. Using $\lambda = e^{i\omega}$:

$$\begin{split} \sum_{k} h[k]\lambda^{-k} &= -\lambda \frac{g(\lambda)}{f(\lambda)} \\ \Rightarrow \sum_{k} h[k]e^{-i\omega k} &= -e^{i\omega} \frac{g(e^{i\omega})}{f(e^{i\omega})} \\ \Rightarrow \sum_{k} h[k]e^{i\omega(n-k)} &= -e^{i(n+1)\omega} \frac{g(e^{i\omega})}{f(e^{i\omega})} \\ \Rightarrow \int_{0}^{2\pi} \sum_{k} h[k]e^{i\omega(n-k)} d\omega &= -\int_{0}^{2\pi} e^{i(n+1)\omega} \frac{g(e^{i\omega})}{f(e^{i\omega})} d\omega \\ \Rightarrow 2\pi h[n] &= -\int_{0}^{2\pi} e^{i(n+1)\omega} \frac{g(e^{i\omega})}{f(e^{i\omega})} d\omega \\ \Rightarrow h[n] &= -\frac{1}{2\pi} \int_{0}^{2\pi} e^{i(n+1)\omega} \frac{g(e^{i\omega})}{f(e^{i\omega})} d\omega \\ \Rightarrow h[n] &= -\frac{1}{2\pi i} \oint_{|z|=1} z^{n} \frac{g(z)}{f(z)} dz \qquad (z = e^{i\omega}, dz = ie^{i\omega} d\omega) \end{split}$$

This is a perfectly nice integral, since the zeros of f(z) are all on the interior of the unit disk (thm. 7.3). There may have been an issue with taking the integral $\int_0^{2\pi} \sum_k h[k] e^{i\omega(n-k)} d\omega$, since we can only assume that $h[n] \in \ell^2$ (is square-summable). However, as will be seen shortly, h[n] is composed of exponentially decaying signals which is ideal for integrals of this form.

So, the impulse response is:

$$h[n] = -\frac{1}{2\pi i} \oint_{|z|=1} z^n \frac{g(z)}{f(z)} dz = -\frac{g_0}{2\pi i} \oint_{|z|=1} z^{n-s} \prod_k \frac{1 - z\eta_k^*}{z - \eta_k} dz$$
(37)

and again, this can be used to find the response to any incoming signal, x[n], through convolution: y[n] = (x * h)[n]. Using residue calculus we can solve this directly

$$\begin{split} h[n] \\ &= -\frac{g_0}{2\pi i} \oint_{|z|=1} z^{n-s} \prod_k \frac{1-z\eta_k^*}{z-\eta_k} dz \\ &= -g_0 \prod_k \left(\frac{1}{-\eta_k}\right) \delta[n-s+1] - g_0 \sum_j (1-|\eta_j|^2) \prod_{k\neq j} \left(\frac{1-\eta_j \eta_k^*}{\eta_j - \eta_k}\right) \eta_j^{n-s} \\ &= \Omega_0 \delta[n-s+1] + \sum_j \Omega_j \eta_j^n \\ &\text{where } \Omega_j = \begin{cases} -g_0 \prod_k \left(\frac{1}{-\eta_k}\right) &, j = 0 \\ -g_0 \frac{1-|\eta_j|^2}{\eta_j^s} \prod_{k\neq j} \left(\frac{1-\eta_j \eta_k^*}{\eta_j - \eta_k}\right) &, j \neq 0 \end{cases}$$

So the impulse response is a set of exponentially decaying signals corresponding to the zeros of f(z).

7.3.1 Bound, Semi-bound, and Unbound Eigenstates

Define \mathbf{U} as the time step operator corresponding to $\alpha = 0$. That is, $\mathbf{U}|0,1\rangle = 0$. Trivially, $|z\mathbf{I} - \mathbf{U}| = b(z)f(z)$. These eigenvalues of \mathbf{U} come in three forms.

Bound eigenvalues have modulus 1 and are roots of b(z). The corresponding eigenvectors are entirely contained within G and can be ignored in the context of sending and receiving signals from the graph.

Semi-bound eigenvalues take the form $0 < |\eta_j| < 1$ and correspond to the exponentially decaying signals.

Unbound eigenvectors are those with eigenvalue zero. Their contribution is a simple delay (of s - 2 time steps, where s is the multiplicity of the 0-eigenvalue) and constant phase change.

7.3.2 Example

The first few terms of the impulse response of the bolo graph can be found by direct computation:

Alternatively,

$$\begin{split} \Omega_0 &= -\left(\frac{9}{(1+i\sqrt{2})(1-i\sqrt{2})}\right) = -3\\ \Omega_1 &= -\frac{1-\left|\frac{1+i\sqrt{2}}{3}\right|^2}{\left(\frac{1+i\sqrt{2}}{3}\right)^2} \left(\frac{1-\left(\frac{1+i\sqrt{2}}{3}\right)\left(\frac{1+i\sqrt{2}}{3}\right)}{\left(\frac{1+i\sqrt{2}}{3}\right)-\left(\frac{1-i\sqrt{2}}{3}\right)}\right) = 2 - i\sqrt{2}\\ \Omega_2 &= -\frac{1-\left|\frac{1-i\sqrt{2}}{3}\right|^2}{\left(\frac{1-i\sqrt{2}}{3}\right)^2} \left(\frac{1-\left(\frac{1-i\sqrt{2}}{3}\right)\left(\frac{1-i\sqrt{2}}{3}\right)}{\left(\frac{1-i\sqrt{2}}{3}\right)-\left(\frac{1+i\sqrt{2}}{3}\right)}\right) = 2 + i\sqrt{2} \end{split}$$

So for $n \ge 1$, $h[n] = -3\delta[n-1] + (2 - i\sqrt{2})\left(\frac{1+i\sqrt{2}}{3}\right)^n + (2 + i\sqrt{2})\left(\frac{1-i\sqrt{2}}{3}\right)^n$. We find

that this yields precisely the same results as the direct computation (and with substantially greater ease).

The bound eigenstate of the Bolo graph is:

$$\left\{\lambda = -1, |\psi^{(-1)}\rangle = \frac{|A,0\rangle - |b\rangle + |0,A\rangle}{\sqrt{3}}\right\}.$$

The two semi-bound eigenstates are:

$$\left\{\lambda = \frac{1 \pm \sqrt{2}i}{3}, |\psi^{(\pm)}\rangle = \frac{1 \pm 2\sqrt{2}i}{3\sqrt{6}} |A,0\rangle + \frac{2 \pm \sqrt{2}i}{3\sqrt{6}} |b\rangle + \frac{1 \pm \sqrt{2}i}{3\sqrt{6}} |0,A\rangle + \sqrt{\frac{2}{3}} |0,1\rangle\right\}.$$

Finally, there is a unbound eigenstate and an unbound generalized eigenstate:

$$\{\lambda = 0, |\psi^{(0)}\rangle = |0,1\rangle, |\psi^{(0)'}\rangle = -\frac{1}{3}|1,0\rangle + \frac{2}{3}|A,0\rangle + \frac{2}{3}|b\rangle\}.$$

Here $\mathbf{U}^2 |\psi^{(0)'}\rangle = \mathbf{U} |\psi^{(0)}\rangle = 0.$

7.4 Detecting Poles

When $\eta = (1-\delta)e^{i\tau}$, for small δ , we find that the pole is difficult to detect when the signal frequency differs from τ . By the inscribe angle theorem, we know that $\arg(e^{i\theta}+1) = \frac{\theta}{2}$ for $\theta \neq \pi$. It follows that $2\arg(e^{i\theta}-\eta) = 2(\tau+\pi) + 2\arg(e^{i(\theta-\tau-\pi)}+(1-\delta)) \approx 2\tau + 2\pi + [\theta-\tau-\pi] = \theta + (\tau+\pi)$. That is, a given pole may change the phase of the reflection coefficient by approximately the same amount for all $\theta \not\approx \tau$.

A little trigonometry reveals that $\tan\left(\arg(e^{i\theta} - (1-\delta)\right) = \frac{\sin(\theta)}{\cos(\theta) - 1 + \delta}$. For $|\theta| < \delta$:

$$2\arg\left(e^{i\theta} - (1-\delta)\right) = \frac{2\theta}{\delta} + O\left(\delta\right)$$
(38)

But for $|\theta| > \delta$:

$$2\arg\left(e^{i\theta} - (1-\delta)\right) = \theta \pm \pi - \frac{2\delta}{\theta} + O\left(\left(\frac{\delta}{\theta}\right)^3\right)$$
(39)

This means that the reflection coefficient jumps by 2π as it passes a pole, η , and that the width of that jump is $O(\delta)$, where $|\eta| = 1 - \delta$.

7.5 Important Points

- A graph G has an effective reflection coefficient $R(\lambda) = -\lambda^2 \frac{g(\lambda)}{f(\lambda)} = -\frac{g_0}{\lambda^{s-2}} \prod_j \frac{1-\lambda\eta_j^*}{\lambda-\eta_j}$ where $|\eta_j| < 1 \ \forall j$.
- f(z) and g(z) can be found by finding the characteristic polynomial of the time step operator that acts on G with the first vertex in the attached tail replaced by a vertex with reflection coefficient α . This characteristic equation takes the form $|z\mathbf{I} - \mathbf{U}| =$ $b(z) (f(z) + \alpha g(z)) = b(z) \left(z^s \prod_{j=1}^d (z - \eta_j) + \alpha g_0 \prod_{j=1}^d (1 - z\eta_j^*) \right)$. The roots of b(z) all have modulus 1 and correspond to bound states, which are not involved with the reflection coefficient.
- The impulse response, h[n], can be used to find the returned signal, y[n], that is the response of the graph to any incoming signal, x[n], using convolution, y[n] = (h*x)[n]. We find that $h[n] = -\frac{1}{2\pi i} \oint_{|z|=1} z^n \frac{g(z)}{f(z)} dz$.
- This response is made up of a set of infinite and exponentially decaying signals, and a single finite signal. These correspond to the non-zero eigenvalues and zero eigenvalue respectively of the time step operator when α = 0.
- The effective reflection coefficient, $R(\lambda)$, increases suddenly by 2π in the neighborhood of poles that are close to the edge of the unit circle. For a given pole, η , the

width of this jump is $\approx 2\delta$ across, where $|\eta| = 1 - \delta$.

8 Application to Classes of Graphs

The only information we can hope to gain from a signal are the zeros of f(z), s, and g_0 . Every other quantity described so far can be determined from these.

However, a graph with d' edge states can have any of a huge number of arrangements, and each vertex in that graph can have any appropriate unitary operator. It is unreasonable to hope for a way of determining the structure of a completely arbitrary graph by studying its responses to signals.

However, if we restrict the graph to being one of a restricted family of graphs, then we can expect to get some information about the structure.

8.1 Star Graphs with Differently Marked Edges

Assume that we know that there are N edges, that the terminating vertex of some of these reflect without phase change, and that some flip the phase (multiply by -1). The question is: can we determine the number of each type of edge?

Define the states

$$\begin{aligned} |\psi_1\rangle &= |0, A\rangle \\ |\psi_2\rangle &= |A, 0\rangle \\ |\psi_3\rangle &= \frac{1}{\sqrt{M}} \sum_{j=1}^M |0, j\rangle \\ |\psi_4\rangle &= \frac{1}{\sqrt{M}} \sum_{j=1}^M |j, 0\rangle \\ |\psi_5\rangle &= \frac{1}{\sqrt{N-M}} \sum_{j=M+1}^N |0, j\rangle \\ |\psi_6\rangle &= \frac{1}{\sqrt{N-M}} \sum_{j=M+1}^N |j, 0\rangle \end{aligned}$$

$$r = -1 + \frac{2}{N+1}, \, t = \frac{2}{N+1}$$

Then the time step operator can be written /

$$\begin{split} \mathbf{U} &= \begin{pmatrix} 0 & -1 + \frac{2}{N+1} & 0 & 2\frac{\sqrt{M}}{N+1} & 0 & 2\frac{\sqrt{N-M}}{N+1} \\ \alpha & 0 & 0 & 0 & 0 & 0 \\ 0 & 2\frac{\sqrt{M}}{N+1} & 0 & -1 + \frac{2M}{N+1} & 0 & 2\frac{\sqrt{M(N-M)}}{N+1} \\ 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 2\frac{\sqrt{N-M}}{N+1} & 0 & 2\frac{\sqrt{M(N-M)}}{N+1} & 0 & -1 + \frac{2(N-M)}{N+1} \\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix} \\ C(z) &= z^{6} + \left(\alpha - \frac{2\alpha}{N+1} + \frac{4M}{1+N} - \frac{2N}{1+N}\right)z^{4} + \left(-1 + \frac{4M\alpha}{N+1} + \frac{2N}{1+N} - \frac{2N\alpha}{1+N}\right)z^{2} + \alpha \\ &= \begin{cases} \frac{z^{2} \left(z^{4} + \left(\frac{4M}{1+N} - \frac{2N}{1+N}\right)z^{2} + \left(1 - \frac{2}{1+N}\right)\right)}{f(z)} \\ + \alpha \underbrace{\left(\left(1 - \frac{2}{N+1}\right)z^{4} + \left(\frac{4M}{N+1} - \frac{2N}{1+N}\right)z^{2} + 1\right)}{g(z)} \end{cases} \end{split}$$

The non-zero roots of f(z) are

$$\eta = \pm \sqrt{1 - \frac{2M+1}{N+1} \pm \frac{\sqrt{1 - 4M(N-M)}}{N+1}}$$
(40)

These four roots are negatives and/or complex conjugates of each other. We find that there is a simple formula for $|\eta|$:

$$\begin{split} &|\eta|^4 = \left| \stackrel{\circ}{\pm} \sqrt{1 - \frac{2M+1}{N+1} \pm \frac{\sqrt{1-4M(N-M)}}{N+1}} \right|^4 \\ &= \left| 1 - \frac{2M+1}{N+1} \pm \frac{\sqrt{1-4M(N-M)}}{N+1} \right|^2 \\ &= \left(1 - \frac{2M+1}{N+1} \right)^2 + \left(\frac{\sqrt{4M(N-M)-1}}{N+1} \right)^2 \\ &= 1 - \frac{4M+2}{N+1} + \frac{4M^2 + 4M+1}{(N+1)^2} + \frac{4M(N-M)-1}{(N+1)^2} \\ &= 1 + \frac{-4MN - 4M - 2N - 2 + 4M^2 + 4M + 1 + 4MN - 4M^2 - 1}{(N+1)^2} \\ &= 1 - \frac{2N+2}{(N+1)^2} \\ &= 1 - \frac{2}{N+1} \\ &\Rightarrow |\eta| = \sqrt[4]{1 - \frac{2}{N+1}} = 1 - \frac{1}{2N} + O\left(\frac{1}{N^2}\right) \end{split}$$

This means that the value of M does not affect how difficult it is to get a result. Instead we find the phase of η retains information about the value of M. Define $R \equiv \frac{M}{N}$. $\eta^2 = \left(1 - \frac{2M+1}{N+1}\right) \pm i\left(\frac{\sqrt{4M(N-M)-1}}{N+1}\right)$, so if the phase of η is τ , then we find that:

$$\begin{aligned} \sin(2\tau) &= \frac{\frac{\sqrt{4M(N-M)-1}}{N+1}}{\sqrt{\left(1-\frac{2M+1}{N+1}\right)^2 + \left(\frac{\sqrt{4M(N-M)-1}}{N+1}\right)^2}} \\ &= \frac{\sqrt{4M(N-M)-1}}{\sqrt{(N+1-2M-1)^2 + \left(\sqrt{4M(N-M)-1}\right)^2}} \\ &= \frac{\sqrt{4M(N-M)-1}}{\sqrt{(N-2M)^2 + 4M(N-M)-1}} \\ &= \sqrt{\frac{4M(N-M)-1}{N^2 - 4MN + 4M^2 + 4MN - 4M^2 - 1}} \\ &= \sqrt{\frac{4M(N-M)-1}{N^2 - 1}} \\ &= \sqrt{\frac{4M(N-M)-1}{N^2 - 1}} \\ &= \sqrt{\frac{4RN(N-RN)-1}{N^2 - 1}} \\ &= \frac{1}{\sqrt{1-\frac{1}{N^2}}} \sqrt{4R(1-R) - \frac{1}{N^2}} \\ &= 2\sqrt{R(1-R)} \sqrt{1 - \frac{1}{4R(1-R)N^2}} \left(1 + O\left(\frac{1}{N^2}\right)\right) \\ &\Rightarrow \begin{cases} \sin(2\tau) = 2\sqrt{R(1-R)} + O\left(\frac{1}{N}\right) \\ \tau = \sqrt{\frac{M}{N}} + O\left(\frac{1}{N}\right) \end{cases}, R = O\left(\frac{1}{N}\right) \end{aligned}$$

The problem of finding $R = \frac{M}{N}$ can now be reduced to finding the phase of the root of f(z) in the first quadrant. Noting that $g_0 = 1$, s = 2, d = 4, and assuming that $\theta \not\approx \tau$:

$$\arg(R(e^{i\theta}))$$

$$= \arg(-g_0) + (2 - s + d)\theta - \sum_j 2\arg(e^{i\theta} - \eta_j)$$

$$= \pi + 4\theta - \sum_{j=1}^4 2\arg(e^{i\theta} - \eta_j)$$

$$\approx \pi + 4\theta - \sum_{j=1}^4 \theta + \pi + \arg(\eta_j)$$

$$= \pi - \sum_{j=1}^4 \arg(\eta_j)$$

$$= \pi - [\tau + \pi] - [\tau] - [-\tau + \pi] - [-\tau - \pi]$$

$$= \pi$$

This is precisely the frequency response of a reflection by -1 at vertex 0 (which is approximately what the graph is).

However, when $e^{i\theta}$ passes around the "far side" of η_j , we find that $\arg(e^{i\theta} - \eta_j)$ jumps by π and the phase of the reflection coefficient jumps by 2π . The closer η_j is to the unit circle, the quicker the jump.

From the results of section 7.4, when $\theta = O(\frac{1}{N})$,

$$\arg\left(e^{i\theta} - \left(1 - \frac{1}{2N}\right)\right) = 2N\theta + O\left(\frac{1}{N}\right) \tag{41}$$

This means that in order to detect one of the η 's we need to detect an interval in which $R(e^{i\theta}) \neq \pi$, and that difference is only detectable within $O\left(\frac{1}{N}\right)$ of the correct value.

So, if a pulse is sent and it is found that $R(e^{i\theta}) \neq \pi$, then $sin(2\theta) = 2\sqrt{R(1-R)}$. However, since the target window is only $O\left(\frac{1}{N}\right)$ wide, we can expect that the pulse must be O(N) long. This is an unimpressive result, since simply counting and tallying up the edges (a brute force classical algorithm) takes O(N) time.



Figure 7: The frequency response for N=100, M=40. $\sin(2\theta) = 2\sqrt{0.4(1-0.4)} \Rightarrow \theta \approx \{0.68, 2.46, 3.82, 5.60\}.$

8.2 Logic Tree Graphs

We can encode bits into reflection coefficients of vertices on the tree. Define:

$$b \to R_b = (-1)^b \tag{42}$$

That is, $R_0 = 1$ and $R_1 = -1$. Since a non-trivial graph has a non-trivial reflection, we need to specify a frequency at which the reflection functions are evaluated. The phase necessary for useful logical operations is $\pm i$. It turns out that there are no other frequencies or reflection coefficients that are similarly useful. This can be shown by starting with $R_0 = e^{i\phi_0}$ and $R_1 = e^{i\phi_1}$ and assuming, for example, that $\{R_0, R_1\} \to R_0$. Either $R_i = \pm 1$, or we find that the logical operation is a tautology.



Figure 8: The model for a non-terminating vertex in the tree.

The Logic Tree graph performs a logic operation at each vertex. The input of the operation performed at vertex C are the reflection coefficients $R_A(\pm i)$, $R_B(\pm i)$, and the output is $R_C(\pm i)$.

For example, the NAND gate is the standard diffusive vertex, with $r = \frac{2}{3}$ and $t = -\frac{1}{3}$. The time step operator for this toy graph is,

$$\mathbf{U} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & \alpha \\ 0 & 0 & 0 & 0 & R_B & 0 \\ 0 & 0 & 0 & R_A & 0 & 0 \\ \frac{2}{3} & \frac{2}{3} & -\frac{1}{3} & 0 & 0 & 0 \\ \frac{2}{3} & -\frac{1}{3} & \frac{2}{3} & 0 & 0 & 0 \\ -\frac{1}{3} & \frac{2}{3} & \frac{2}{3} & 0 & 0 & 0 \end{pmatrix} |\psi_1\rangle = |D, C\rangle$$
where
$$|\psi_2\rangle = |A, C\rangle$$
where
$$|\psi_3\rangle = |B, C\rangle$$
where
$$|\psi_4\rangle = |C, B\rangle$$

$$|\psi_5\rangle = |C, A\rangle$$

$$|\psi_6\rangle = |C, D\rangle$$

The effective reflection coefficient at C, to a signal from the direction of vertex D, can be calculated from the characteristic equation:

$$C(z) = z^2 \left[z^4 + \frac{R_A + R_B}{3} z^2 - \frac{R_A R_B}{3} \right] + \alpha \left[\frac{1}{3} z^4 - \frac{R_A + R_B}{3} z^2 - R_A R_B \right]$$

From the earlier results:

$$R_C\left(e^{i\theta}\right) = -\left(e^{i\theta}\right)^2 \frac{g\left(e^{i\theta}\right)}{f\left(e^{i\theta}\right)} = -\frac{e^{i4\theta} - \left(R_A + R_B\right)e^{i2\theta} - 3R_A R_B}{3e^{i4\theta} + \left(R_A + R_B\right)e^{i2\theta} - R_A R_B}$$
(43)

Recall that these reflection coefficients are functions of $e^{i\theta}$ themselves and are being evaluated at $e^{i\theta} = \pm i$.

If the parent vertices reflect with $R_A = R_B = R_1 = -1$, then the vertex C reflects with:

$$R_{1,1}(\pm i) = -\frac{i^4 - (R_1 + R_1)i^2 - 3R_1R_1}{3i^4 + (R_1 + R_1)i^2 - R_1R_1} = -\frac{1 - 2 - 3}{3 + 2 - 1} = 1 = R_0$$
(44)

For $R_A = R_0$ and $R_B = R_1$, vertex C reflects with:

$$R_{0,1}(\pm i) = -\frac{i^4 - (R_0 + R_1)i^2 - 3R_0R_1}{3i^4 + (R_0 + R_1)i^2 - R_0R_1} = -\frac{1+0+3}{3+0+1} = -1 = R_1$$
(45)

For $R_A = R_B = R_0$, there seems to be an issue with calculating the reflection:

$$R_{0,0}(\pm i) = -\frac{i^4 - 2i^2 - 3}{3i^4 + 2i^2 - 1} = -\frac{1 + 2 - 3}{3 - 2 - 1} = \frac{0}{0}$$
(46)

However, all that's happening is that a bound $\pm i$ -eigenstate exists when $R_A = 1 = R_B$. This means that $\pm i$ is a root of the characteristic polynomial, and $z^2 + 1$ must appear in both f(z) and g(z) (that is, it *should* have been included in b(z) and removed already). Indeed, we find:

$$R_{0,0}(\lambda) = -\frac{\lambda^4 - 2\lambda^2 - 3}{3\lambda^4 + 2\lambda^2 - 1} = -\frac{(\lambda^2 + 1)(\lambda^2 - 3)}{(\lambda^2 + 1)(3\lambda^2 - 1)} = -\frac{\lambda^2 - 3}{3\lambda^2 - 1}$$

And therefore,

$$R_{0,0}(\pm i) = -\frac{i^2 - 3}{3i^2 - 1} = -\frac{-1 - 3}{-3 - 1} = -1 = R_1$$
(47)

But this is exactly the logical structure of a NAND gate:

R_A	R_B	R_C
R_0	R_0	R_1
R_0	R_1	R_1
R_1	R_0	R_1
R_1	R_1	R_0

8.2.1 **Different Gates**

In the last subsection
$$\mathbf{U} = \begin{pmatrix} 0 & \mathbf{B} \\ \mathbf{G}_{NAND} & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & \alpha \\ 0 & 0 & 0 & 0 & R_B & 0 \\ 0 & 0 & 0 & R_A & 0 & 0 \\ \frac{2}{3} & \frac{2}{3} & -\frac{1}{3} & 0 & 0 & 0 \\ \frac{2}{3} & -\frac{1}{3} & \frac{2}{3} & 0 & 0 & 0 \\ -\frac{1}{3} & \frac{2}{3} & \frac{2}{3} & 0 & 0 & 0 \end{pmatrix}$$

The "bits matrix", $\mathbf{B} = \begin{pmatrix} 0 & 0 & \alpha \\ 0 & R_B & 0 \end{pmatrix}$, encode the input bits to the gate in the

The "bits maximum of the reflection coefficients. The gate matrix, $\mathbf{G}_{NAND} = \begin{pmatrix} \frac{2}{3} & \frac{2}{3} & -\frac{1}{3} \\ \frac{2}{3} & -\frac{1}{3} & \frac{2}{3} \\ -\frac{1}{3} & \frac{2}{3} & \frac{2}{3} \end{pmatrix}$, encodes the Uning exactly the same set of

form

steps (characteristic equation \rightarrow frequency response equation \rightarrow responses for $\{R_A, R_B\}$ = $\{1,1\},\{1,-1\},\{-1,-1\}$), we find that
$$\mathbf{G}_{NAND} = \mathbf{G}_{\overline{\wedge}} = \begin{pmatrix} \frac{2}{3} & \frac{2}{3} & -\frac{1}{3} \\ \frac{2}{3} & -\frac{1}{3} & \frac{2}{3} \\ -\frac{1}{3} & \frac{2}{3} & \frac{2}{3} \end{pmatrix}, \\ \mathbf{G}_{AND} = \mathbf{G}_{\wedge} = \begin{pmatrix} \frac{2}{3} & \frac{2}{3} & -\frac{1}{3} \\ \frac{2}{3} & -\frac{1}{3} & \frac{2}{3} \\ \frac{1}{3} & -\frac{2}{3} & -\frac{2}{3} \end{pmatrix}, \\ \frac{1}{3} & -\frac{2}{3} & -\frac{2}{3} \end{pmatrix}, \\ \mathbf{G}_{NOR} = -\mathbf{G}_{NAND} = \mathbf{G}_{\nabla} = \begin{pmatrix} -\frac{2}{3} & -\frac{2}{3} & \frac{1}{3} \\ -\frac{2}{3} & \frac{1}{3} & -\frac{2}{3} \\ \frac{1}{3} & -\frac{2}{3} & -\frac{2}{3} \end{pmatrix} \\ \mathbf{G}_{OR} = -\mathbf{G}_{AND} = \mathbf{G}_{\vee} = \begin{pmatrix} -\frac{2}{3} & -\frac{2}{3} & \frac{1}{3} \\ -\frac{2}{3} & \frac{1}{3} & -\frac{2}{3} \\ -\frac{2}{3} & \frac{1}{3} & -\frac{2}{3} \end{pmatrix}$$

We can therefore express any sequence of AND, OR, NAND, and NOR operations on a set of input bits by mapping those bits into the ± 1 reflection coefficients of the leaves, and mapping the gates into the local time step operators of each of the other vertices. The result of one level of computation is fed into the next in the form of the effective reflection coefficient of each intermediate vertex.

,

The reflection coefficient of a given vertex, in terms of the reflection coefficients of the

previous two vertices, A and B, are:

$$R_{AND} = R[A \land B] = \frac{z^4 - (A+B)z^2 - 3AB}{3z^4 + (A+B)z^2 - AB}$$
(48)

$$R_{OR} = R[A \lor B] = -\frac{z^4 + (A+B)z^2 - 3AB}{3z^4 - (A+B)z^2 - AB}$$
(49)

$$R_{NAND} = R[A \overline{\wedge} B] = -\frac{z^4 - (A+B)z^2 - 3AB}{3z^4 + (A+B)z^2 - AB}$$
(50)

$$R_{NOR} = R[A \nabla B] = \frac{z^4 + (A+B)z^2 - 3AB}{3z^4 - (A+B)z^2 - AB}$$
(51)

(52)

8.2.2 Signal Window

To execute a calculation on a logic tree it is necessary to use an input signal that is very close to the pure momentum state with phase $\pm i$. The response is returned in the form of the reflection coefficient at the base of the tree graph. However, the larger the tree, the more poles exist and the more rapidly the reflection coefficient changes. This forces us to use a signal with a narrower spectrum. By the uncertainty principle, the size of the allowable spectrum is inversely proportional to the minimum length of the signal and thus dictates the computational time.

We define the "window" for a given R(z) as $\left[\frac{\pi}{2} - L, \frac{\pi}{2} + L\right]$, where $Re\left[R\left(e^{i\left(\frac{\pi}{2}\pm L\right)}\right)\right] = 0$. Within this window the real part of R is either entirely positive (for logical 0) or entirely negative (for logical 1).



Figure 9: $Re\left[R\left(e^{i\theta}\right)\right]$ for a logic tree of depth 6. Since $Re\left[R\left(i\right)\right] = R\left(i\right) = 1$ the result was a logical zero, but in order to see that we would need to send the graph a signal with a frequency spread of no more than approximately 0.1. The "spiking" effect caused by poles near the edge of the unit circle is clearly visible here.

Not surprisingly, it is remarkably difficult to predict the size of the window, which can vary widely even among trees of the same depth. We do find however, that the *average* size of the window follows the familiar $O\left(\frac{1}{\sqrt{N}}\right)$ pattern. Finding a quick method for predicting the window size for a given tree is a clear and important next step, and will be the subject of future work.



Figure 10: Top: the mean window size for trees of depths 2-6 vs. $N = 2^D$. Bottom: the window sizes of 100 trees (each) of depths 2-6 vs. $N = 2^D$. While the mean closely follows the curve $\frac{1}{\sqrt{N}}$, the individual trees may have substantially smaller or larger windows. We find that depth is merely a rough predictor of computational time.

9 Tables

What follows is a table of the reflection coefficients for several small Logic Trees. It lists the reflection function itself (with bound states factored out), the position of all of the poles, and the window size. In order to save room, we will use the notation: ${}^{4}(a + bi) \equiv$ $\{a + bi, a - bi, -a + bi, -a - bi\}.$

Logic	R(z)	Poles	W
0	1		_
1	-1		-
0 \(\no 0)	$\frac{z^2+3}{3z^2+1}$	$\pm 0.577i$	0.92
$1 \overline{\vee} 0$	$\frac{z^4+3}{3z^4+1}$	$^{4}(0.537+0.537i)$	1.10
$1 \overline{\vee} 1$	$\frac{z^2-3}{3z^2-1}$	± 0.577	2.22
$0 \lor 0$	$-\frac{z^2+3}{3z^2+1}$	$\pm 0.577i$	0.92
$1 \lor 0$	$-\frac{z^4+3}{3z^4+1}$	4(0.537+0.537i)	1.10
$1 \lor 1$	$-\frac{z^2-3}{3z^2-1}$	± 0.577	2.22
0⊼0	$-\frac{z^2-3}{3z^2-1}$	± 0.577	2.22
$1\overline{\wedge}0$	$-\frac{z^4+3}{3z^4+1}$	4(0.537+0.537i)	1.10
$1\overline{\wedge}1$	$-\frac{z^2+3}{3z^2+1}$	$\pm 0.577i$	0.92
$0 \wedge 0$	$\frac{z^2-3}{3z^2-1}$	± 0.577	2.22
$1 \wedge 0$	$\frac{z^4+3}{3z^4+1}$	4(0.537+0.537i)	1.10
$1 \wedge 1$	$\frac{z^2+3}{3z^2+1}$	$\pm 0.577i$	0.92

Logic	R(z)	Poles	W	
$\boxed{[1 \land 1] \land [1 \land 1]}$	$\frac{3z^4 - 2z^2 - 9}{9z^4 + 2z^2 - 3}$	$\pm 0.691, \pm 0.836i$	0.32	
	$3z^6 - z^4 - 3z^2 + 9$	$\pm 0.802i,$	0.38	
	$9z^6 - 3z^4 - z^2 + 3$	$^4(0.777 + 0.340i)$	0.00	
$[1 \wedge 1] \wedge [1 \vee 0]$	$\frac{3z^6-z^4-3z^2+9}{2z^6-z^4-3z^2+9}$	$\pm 0.802i,$	0.38	
	$9z^{0}-3z^{*}-z^{2}+3$	$^4(0.777 + 0.340i)$		
$\boxed{[1\vee 0]\wedge [1\vee 0]}$	$\frac{3z^6+3z^4+z^2+9}{2z^6+3z^4+z^2+9}$	$\pm 0.752,$	0.46	
	$9z^6+z^4+3z^2+3$	$^4(0.705 + 0.520i)$	0.10	
$[1 \land 0] \lor [1 \lor 0]$	$-\frac{9z^{12}+9z^8+19z^4+27}{27z^{12}+19z^8+9z^4+9}$	$^4(0.670 + 0.670i),$		
		$^4(0.327 + 0.834i),$	0.54	
		$^4(0.834 + 0.327i)$		
$\boxed{[0 \land 0] \lor [0 \land 0]}$	$-\frac{3z^4+2z^2-9}{9z^4-2z^2-3}$	$\pm 0.836, \pm 0.691i$	0.62	
$[1 \land 1] \lor [1 \lor 0]$	$-\frac{9z^8-6z^6+20z^4-18z^2+27}{27z^8-18z^6+20z^4-6z^2+9}$	$^4(0.492 + 0.668i),$	0.90	
		$^4(0.829 + 0.389i)$		
$[0 \land 1] \land [0 \lor 0]$	$\frac{9z^8 - 6z^6 + 20z^4 - 18z^2 + 27}{27z^8 - 18z^6 + 20z^4 - 6z^2 + 9}$	$^4(0.492 + 0.668i)$	0.90	
		$^4(0.829 + 0.389i)$		
$[1 \land 0] \land [1 \land 0]$	$3z^6 - 3z^4 + z^2 - 9$	$\pm 0.752,$	0.96	
	$9z^6 - z^4 + 3z^2 - 3$	$^4(0.520 + 0.705i)$		

Logic	R(z)	Poles	W
$[0 \land 1] \land [0 \land 1]$	$\frac{3z^6-3z^4+z^2-9}{2z^6-3z^4+z^2-9}$	$\pm 0.752,$	0.96
	$9z^{0}-z^{4}+3z^{2}-3$	$^4(0.520 + 0.705i)$	
$[0 \land 0] \land [0 \lor 0]$	$\frac{z^4+3}{3z^4+1}$	$^{4}(0.537 + 0.537i)$	1.10
$\boxed{[0 \land 0] \land [0 \land 0]}$	$\frac{3z^4 - 4z^2 + 9}{9z^4 - 4z^2 + 3}$	$^{4}(0.632 + 0.421i)$	1.40

Logic	R(z)	Poles	W
$[(1 \land 1) \land (1 \land 1)] \land \\[1ex] [(1 \land 1) \land (1 \land 1)]$	$\frac{9z^6 - 7z^4 + 3z^2 + 27}{27z^6 + 3z^4 - 7z^2 + 9}$	$\pm 0.928i,$ $^{4}(0.706 + 0.351i)$	0.137
$ [(1 \land 0) \land (1 \land 0)] \land \\ [(1 \land 0) \lor (0 \lor 0)] $	$\frac{81z^{12} - 36z^{10} + 153z^8 - 112z^6 + 291z^4 - 108z^2 + 243}{243z^{12} - 108z^{10} + 291z^8 - 112z^6 + 153z^4 - 36z^2 + 81}$	${}^{4}(0.416 + 0.763i),$ ${}^{4}(0.704 + 0.669i),$ ${}^{4}(0.835 + 0.338i)$	0.72
$[(0 \land 0) \land (0 \land 0)]$ \land $[(0 \land 0) \land (0 \land 0)]$	$\frac{9z^6 - 13z^4 + 15z^2 - 27}{27z^6 - 15z^4 + 13z^2 - 9}$	$\pm 0.794,$ $^4(0.587 + 0.618i)$	1.134

A Appendix

A.1 The Bolo Subgraph

The bolo graph (which resembles a bolo tie) has a bound state, and 4 Right side active eigenvectors. Using techniques established earlier we can quickly decide on the best eigenvalue and Left side eigenvector to use as an approximate initial state to ensure the quickest search. For the purposes of this example, $N = 10^6$.



Figure 11: The Right side of this graph is the "Bolo Graph".

We can get all the information we need from \mathbf{U}_0 , so we can ignore the Left side entirely. Define the basis vectors as:

$$\begin{split} |\Psi_1\rangle &= |0,1\rangle \\ |\Psi_2\rangle &= |A,1\rangle \\ |\Psi_3\rangle &= |b\rangle \\ |\Psi_4\rangle &= |1,A\rangle \\ |\Psi_5\rangle &= |1,0\rangle \end{split}$$

And in this basis define the effect of \mathbf{U}_0 as:

 $\mathbf{U}_{0} = \begin{pmatrix} 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & -1 & 0 \\ \frac{2}{3} & \frac{2}{3} & -\frac{1}{3} & 0 & 0 \\ \frac{2}{3} & -\frac{1}{3} & \frac{2}{3} & 0 & 0 \\ -\frac{1}{3} & \frac{2}{3} & \frac{2}{3} & 0 & 0 \end{pmatrix}$

This is an equal scattering in three directions at vertex 1. The difference is that a signal returns from the b arm in 1 time step, and from the A arm in 2.

Step 1) Find the eigenvalues and eigenvectors of the Right side.

The characteristic polynomial is $C_0(z) = z^5 + \frac{1}{3}z^4 - \frac{2}{3}z^3 + \frac{2}{3}z^2 - \frac{1}{3}z - 1$, and the five eigenvalues are then found to be: $\lambda = \{-1, -1, 1, \frac{1}{3}(1 + i2\sqrt{2}), \frac{1}{3}(1 - i2\sqrt{2})\}.$

Already we know that there must be at least one bound eigenstate with eigenvalue -1, since the active eigenvector for each eigenvalue is unique and -1 is degenerate (thm. 4.8). The eigenvectors, in the same order, are:

$$\begin{split} |bound^{(-1)}\rangle &= \frac{1}{\sqrt{3}} \left[|A,1\rangle - |b\rangle + |1,A\rangle \right] \\ |\mathfrak{r}^{(-1)}\rangle &= \sqrt{\frac{3}{8}} \left[|0,1\rangle - \frac{1}{3}|A,1\rangle - \frac{2}{3}|b\rangle - \frac{1}{3}|1,A\rangle + |1,0\rangle \right] \\ |\mathfrak{r}^{(1)}\rangle &= \frac{1}{2} \left[-|0,1\rangle + |A,1\rangle - |1,A\rangle + |1,0\rangle \right] \\ \left| \mathfrak{r}^{\left(\frac{1+i2\sqrt{2}}{3}\right)} \right\rangle &= \frac{\sqrt{3}}{4} \left[\left(-\frac{1}{3} + \frac{2\sqrt{2}}{3}i \right) |0,1\rangle + \left(-\frac{1}{3} + \frac{2\sqrt{2}}{3}i \right) |A,1\rangle + \left(\frac{2}{3} + \frac{2\sqrt{2}}{3}i \right) |b\rangle + |1,A\rangle + |1,0\rangle \right] \\ \left| \mathfrak{r}^{\left(\frac{1-i2\sqrt{2}}{3}\right)} \right\rangle &= \frac{\sqrt{3}}{4} \left[\left(-\frac{1}{3} - \frac{2\sqrt{2}}{3}i \right) |0,1\rangle + \left(-\frac{1}{3} - \frac{2\sqrt{2}}{3}i \right) |A,1\rangle + \left(\frac{2}{3} - \frac{2\sqrt{2}}{3}i \right) |b\rangle + |1,A\rangle + |1,0\rangle \right] \\ All of the last four eigenvectors are active eigenvectors. This is immediately obvious \\ \end{split}$$

because $\langle 0,1|\mathfrak{r}^{(j)}\rangle \neq 0$ for each of them, so they are hub adjacent. The $\lambda_0 = -1$ active

eigenvector can be found by first finding the unique bound eigenvector. What remains in the -1 eigenspace must be the active eigenvector.

The active eigenspace is 6-dimensional and is spanned by these four Right side and the two Left side active eigenvectors. Paired, or otherwise dependent on ϵ , eigenvectors are always expressible as superpositions of these six active eigenvectors. Even if the Left side were replaced with something more interesting, the four active eigenvectors listed above would provide all the information necessary to analyze how the Right side interacts.

Step 2) Select a target eigenvalue.

We already have enough information to see which of these states, or rather which of these eigenvalues, is the best target for a search. Because the optimal number of iterations for a quadratic search is is given by $m = \lfloor \frac{\pi}{2c} \sqrt{N} \rfloor$ (thm. 4.13), and since $c = |\langle \ell_0 | \mathbf{U}_1 | \mathbf{r}_0 \rangle| = \sqrt{2} |\langle 1, 0 | \mathbf{r}_0 \rangle|$ (thm. 4.12), the state that overlaps $|1, 0\rangle$ most will yield the shortest search time. Additionally, a large value of $c^{(j)}$ means that the Right side active eigenvector is concentrated closer to the hub, which means that states on the edge between 0 and 1 are more likely to be measured, which is important if we assume that the states in G are unmeasurable (i.e., cannot be the result of a measurement).

$$\begin{split} &\sqrt{\frac{3}{4}} = c^{(-1)} = \sqrt{2} \left| \left< 1, 0 | \mathfrak{r}^{(-1)} \right> \right| \\ &\sqrt{\frac{1}{2}} = c^{(1)} = \sqrt{2} \left| \left< 1, 0 | \mathfrak{r}^{(1)} \right> \right| \\ &\sqrt{\frac{3}{8}} = c^{\left(\frac{1}{3} + i\frac{2\sqrt{2}}{3}\right)} = \sqrt{2} \left| \left< 1, 0 \right| \mathfrak{r}^{\left(\frac{1}{3} + i\frac{2\sqrt{2}}{3}\right)} \right> \right| \\ &\sqrt{\frac{3}{8}} = c^{\left(\frac{1}{3} - i\frac{2\sqrt{2}}{3}\right)} = \sqrt{2} \left| \left< 1, 0 \right| \mathfrak{r}^{\left(\frac{1}{3} - i\frac{2\sqrt{2}}{3}\right)} \right> \right| \end{split}$$

Clearly, $\lambda_0 = -1$ is the best choice, since $max\{c^{(j)}\} = c^{(-1)} = \sqrt{\frac{3}{4}}$. We know (thm. 4.14) that there is always some $c^{(j)} \ge \sqrt{\frac{2}{d}} = \sqrt{\frac{2}{4}} = \frac{1}{\sqrt{2}}$, so a value of $\sqrt{\frac{3}{4}}$ is not surprising.

Step 3) Tune the Left side eigenvalues.

The Left side $\lambda_0 = -1$ active eigenvector is $|\ell^{(-1)}\rangle = \frac{1}{\sqrt{2}} (|out\rangle - |in\rangle)$, and this eigenstate is only possible when $e^{i\phi} = \lambda_0^2 = (-1)^2 = 1$. So, by setting $\phi = 0$, the eigenvalues on the Left become ± 1 . This does mean that, since both sides now share both 1 and -1 as eigenvalues, paired states can exist for both eigenspaces. However, by initializing with the -1 eigenstate, the +1 state is unimportant. We want to match the -1 state because it is the fastest (largest value of $c^{(j)}$).

Step 4) Initialize the system with the state $|\Psi\rangle = \frac{1}{\sqrt{2 \cdot 10^6}} \sum_{j=1}^{10^6} (|0, j\rangle - |j, 0\rangle).$

To within an error of $O(0.1\%) = O\left(\frac{1}{\sqrt{10^6}}\right)$, this is equal to the Left side $\lambda_0 = -1$ eigenstate, $\left|\ell^{(-1)}\right\rangle = \frac{1}{\sqrt{2(10^6-1)}} \sum_{j=2}^{10^6} \left(\left|0,j\right\rangle - \left|j,0\right\rangle\right)$. Since we assume that we don't know to which edge the Bolo graph is attached, we can't start *entirely* in the -1 Left active eigenstate. That said, $\left<\ell^{(-1)}\right|\Psi\rangle = \frac{2(10^6-1)}{2\cdot 10^3\sqrt{(10^6-1)}} = 0.9999995$, so these two states are

essentially equal.

Step 5) Iterate the time step operator, \mathbf{U} .

Use **U** to step time forward $m = 1813 = \left\lfloor \frac{\pi}{\sqrt{3}} \sqrt{10^6} \right\rfloor = \left\lfloor \frac{\pi}{2c^{(-1)}} \sqrt{10^6} \right\rfloor$ times. This process will cause the state to rotate from $|\ell^{(-1)}\rangle$ to $|\mathfrak{r}^{(-1)}\rangle$, to within an additional error of O(0.1%) produced by the rounding of the floor function, and the fact that the paired eigenvectors, $|V^{\pm}\rangle$, are only very closely approximated by combinations of $|\ell^{(-1)}\rangle$ and $|\mathfrak{r}^{(-1)}\rangle$.

Step 6) Measure the system. The probability of the particle being detected on the edge between vertices 0 and 1 is $p = \left|\left\langle 0, 1 \left| \mathfrak{r}^{(-1)} \right\rangle\right|^2 + \left|\left\langle 1, 0 \left| \mathfrak{r}^{(-1)} \right\rangle\right|^2 = \left|\sqrt{\frac{3}{8}}\right|^2 + \left|\sqrt{\frac{3}{8}}\right|^2 = \frac{3}{4}$. This " $\frac{3}{4}$ " is good news, since it means that the algorithm won't need to be repeated extensively.

Finally, the Left and Right eigenvalues need not be exact. According to theorem 5.5, the search will still work more than half of the time when the difference between the Left and Right eigenvalues, δ , satisfies $\delta < c^{(-1)}\sqrt{\frac{2}{N}} = \sqrt{\frac{3}{4}}\sqrt{\frac{2}{10^6}} \approx 0.001$. So, for $N = 10^6$, the complex phase of the Left eigenvalue should be in the range $[\pi - 0.001, \pi + 0.001]$.

Notice that, aside from finding the value of m and estimating errors, N (or ϵ) was never considered at all. Indeed the the Left and Right sides are handled separately from beginning to end.

A.2 Proofs from section 3 (Algebraic Functions and the Behavior of Zeros)

Theorem. 3.1 If F(z) is globally analytic in an annulus around 0, and is m-valued, then F(z) can be expressed as a Puiseux series (a Laurent series with certain rational powers) of the form $F(z) = \sum_{n=-\infty}^{\infty} A_n z^{\frac{n}{m}}$. Moreover, the *m* different branches of *F*, $F^{(j)}$, can be separated by an arbitrary branch cut through the annulus and expressed as $F^{(j)}(z) = \sum_{n=-\infty}^{\infty} A_n \omega^{jn} z^{\frac{n}{m}}$, where ω is a primitive mth root of unity, $\omega = e^{i\frac{2\pi}{m}}$.

Proof Consider the annulus in the z-plane defined by $D_z = \{z : 0 < r < |z| < R\}$, and the mapping $z = \zeta^m$. Define $G(\zeta) \equiv F(\zeta^m)$ on the annulus $D_{\zeta} = \{\zeta : 0 < r^{\frac{1}{m}} < |\zeta| < R^{\frac{1}{m}}\}$. *G* inherits its analyticity from *F*, since $\frac{d}{d\zeta}G(\zeta) = \frac{d}{d\zeta}F(\zeta^m) = \frac{dz}{d\zeta}\frac{d}{dz}F(z)$. In addition, *G* is single valued. Defining any one of the branches of *F* to be the principle branch, f_0 , and taking the value of $G(x) = F^{(0)}(x^m)$, $x \in \mathbb{R}$, we can then define G(z) to be the terminal value of any analytic continuation of *G* from *x*. While F(z) has *m* branches, $G(\zeta)$ has *m* corresponding $\frac{2\pi}{m}$ wedges.

Continuation along a path, C_{ζ} , that starts at $x \in \mathbb{R}^+$ and traverses once around the circle $|\zeta| = x$ corresponds to traversing the circle C_z , defined by $|z| = x^m$, in D_z , m times. But since F(z) is m valued, traversing $|z| = x^m m$ times will return F to the principle branch. Thus, $G(xe^{2\pi i}) = G(x)$, and more generally $G(\zeta e^{2\pi i}) = G(\zeta)$, for $\zeta \in D_{\zeta}$.

Since $G(\zeta)$ is analytic and single-valued in the annulus D_{ζ} , it admits a Laurent series: $G(\zeta) = \sum_{n=-\infty}^{\infty} A_n \zeta^n$. Therefore, the globally analytic *m*-valued function *F* can be written as $F(z) = G(z^{\frac{1}{m}}) = \sum_{n=-\infty}^{\infty} A_n z^{\frac{n}{m}}.$

Notice that if the initial branch, $F^{(0)}(z) = \sum_{n=-\infty}^{\infty} A_n z^{\frac{n}{m}}$, is analytically continued once around C_z a 2π phase is added to z and we find the function taking values on the next branch cut (so a very natural ordering of the branch cuts is here defined by subsequent loops around z = 0). We find that $F^{(1)}(z) = \sum_{n=-\infty}^{\infty} A_n (e^{2\pi i})^{\frac{n}{m}} z^{\frac{n}{m}} = \sum_{n=-\infty}^{\infty} A_n \omega^n z^{\frac{n}{m}}$, where $\omega = e^{i\frac{2\pi}{m}}$. j loops around z = 0 yields $F^{(j)}(z) = \sum_{n=-\infty}^{\infty} A_n \omega^{jn} z^{\frac{n}{m}}$.

Theorem. 3.2 If $P(z, \epsilon)$ is a degree d polynomial in z, then there exists an open disk D, containing 0, and d analytic functions, $f^{(1)}, \dots, f^{(d)}$, such that:

- (i) $P(f^{(k)}(\epsilon), \epsilon) = 0, \epsilon \in D$
- $(ii) \quad f^{(k)}(0) = \lambda^{(k)}$

(*iii*)
$$P(\lambda, \epsilon) = 0, \epsilon \in D \Rightarrow \lambda = f^{(k)}(\epsilon), \text{ for some } k$$

Note that $f^{(k)}$ are indexed functions, and not necessarily branches of the same globally analytic function. While it is true that when $P(z, \epsilon)$ is not simultaneously reducible in both z and ϵ , the zeros (as functions or ϵ) are all branches of the same globally analytic function, it is not necessary to know that here.

Proof Since the zeros of P(z,0) are distinct, $\exists \delta$ such that $|z - \lambda^{(k)}| \leq \delta$ contains no zeros other than $\lambda^{(k)}$. Define C_k to be the loop defined by $|z - \lambda^{(k)}| = \delta$. By the argument principle $\frac{1}{2\pi i} \oint_{C_k} \frac{\partial_z P(z,0)}{P(z,0)} dz = 1$. Here we are assuming that the zeros of P(z,0) are all of degree 1, and there is only one zero inside of C_k . The case of higher degree zeros is dealt with in theorem 3.3.

The zeros of $P(z, \epsilon)$ are continuous functions of the coefficients of $P(z, \epsilon)$ (other than a_d at $a_d = 0$), and the coefficients of $P(z, \epsilon)$ are continuous functions of ϵ . By definition $\exists \sigma > 0$ such that when $\epsilon < \sigma$, $|f^{(k)}(\epsilon) - \lambda^{(k)}| < \delta$. In other words, the zero will stay within C_k , so for small values of ϵ , $\frac{1}{2\pi i} \oint_{C_k} \frac{\partial_z P(z,\epsilon)}{P(z,\epsilon)} dz = 1$. Notice that we've only used the definition of $f_k(\epsilon)$ as the zero of $P(z,\epsilon)$ corresponding to $\lambda^{(k)}$, independent of its analytic properties.

This integral can be used to pick out the value of the zero, $f^{(k)}(\epsilon)$, by multiplying the argument of the integral by z. By the residue calculus:

$$f^{(k)}(\epsilon) = \frac{1}{2\pi i} \oint_{C_k} z \frac{\partial_z P(z,\epsilon)}{P(z,\epsilon)} dz$$

The important thing to notice here is that, since $P(z, \epsilon)$ is a polynomial of ϵ , near $\epsilon = 0$ $f_k(\epsilon)$ is analytic.

Repeating this process for each of the *d* simple zeros of P(z, 0) yields the *d* analytic functions $f^{(1)}(\epsilon), \dots, f^{(d)}(\epsilon)$ that are the zeros of $P(z, \epsilon)$.



Theorem. 3.3 If $P(z, \epsilon)$ is an irreducible polynomial in z and ϵ , then all of the double roots of P are isolated in the ϵ -plane. That is, if for some value of $\epsilon_0 P(z, \epsilon_0)$ has a double root, then there exists $\delta > 0$ such that when $0 < |\epsilon - \epsilon_0| < \delta$, $P(z, \epsilon)$ does not have a double root in z.

The proof of this requires the introduction of a new object: the discriminant.

Definition The "discriminant of P", $\mathcal{D}[P]$, is a function of the coefficients of a polynomial P, and $\mathcal{D}[P] \equiv a_d^{2d-2} \prod_{j>k} (\lambda^{(j)} - \lambda^{(k)})^2$, where a_d is the leading coefficient of P, and $\{\lambda^{(k)}\}$ are the zeros of P.

Clearly the discriminant is zero if and only if P has a repeated root, and this is the property that makes it so appealing.

A known fact about the discriminant is that it is the resultant of P and $\partial_z P$, which is in some sense like being the $gcd(P, \partial_z P)$. One of the methods of finding the discriminant is very much like Euclid's algorithm for finding the gcd of two numbers, but rather than finding combinations of the two numbers that produce the lowest non-zero value, the discriminant involves finding the combination of polynomials that produces the lowest degree non-zero polynomial. For example, if $P(z) = Az^2 + Bz + C$, then $\partial_z P(z) = 2Az + B$, and

$$2P - z\partial_z P = Bz + 2C$$

$$\Rightarrow 2A(2P - z\partial_z P) - B\partial_z P = 4AC - B^2$$

Which is the well-known discriminant for quadratic equations. So, $\mathcal{D}[P] = B^2 - 4AC =$ $(-4A)P + (2Az + B)\partial_z P.$

The things to keep in mind here are:

- i) $\mathcal{D} = 0$ if and only if P(z) has a repeated zero.
- *ii*) \mathcal{D} is <u>not</u> a function of z.
- *iii*) \mathcal{D} is a polynomial in the coefficients of P.
- *iv*) If the coefficients of P are polynomials of ϵ , then so is \mathcal{D} .

Proof $\mathcal{D}(\epsilon)$ inherits its analyticity from $P(z, \epsilon)$. Because \mathcal{D} is analytic, if it has a non-

isolated zero, then it must be identically zero. But if the discriminant of P is always zero, then P always has a double root, and must therefore be reducible into factors. Because the original assumption was that $P(z, \epsilon)$ is irreducible, \mathcal{D} cannot be identically zero, and therefore any zeros of $\mathcal{D}(\epsilon)$ are isolated. This means that changing ϵ splits a multiple zero into simple zeros in general, and if P(z, 0) has a repeated root, then within a small punctured disk about $\epsilon = 0$, $P(z, \epsilon)$ has only simple roots.

Theorem. 3.4 In the neighborhood of a zero of $P(z, \epsilon)$ of multiplicity s > 1, the zeros take the form $f^{(j)}(\epsilon) = \sum_{n=-\infty}^{\infty} A_n \omega^{jn} \epsilon^{\frac{n}{H}}$, where H < s. Specifically, the zeros are branches of one or more H_i -valued global analytic functions, with the given Puiseux series expansion, such that $\sum H_i = s$.

Proof Without loss of generality, assume that the zero of multiplicity s is found at $\epsilon = 0$, so $f^{(1)}(0) = f^{(2)}(0) = \cdots = f^{(s)}(0)$. In the last theorem it was shown that within a small disk excluding $\epsilon = 0$ these s functions are different. For some ϵ_0 within this punctured disk we can apply theorem 3.2 verbatim to show that $f^{(1)}(\epsilon), \cdots, f^{(s)}(\epsilon)$ are analytic functions.

However, they may not necessarily be single-valued. If they are analytically continued in a loop around $\epsilon = 0$ they may come back with a different value. By definition $P(f^{(k)}(\epsilon), \epsilon) = 0$, and there are only *d* possible such functions. As a result, if $f^{(k)}(\epsilon)$ does not return to its original value it must return as one of the other functions. Therefore, looping around $\epsilon = 0$ permutes $f^{(1)}, \dots, f^{(s)}$. If *H* loops brings f_k back to its original value, then $f^{(k)}$ is a branch of an *H*-valued global analytic function. Clearly, H < s since there are only *s* available functions to permute. The *s* different functions can be grouped according to which of the global analytic functions they're branches of, $\{f^{(1)}, f^{(2)}, \dots, f^{(H_1)}\}\{f^{(H_1+1)}, \dots, f^{(H_1+H_2)}\}\dots$, where $\sum H_i = s$

Since these functions are branches of a global analytic function in an annulus, by theorem 3.4 these functions must be of the form $f^{(j)}(\epsilon) = \sum_{n=-\infty}^{\infty} A_n \omega^{jn} \epsilon^{\frac{n}{H}}$.

Proof That the Characteristic Polynomial is Affine in ϵ

For a hub vertex with reflection coefficients r and t, we know that unitarity implies $|r|^2 + (N-1)|t|^2 = 1$ and $2Re(r^*t) + (N-2)|t|^2 = 0$. The most commonly used solution, and the one assumed throughout this thesis, is $r = -1 + 2\epsilon$, $t = 2\epsilon$. The generalized solution is handled in section 7.

In the automorphism graph we found that the reflection coefficients are $R_L = r + (N-2)t = 1 - 2\epsilon$ and $R_R = r = -1 + 2\epsilon$, for the Left and Right sides respectively, and the transmission coefficients between the two sides is $T = t\sqrt{N-1} = 2\sqrt{\epsilon - \epsilon^2}$.

Theorem. 3.5 Assume that **U** is a time step matrix as described so far. That is, there is a Left and Right side and these are connected only through a hub vertex with N edges where the reflection and transmission coefficients are $r = -1 + \frac{2}{N}$ and $t = \frac{2}{N}$. Then $C(z, \epsilon) =$ $|\mathbf{U} - z\mathbf{I}|$ is an affine polynomial of $\epsilon = \frac{1}{N}$, and can be written $C(z, \epsilon) = C_0(z) + \epsilon f(z)$. Proof First, some cumbersome notation. Define $|\mathbf{M}|$ to be the determinant of the matrix \mathbf{M} , $|\mathbf{M}|_{(i,j)}$ to be the determinant with the (i, j) term replaced with a zero, and $|\mathbf{M}|_{\langle i,j \rangle}$ to be the determinant of \mathbf{M} with the *i*th column and *j*th row removed. Note that if \mathbf{M} is an $n \times n$ matrix, then $|\mathbf{M}|_{(i,j)}$ is also $n \times n$, and $|\mathbf{M}|_{\langle i,j \rangle}$ is $(n-1) \times (n-1)$.

In what follows we will make use of the fact that we can remove an element from the determinant of \mathbf{M} , but must include a determinant of a minor matrix. For example,

$$\begin{vmatrix} a & b & c \\ d & e & f \\ g & h & i \end{vmatrix} = a \begin{vmatrix} e & f \\ h & i \end{vmatrix} - d \begin{vmatrix} b & c \\ h & i \end{vmatrix} + g \begin{vmatrix} b & c \\ e & f \end{vmatrix} = \begin{vmatrix} a & b & c \\ d & e & f \\ 0 & h & i \end{vmatrix} + g \begin{vmatrix} b & c \\ e & f \end{vmatrix}$$

This is can be more succinctly written, $|\mathbf{M}| = |\mathbf{M}|_{(1,3)} + g|\mathbf{M}|_{<1,3>}$. Notice that $|\mathbf{M}|_{(1,3)}$

is 3×3 , while $|\mathbf{M}|_{<1,3>}$ is 2×2 .

If we list all of the Left side states first, then

$$\mathbf{U} \equiv \left(\begin{array}{c|c} \mathbf{U}_L & T_{ij} \\ \hline \\ \hline \\ T_{kl} & \mathbf{U}_R \end{array} \right)$$

where \mathbf{U}_L and \mathbf{U}_R are the restrictions of \mathbf{U} to the Left and Right sides, and T_{ij} and T_{kl} are all zero except for a single $T = 2\sqrt{\epsilon - \epsilon^2}$ at the indicated coordinate. Note that if the T's are at the coordinates (i, j) and (k, l), then the reflection coefficient for the left side, R_L , can be found at (k, j) and similarly R_R can be found at (i, l). It is now straightforward to see,

$$C(z,\epsilon) = \frac{\begin{vmatrix} \mathbf{U}_L - z\mathbf{I} & T_{ij} \end{vmatrix}}{T_{kl} & \mathbf{U}_R - z\mathbf{I} \end{vmatrix}$$

There's a slight abuse of notation in this step. Since the third term has had the jth

row removed, the coordinate of T_{kl} is not (k, l), but is instead (k, l-1). It follows that,

The second and third terms of this last line are both equal to zero. In the second term the *l*th column is removed, but since $\mathbf{U}_R - z\mathbf{I}$ is a square matrix, removing a row leaves the columns linearly dependent. Thus the matrix is degenerate, and the determinant is zero. A similar argument holds for the third term. Both of the non-zero blocks of the fourth term are square matrices, and are therefore the determinant is not necessarily zero. We now have,

This is enough to show that $C(z, \epsilon)$ is a polynomial in both z and ϵ . However, this can be taken a step further. R_R is the i, l term and R_L is the k, j term. Repeating the same trick we find that

And finally, using the fact that $R_R = -1 + 2\epsilon$, $R_L = 1 - 2\epsilon$, and $T = 2\sqrt{\epsilon - \epsilon^2}$,

it is worth noting that $R_R R_L - T^2 = -1$ is not a coincidence dependent on how the solutions to the unitarity condition are chosen, but is in fact the unitarity condition itself. Thus, if we had used a solution different from $r = -1 + 2\epsilon$, $t = 2\epsilon$, we would find that $R_R R_L - T^2$ is always a constant.

The long manipulation in this proof is nothing more than a careful removal of every ϵ dependent element of **U**, so the explicit ϵ in the above equation is in fact the *only* remaining ϵ . Clearly, the characteristic polynomial is a polynomial in z and an affine polynomial in ϵ . With $C_0(z) \equiv |\mathbf{U}_0 - z\mathbf{I}|$ we can now write

$$C(z,\epsilon) \equiv |\mathbf{U} - z\mathbf{I}| = C_0(z) + \epsilon f(z)$$
(55)

A.3 Proofs from section 4 (Pairing)

Theorem. 4.2 $||\mathbf{P}^{(k)}(\epsilon) - \mathbf{P}^{(k)}(0)|| = O(\sqrt{\epsilon}) \text{ and } |V^{(k)}(\epsilon)\rangle = |V^{(k)}(0)\rangle + O(\sqrt{\epsilon}).$

Proof The "resolvent" is a matrix defined as $\mathbf{R}(\zeta, \epsilon) = (\mathbf{U} - \zeta \mathbf{I})^{-1}$.

When ζ_0 is not an eigenvalue of **U**,

$$\mathbf{U} - \zeta \mathbf{I}$$

$$= \mathbf{U}_0 - \zeta_0 \mathbf{I} - (\zeta - \zeta_0) \mathbf{I} + (\mathbf{U} - \mathbf{U}_0)$$

$$= \mathbf{U}_0 - \zeta_0 \mathbf{I} - (\zeta \mathbf{I} - \zeta_0 \mathbf{I} + \mathbf{U} - \mathbf{U}_0) \mathbf{R}(\zeta_0, 0) (\mathbf{U}_0 - \zeta_0 \mathbf{I})$$

$$= [\mathbf{I} - (\zeta \mathbf{I} - \zeta_0 \mathbf{I} + \mathbf{U} - \mathbf{U}_0) \mathbf{R}(\zeta_0, 0)] (\mathbf{U}_0 - \zeta_0 \mathbf{I})$$

$$\Rightarrow \mathbf{R}(\zeta, \epsilon) = \mathbf{R}(\zeta_0, 0) [\mathbf{I} - ((\zeta - \zeta_0) \mathbf{I} + \mathbf{U} - \mathbf{U}_0) \mathbf{R}(\zeta_0, 0)]^{-1}$$

Since \mathbf{U}_0 is a known unitary matrix, for which ζ_0 is not an eigenvalue, we know that $\mathbf{R}(\zeta_0, 0)$ is well-defined. The entries of \mathbf{U} can be expanded as power series in $\sqrt{\epsilon}$, and since the entries of \mathbf{U} are continuous functions of ϵ , $||\mathbf{U} - \mathbf{U}_0||$ can be made arbitrarily small. Therefore, for small values of ϵ and $(\zeta - \zeta_0)$ we find that $||(\zeta - \zeta_0)\mathbf{I} + (\mathbf{U} - \mathbf{U}_0)|| < ||\mathbf{R}(\zeta_0, 0)||^{-1}$, and therefore $\mathbf{R}(\zeta, \epsilon)$ can be written as a double power series in ζ and $\sqrt{\epsilon}$.

Interesting things happen when $\zeta = \lambda^{(k)}$. The projection operator onto the $\lambda^{(k)}$ eigenspace can be expressed as $\mathbf{P}^{(k)} = -\frac{1}{2\pi i} \oint \mathbf{R}(\zeta, \epsilon) d\zeta$, where the integral is taken over
a curve that loops once around $\lambda^{(k)}$, and no other eigenvalues. This can be shown by
applying $\mathbf{P}^{(k)}$ to the eigenvector $|V^{(j)}\rangle$.

Since $|V^{(j)}\rangle = \mathbf{R}(\zeta, \epsilon)(\mathbf{U}-\zeta\mathbf{I})|V^{(j)}\rangle = (\lambda^{(j)}-\zeta)\mathbf{R}(\zeta, \epsilon)|V^{(j)}\rangle$ we know that $\mathbf{R}(\zeta, \epsilon)|V^{(j)}\rangle = \frac{1}{\lambda^{(j)}-\zeta}|V^{(j)}\rangle.$

It follows that,

$$\begin{aligned} \mathbf{P}^{(k)} | V^{(j)} \rangle \\ &= -\frac{1}{2\pi i} \oint \mathbf{R}(\zeta, \epsilon) d\zeta | V^{(j)} \rangle \\ &= -\frac{1}{2\pi i} \oint \mathbf{R}(\zeta, \epsilon) | V^{(j)} \rangle d\zeta \\ &= -\frac{1}{2\pi i} \oint \frac{1}{\lambda^{(j)} - \zeta} | V^{(j)} \rangle d\zeta \\ &= \frac{1}{2\pi i} \oint \frac{1}{\zeta - \lambda^{(j)}} d\zeta | V^{(j)} \rangle \\ &= \delta_{jk} | V^{(j)} \rangle \end{aligned}$$

The last step follows from the residue theorem, and the assumption that the integral is over a path that encloses only $\lambda^{(k)}$. $[\mathbf{P}^{(k)}]^2 = \mathbf{P}^{(k)}$, so $\mathbf{P}^{(k)}$ is a projection, and $\mathbf{P}^{(j)}\mathbf{P}^{(k)} = \delta_{jk}\mathbf{P}^{(k)}$, by the orthogonality of eigenvectors with different eigenvalues. Notice that this is not a projection onto a particular eigenvector with eigenvalue $\lambda^{(k)}$, but is a projection onto the eigenspace for $\lambda^{(k)}$.

The important thing is that since $\mathbf{R}(\zeta, \epsilon)$ is expressible as a power series in $\sqrt{\epsilon}$, then so is $\mathbf{P}^{(k)}$.

Away from $\epsilon = 0$ the eigenvalues are distinct, and thus the eigenprojections are 1dimensional and can be written $\mathbf{P}^{(k)} = |V^{(k)}\rangle\langle V^{(k)}|$. So if the entries of $\mathbf{P}^{(k)}$ take the form of $\sum_{n=0}^{\infty} c_n(\sqrt{\epsilon})^n$, then so do the entries in the corresponding eigenvector.

Theorem. 4.4

 $\mathbf{U}|V^{(k)}(\epsilon)\rangle = \lambda^{(k)}(\epsilon)|V^{(k)}(\epsilon)\rangle \text{ for all } k. \text{ Define } \mathcal{S} = span\{|V^{(1)}(0)\rangle, \cdots, |V^{(j)}(0)\rangle\} \text{ to be}$ some subset of eigenvectors of \mathbf{U}_0 , and $\mathbf{P}_{\mathcal{S}}$ as the projection operator onto \mathcal{S} . If $|u\rangle \in S$, then $\forall m$

- $i) \quad \mathbf{P}_{\mathcal{S}^{\perp}} \mathbf{U}_0^m | u \rangle = 0$
- $ii) \quad \mathbf{P}_{\mathcal{S}^{\perp}} \mathbf{U}^m | u \rangle = O(\sqrt{\epsilon})$

That is, if $|u\rangle \in S$, then $\mathbf{U}_0^m |u\rangle$ is also in S, and $\mathbf{U}^m |u\rangle$ is almost entirely in S.

$$Proof i)$$

$$|u\rangle \in S$$

$$\Rightarrow |u\rangle = \alpha_1 |V^{(1)}(0)\rangle + \dots + \alpha_j |V^{(j)}(0)\rangle$$

$$\Rightarrow \mathbf{U}_0^m |u\rangle = \alpha_1 \left[\lambda^{(1)}(0)\right]^m |V^{(1)}(0)\rangle + \dots + \alpha_j \left[\lambda^{(j)}(0)\right]^m |V^{(j)}(0)\rangle$$

$$\Rightarrow \mathbf{U}_0^m |u\rangle \in S$$

$$ii)$$

Notice first that \mathbf{U}_0 is unitary, so $||\mathbf{U}_0|| = 1$. Since it has entries of $O(\sqrt{\epsilon})$, $||\mathbf{U} - \mathbf{U}_0|| = O(\sqrt{\epsilon})$ and therefore $||\mathbf{U}|| \le ||\mathbf{U}_0|| + O(\sqrt{\epsilon}) = 1 + O(\sqrt{\epsilon})$. When on the "unitary preserving path" ($\epsilon \in \mathbb{R}^+, 0 \le \epsilon \le \frac{1}{2}$), $||\mathbf{U}|| = 1$.

$$\begin{split} |u\rangle \in \mathcal{S} \\ \Rightarrow |u\rangle &= \alpha_1 |V^{(1)}(0)\rangle + \dots + \alpha_j |V^{(j)}(0)\rangle \\ &= |u\rangle = \alpha_1 |V^{(1)}(\epsilon)\rangle + \dots + \alpha_j |V^{(j)}(\epsilon)\rangle + O(\sqrt{\epsilon}) \qquad \text{thm. 4.3} \\ \Rightarrow \mathbf{U}^m |u\rangle &= \alpha_1 [\lambda^{(1)}(\epsilon)]^m |V^{(1)}(\epsilon)\rangle + \dots + \alpha_j [\lambda^{(j)}(\epsilon)]^m |V^{(j)}(\epsilon)\rangle + \mathbf{U}^m O(\sqrt{\epsilon}) \\ &= \alpha_1 [\lambda^{(1)}(\epsilon)]^m |V^{(1)}(\epsilon)\rangle + \dots + \alpha_j [\lambda^{(j)}(\epsilon)]^m |V^{(j)}(\epsilon)\rangle + O(\sqrt{\epsilon}) \qquad \text{unitarity} \\ &= \alpha_1 [\lambda^{(1)}(\epsilon)]^m |V^{(1)}(0)\rangle + \dots + \alpha_j [\lambda^{(j)}(\epsilon)]^m |V^{(j)}(0)\rangle + O(\sqrt{\epsilon}) \qquad \text{thm. 4.3} \\ &\text{Since } \alpha_1 [\lambda^{(1)}(\epsilon)]^m |V^{(1)}(0)\rangle + \dots + \alpha_j [\lambda^{(j)}(\epsilon)]^m |V^{(j)}(0)\rangle \in \mathcal{S}, \ \mathbf{P}_{\mathcal{S}^{\perp}} \mathbf{U}^m |u\rangle = O(\sqrt{\epsilon}). \end{split}$$

Theorem. 4.8

Assume that the Right side λ_0 -eigenspace of \mathbf{U}_0 is D dimensional.

1) If the λ_0 -eigenspace of \mathbf{U}_0 is bound in G, then the λ_0 -eigenspace of \mathbf{U} is D dimensional and all of the associated eigenvectors are constant. This is case i) of the Three Case Theorem.

2) If the λ_0 -eigenspace of \mathbf{U}_0 is in contact with the hub vertex, then the Right sided λ_0 -eigenspace of \mathbf{U} is D-1 dimensional and the D-1 associated eigenvectors are constant and bound in G. This leaves one eigenvector which is non-constant in ϵ , and is in contact with the hub vertex. This is either case ii or case iii of the Three Case Theorem.

Proof The first result is trivial. If an eigenvector is bound in G, then varying ϵ (which only affects reflection and transmission across the hub vertex) can't have any impact on it. So, for eigenvectors bound in G, $\mathbf{U}|V\rangle = \mathbf{U}_0|V\rangle = \lambda_0|V\rangle$.

For the second result we assume that the λ_0 -eigenspace is in contact with the hub vertex, and we will use the set up described in section 2. Define $|V\rangle = \alpha |in\rangle + \beta |out\rangle + \gamma |1,0\rangle + \delta |0,1\rangle + |G\rangle$, where $|G\rangle = \mathbf{P}_G |V\rangle$ and $\mathbf{U}|V\rangle = \lambda_0 |V\rangle$. So $|V\rangle$ is in contact with the hub vertex, is an eigenvector of \mathbf{U} , and has a constant eigenvalue. It may seem too restrictive to assume that the Left side has a particular form, but we will find that it makes no difference.

The rough idea of the proof is to show that if $|V_0\rangle$ is a hub-adjacent λ_0 eigenvector of \mathbf{U}_0 , then $|V\rangle$ cannot be a λ_0 eigenvector of \mathbf{U} . Instead, the eigenvalue must be a non-

constant function of ϵ . Since a λ_0 eigenvector is lost when we change from the $\epsilon = 0$ case to the $\epsilon \neq 0$ case, we can say that if the λ_0 -eigenspace of \mathbf{U}_0 is D dimensional, then the λ_0 -eigenspace of \mathbf{U} is D-1 dimensional.

Assume that there is no Left side λ_0 -eigenspace. By the Three Case theorem and theorem 4.7, the only possibilities are that all of the eigenvectors in the λ_0 family are constant, or there is one unique non-constant eigenvector. Since the λ_0 space of \mathbf{U}_0 is entirely Right sided, $|V_0\rangle$ takes the form $|V_0\rangle = \gamma_0 |1, 0\rangle + \delta_0 |0, 1\rangle + |G_0\rangle$. It follows that,

$$\begin{split} \mathbf{U}_{0}|V_{0}\rangle &= \lambda_{0}|V_{0}\rangle \\ \Rightarrow &-\gamma_{0}|0,1\rangle + \mathbf{U}_{0}\left[\delta_{0}|0,1\rangle + |G_{0}\rangle\right] = \gamma_{0}\lambda_{0}|1,0\rangle + \delta_{0}\lambda_{0}|0,1\rangle + \lambda_{0}|G_{0}\rangle \\ \Rightarrow &\begin{cases} \gamma_{0} &= -\delta_{0}\lambda_{0} \\ \mathbf{U}_{0}\left[\delta_{0}|0,1\rangle + |G_{0}\rangle\right] = \gamma_{0}\lambda_{0}|0,1\rangle + \lambda_{0}|G_{0}\rangle \\ \text{Keep both of these innocent looking results in mind for a moment.} \end{cases}$$

Now extending to the $\epsilon \neq 0$ case,

$$\begin{split} \mathbf{U}|V\rangle &= \\ \alpha \left[(1-2\epsilon)|out\rangle + 2\sqrt{\epsilon - \epsilon^2}|0,1\rangle \right] + \beta e^{i\phi}|in\rangle + \gamma \left[(-1+2\epsilon)|0,1\rangle + 2\sqrt{\epsilon - \epsilon^2}|out\rangle \right] + \mathbf{U} \left[\delta|0,1\rangle + |G\rangle \right] \\ \mathbf{U}|V\rangle &= \lambda_0 |V\rangle \Rightarrow \begin{cases} |in\rangle : \quad \beta e^{i\phi} = \alpha\lambda_0 \\ |out\rangle : \quad \alpha(1-2\epsilon) + \gamma 2\sqrt{\epsilon - \epsilon^2} = \beta\lambda_0 \\ |0,1\rangle : \quad \alpha 2\sqrt{\epsilon - \epsilon^2} + \gamma(-1+2\epsilon) = \delta\lambda_0 \\ \mathbf{U} \left[\delta|0,1\rangle + |G\rangle \right] = \gamma\lambda_0 |1,0\rangle + \lambda_0 |G\rangle \end{split}$$

This is difficult to solve directly, but fortunately the last of these four relations can be used to eliminate a variable. Notice that $\mathbf{U}[\delta|0,1\rangle + |G\rangle] = \mathbf{U}_0[\delta|0,1\rangle + |G\rangle]$ since both $|0,1\rangle$ and $|G\rangle$ are unaffected by the hub vertex. Beginning with the last relation from both the $\epsilon = 0$ and $\epsilon \neq 0$ cases,

$$\begin{cases} \mathbf{U}_{0} \left[\delta_{0} | 0, 1 \right\rangle + |G_{0} \right] = \gamma_{0} \lambda_{0} | 0, 1 \right\rangle + \lambda_{0} | G_{0} \rangle \\ \mathbf{U} \left[\delta | 0, 1 \right\rangle + |G \rangle \right] = \gamma \lambda_{0} | 1, 0 \rangle + \lambda_{0} | G \rangle \\ \Rightarrow \begin{cases} \mathbf{U}_{0} \left[\delta_{0} | 0, 1 \right\rangle + |G_{0} \rangle \right] = \gamma_{0} \lambda_{0} | 0, 1 \rangle + \lambda_{0} | G \rangle \\ \mathbf{U}_{0} \left[\delta | 0, 1 \rangle + |G \rangle \right] = \gamma \lambda_{0} | 1, 0 \rangle + \lambda_{0} | G \rangle \\ \Rightarrow \left[\delta_{0}^{*} \langle 0, 1 | + \langle G_{0} |] \mathbf{U}_{0}^{\dagger} \mathbf{U}_{0} \left[\delta | 0, 1 \rangle + |G \rangle \right] = \left(\gamma_{0}^{*} \lambda_{0}^{*} \langle 1, 0 | + \lambda_{0}^{*} \langle G_{0} | \rangle \left(\gamma \lambda_{0} | 0, 1 \rangle + \lambda_{0} | G \rangle \right) \right) \\ \Rightarrow \delta_{0}^{*} \delta \langle 0, 1 | 0, 1 \rangle + \langle G_{0} | G \rangle = \gamma_{0}^{*} \gamma \lambda_{0}^{*} \lambda_{0} \langle 1, 0 | 1, 0 \rangle + \lambda_{0}^{*} \lambda_{0} \langle G_{0} | G \rangle \\ \Rightarrow \delta_{0}^{*} \delta + \langle G_{0} | G \rangle = \gamma_{0}^{*} \gamma + \langle G_{0} | G \rangle \\ \Rightarrow \delta_{0}^{*} \delta = \left(-\delta_{0}^{*} \lambda_{0}^{*} \right) \gamma \\ \Rightarrow \delta_{0}^{*} \delta = \left(-\delta_{0}^{*} \lambda_{0}^{*} \right) \gamma \\ \Rightarrow \delta = -\lambda_{0}^{*} \gamma \\ \Rightarrow -\delta \lambda_{0} = \gamma \end{cases}$$

So we now have four straightforward equations and four variables: \mathbf{f}

$$\begin{cases} \beta e^{i\phi} = \alpha \lambda_0 \\\\ \alpha(1-2\epsilon) + \gamma 2\sqrt{\epsilon-\epsilon^2} = \beta \lambda_0 \\\\ \alpha 2\sqrt{\epsilon-\epsilon^2} + \gamma(-1+2\epsilon) = \delta \lambda_0 \\\\ \gamma = -\delta \lambda_0 \end{cases}$$

$$\Rightarrow \begin{cases} \beta = \alpha \lambda_0 e^{-i\phi} \\ \alpha(1 - 2\epsilon) + (-\delta \lambda_0) 2\sqrt{\epsilon - \epsilon^2} = \beta \lambda_0 \\ \alpha 2\sqrt{\epsilon - \epsilon^2} + (-\delta \lambda_0)(-1 + 2\epsilon) = \delta \lambda_0 \end{cases}$$
$$\Rightarrow \begin{cases} \alpha(1 - 2\epsilon) - \delta \lambda_0 2\sqrt{\epsilon - \epsilon^2} = (\alpha \lambda_0 e^{-i\phi}) \lambda_0 \\ \alpha 2\sqrt{\epsilon - \epsilon^2} = \delta \lambda_0 2\epsilon \end{cases}$$
$$\Rightarrow \begin{cases} \alpha(1 - \lambda_0^2 e^{-i\phi} - 2\epsilon) = \delta \lambda_0 2\sqrt{\epsilon - \epsilon^2} \\ \alpha 2\sqrt{\epsilon - \epsilon^2} = \delta \lambda_0 2\epsilon \end{cases}$$
$$\Rightarrow \begin{cases} \alpha(1 - \lambda_0^2 e^{-i\phi} - 2\epsilon) = \delta \lambda_0 2\sqrt{\epsilon - \epsilon^2} \\ \delta = \alpha \frac{\sqrt{\epsilon - \epsilon^2}}{\lambda_0 \epsilon} \end{cases}$$
$$\Rightarrow \alpha(1 - \lambda_0^2 e^{-i\phi} - 2\epsilon) = \left(\alpha \frac{\sqrt{\epsilon - \epsilon^2}}{\lambda_0 \epsilon}\right) \lambda_0 2\sqrt{\epsilon - \epsilon^2}$$
$$\Rightarrow \alpha(1 - \lambda_0^2 e^{-i\phi} - 2\epsilon) = \alpha(2 - 2\epsilon)$$

$$\Rightarrow \alpha (1 - \lambda_0^2 e^{-i\phi} - 2\epsilon) = \alpha (2 - \epsilon)$$
$$\Rightarrow \alpha (\lambda_0^2 + e^{i\phi}) = 0$$

Unless ϕ was specifically chosen so that $e^{i\phi} + \lambda_0^2 = 0$ it follows that $\alpha = \beta = \gamma = \delta = 0$, which contradicts the statement that $|V_0\rangle$ is in contact with the hub vertex. What has just been shown is that if $|V_0\rangle$ is a λ_0 eigenvector of \mathbf{U}_0 in contact with the hub vertex, then $|V\rangle$ either has a different eigenvalue or $e^{i\phi} + \lambda_0^2 = 0$.

First assume that $\lambda_0^2 + e^{i\phi} \neq 0$ and $\lambda_0^2 - e^{i\phi} \neq 0$ (there is no Left side λ_0 -eigenspace). If the λ_0 eigenspace of \mathbf{U}_0 is in contact with the hub vertex, then by moving from the $\epsilon = 0$ case to the $\epsilon \neq 0$ case at least one eigenvector is lost. Since $\lambda_0^2 - e^{i\phi} \neq 0$, by thm. 4.7 there can be no pairing. The Three Case Theorem then implies that there is at most only one non-constant eigenvalue in the λ_0 family. So, only one eigenvector is lost and if the Right side λ_0 -eigenspace of \mathbf{U}_0 is D dimensional, then the Right side λ_0 -eigenspace of \mathbf{U} must be D-1 dimensional.

The Fundamental Pairing Theorem

Theorem. 4.10 The λ_0 -eigenspace is in contact with both the Left and Right sides of the hub vertex if and only if there exists paired vectors $|V^{\pm}\rangle$ with eigenvalues of the form $\lambda_0 e^{\pm ic\sqrt{\epsilon}} + O(\epsilon)$.

Proof Both sides of the λ_0 -eigenspace have an active eigenvector, because both sides are in contact with the hub (thm. 4.8). Define $|\ell_0\rangle$ and $|\mathfrak{r}_0\rangle$ to be the Left and Right side active eigenvectors.

Assume that $|P\rangle$ and $|Q\rangle$ are eigenvectors with eigenvalues in the λ_0 family, and that both are in contact with the hub vertex. They may be paired, or one or both may be constant. $|P\rangle$ and $|Q\rangle$ are in the active subspace, and $|P_0\rangle$ and $|Q_0\rangle$ are in the λ_0 -eigenspace of \mathbf{U}_0 , so it follows that $span\{|P_0\rangle, |Q_0\rangle\} = span\{|\ell_0\rangle, |\mathfrak{r}_0\rangle\}$. Define the eigenvalues of $|P\rangle$ and $|Q\rangle$ to be $\lambda_0 e^{ip(\epsilon)}$ and $\lambda_0 e^{iq(\epsilon)}$, where p(0) = q(0) = 0.

Because the spans are equal and two dimensional there exists a transformation between the orthonormal bases, $\{|\ell_0\rangle, |\mathfrak{r}_0\rangle\}$ and $\{|P_0\rangle, |Q_0\rangle\}$, which we can write

$$\begin{pmatrix} |\ell_0\rangle \\ |\mathfrak{r}_0\rangle \end{pmatrix} = \begin{pmatrix} e^{i\gamma}\cos(\omega) & e^{i\delta}\sin(\omega) \\ e^{i\gamma+i\eta}\sin(\omega) & -e^{i\delta+i\eta}\cos(\omega) \end{pmatrix} \begin{pmatrix} |P_0\rangle \\ |Q_0\rangle \end{pmatrix}.$$

By carefully choosing the relative phases between all four vertices of the relative phases between all four vertices.

By carefully choosing the relative phases between all four vectors, we can assume with-
out loss of generality that
$$\begin{pmatrix} |\ell_0\rangle \\ |\mathfrak{r}_0\rangle \end{pmatrix} = \begin{pmatrix} \cos(\omega) & \sin(\omega) \\ -\sin(\omega) & \cos(\omega) \end{pmatrix} \begin{pmatrix} |P_0\rangle \\ |Q_0\rangle \end{pmatrix}$$
, with $0 \le \omega \le \frac{\pi}{2}$,
and use this to define $|\ell\rangle$ and $|\mathfrak{r}\rangle$ as: $\begin{pmatrix} |\ell\rangle \\ |\mathfrak{r}\rangle \end{pmatrix} = \begin{pmatrix} \cos(\omega) & \sin(\omega) \\ -\sin(\omega) & \cos(\omega) \end{pmatrix} \begin{pmatrix} |P\rangle \\ |Q\rangle \end{pmatrix}$.

Notice that while $|\ell_0\rangle$ and $|\mathfrak{r}_0\rangle$ are eigenvectors of \mathbf{U}_0 , $|\ell\rangle$ and $|\mathfrak{r}\rangle$ are <u>not</u> eigenvectors of \mathbf{U} , they're merely defined in terms of the eigenvectors $|P\rangle$ and $|Q\rangle$. Since eigenvectors can be expressed as power series in $\sqrt{\epsilon}$, we can write $|\ell\rangle = |\ell_0\rangle + \sqrt{\epsilon}|\ell_1\rangle + O(\epsilon)$, and similarly for $|\mathfrak{r}\rangle$.

In the
$$\{|P\rangle, |Q\rangle\}$$
 basis $\mathbf{U} = \lambda_0 \begin{pmatrix} e^{ip(\epsilon)} & 0\\ & & \\ 0 & e^{iq(\epsilon)} \end{pmatrix}$

and a similarity transform allows us to write this in the $\{|\ell\rangle, |\mathfrak{r}\rangle\}$ basis,

$$\mathbf{U} = \begin{pmatrix} \cos(\omega) & \sin(\omega) \\ -\sin(\omega) & \cos(\omega) \end{pmatrix} \begin{pmatrix} \lambda_0 e^{ip(\epsilon)} & 0 \\ 0 & \lambda_0 e^{iq(\epsilon)} \end{pmatrix} \begin{pmatrix} \cos(\omega) & -\sin(\omega) \\ \sin(\omega) & \cos(\omega) \end{pmatrix}$$
$$= \lambda_0 \begin{pmatrix} \cos(\omega) & \sin(\omega) \\ -\sin(\omega) & \cos(\omega) \end{pmatrix} \begin{pmatrix} \cos(\omega) e^{ip(\epsilon)} & -\sin(\omega) e^{ip(\epsilon)} \\ \sin(\omega) e^{iq(\epsilon)} & \cos(\omega) e^{iq(\epsilon)} \end{pmatrix}$$
$$= \lambda_0 \begin{pmatrix} \cos^2(\omega) e^{ip(\epsilon)} + \sin^2(\omega) e^{iq(\epsilon)} & \sin(\omega) \cos(\omega) (-e^{ip(\epsilon)} + e^{iq(\epsilon)}) \\ \sin(\omega) \cos(\omega) (-e^{ip(\epsilon)} + e^{iq(\epsilon)}) & \cos^2(\omega) e^{iq(\epsilon)} + \sin^2(\omega) e^{ip(\epsilon)} \end{pmatrix}$$

Using the trig identities $\cos^2(\omega) = \frac{1+\cos(2\omega)}{2}$, $\sin^2(\omega) = \frac{1-\cos(2\omega)}{2}$, and $\sin(\omega)\cos(\omega) = \frac{1-\cos(2\omega)}{2}$

$$\frac{\sin(2\omega)}{2} \text{ we find}$$

$$\mathbf{U} = \frac{\lambda_0}{2} \begin{pmatrix} e^{ip(\epsilon)} + e^{iq(\epsilon)} + \cos(2\omega) \left(e^{ip(\epsilon)} - e^{iq(\epsilon)} \right) & \sin(2\omega) \left(-e^{ip(\epsilon)} + e^{iq(\epsilon)} \right) \\ \sin(2\omega) \left(-e^{ip(\epsilon)} + e^{iq(\epsilon)} \right) & e^{ip(\epsilon)} + e^{iq(\epsilon)} - \cos(2\omega) \left(e^{ip(\epsilon)} - e^{iq(\epsilon)} \right) \end{pmatrix}$$

This is enough to determine the value of ω .

Notice that $2|\mathbf{U}_{12}| = |\sin(2\omega)||e^{ip(\epsilon)} - e^{iq(\epsilon)}|$ and $|\mathbf{U}_{11} - \mathbf{U}_{22}| = |\cos(2\omega)||e^{ip(\epsilon)} - e^{iq(\epsilon)}|$. It follows that $\frac{4|\mathbf{U}_{12}|^2}{4|\mathbf{U}_{12}|^2 + |\mathbf{U}_{11} - \mathbf{U}_{22}|^2} = \frac{\sin^2(2\omega)|e^{ip(\epsilon)} - e^{iq(\epsilon)}|^2}{\sin^2(2\omega)|e^{ip(\epsilon)} - e^{iq(\epsilon)}|^2 + \cos^2(2\omega)|e^{ip(\epsilon)} - e^{iq(\epsilon)}|^2} = \frac{\sin^2(2\omega)}{\sin^2(2\omega) + \cos^2(2\omega)} = \sin^2(2\omega).$

Or more simply, $\sin^2(2\omega) = \left(1 + \left|\frac{\mathbf{U}_{11} - \mathbf{U}_{22}}{2\mathbf{U}_{12}}\right|^2\right)^{-1}$. We can calculate $|\mathbf{U}_{11} - \mathbf{U}_{22}|$ and

 $|\mathbf{U}_{12}|$ directly:

$$\begin{aligned} |\mathbf{U}_{11} - \mathbf{U}_{22}| \\ &= |\langle \ell | \mathbf{U} | \ell \rangle - \langle \mathbf{r} | \mathbf{U} | \mathbf{r} \rangle | \\ &= |\langle \ell_0 | \mathbf{U}_0 | \ell_0 \rangle - \langle \mathbf{r}_0 | \mathbf{U}_0 | \mathbf{r}_0 \rangle \\ &+ \sqrt{\epsilon} \left(\langle \ell_1 | \mathbf{U}_0 | \ell_0 \rangle + \langle \ell_0 | \mathbf{U}_1 | \ell_0 \rangle + \langle \ell_0 | \mathbf{U}_0 | \ell_1 \rangle - \langle \mathbf{r}_1 | \mathbf{U}_0 | \mathbf{r}_0 \rangle - \langle \mathbf{r}_0 | \mathbf{U}_1 | \mathbf{r}_0 \rangle - \langle \mathbf{r}_0 | \mathbf{U}_0 | \mathbf{r}_1 \rangle) | + O(\epsilon) \end{aligned}$$

$$\begin{aligned} &= |\lambda_0 \langle \ell_0 | \ell_0 \rangle - \lambda_0 \langle \mathbf{r}_0 | \mathbf{r}_0 \rangle \\ &+ \sqrt{\epsilon} \left(\lambda_0 \langle \ell_1 | \ell_0 \rangle + \langle \ell_0 | \mathbf{U}_1 | \ell_0 \rangle + \lambda_0 \langle \ell_0 | \ell_1 \rangle - \lambda_0 \langle \mathbf{r}_1 | \mathbf{r}_0 \rangle - \langle \mathbf{r}_0 | \mathbf{U}_1 | \mathbf{r}_0 \rangle - \lambda_0 \langle \mathbf{r}_0 | \mathbf{r}_1 \rangle) | + O(\epsilon) \end{aligned}$$

$$\begin{aligned} &= |\lambda_0 - \lambda_0 + \sqrt{\epsilon} \left(\lambda_0 [(\langle \ell_1 | \ell_0 \rangle + \langle \ell_0 | \ell_1 \rangle) - (\langle \mathbf{r}_1 | \mathbf{r}_0 \rangle + \langle \mathbf{r}_0 | \mathbf{r}_1 \rangle)] + \langle \ell_0 | \mathbf{U}_1 | \ell_0 \rangle - \langle \mathbf{r}_0 | \mathbf{U}_1 | \mathbf{r}_0 \rangle) | + O(\epsilon) \end{aligned}$$

$$\begin{aligned} &= |0 + \sqrt{\epsilon} \left(\lambda_0 [0 - 0] + \langle \ell_0 | \mathbf{U}_1 | \ell_0 \rangle - \langle \mathbf{r}_0 | \mathbf{U}_1 | \mathbf{r}_0 \rangle) | + O(\epsilon) \end{aligned}$$

$$\begin{aligned} &= \sqrt{\epsilon} |\langle \ell_0 | \mathbf{U}_1 | \ell_0 \rangle - \langle \mathbf{r}_0 | \mathbf{U}_1 | \mathbf{r}_0 \rangle | + O(\epsilon) \end{aligned}$$

$$\begin{aligned} &= \sqrt{\epsilon} |\langle 0 - 0| + O(\epsilon) \end{aligned}$$

In the last step here we used the fact that $|\ell_0\rangle$ and $|\mathfrak{r}_0\rangle$ are one-sided, and since \mathbf{U}_1 is only involved in transmitting between the Left and Right sides, $\langle \ell_0 | \mathbf{U}_1 | \ell_0 \rangle = \langle \mathfrak{r}_0 | \mathbf{U}_1 | \mathfrak{r}_0 \rangle = 0$.

$$\begin{aligned} |\mathbf{U}_{12}| \\ &= |\langle \mathbf{\mathfrak{r}} | \mathbf{U} | \ell \rangle | \\ &= |\langle \mathbf{\mathfrak{r}}_0 | \mathbf{U}_0 | \ell_0 \rangle + \sqrt{\epsilon} \left(\langle \mathbf{\mathfrak{r}}_1 | \mathbf{U}_0 | \ell_0 \rangle + \langle \mathbf{\mathfrak{r}}_0 | \mathbf{U}_1 | \ell_0 \rangle + \langle \mathbf{\mathfrak{r}}_0 | \mathbf{U}_0 | \ell_1 \rangle \right) | + O(\epsilon) \\ &= |\lambda_0 \langle \mathbf{\mathfrak{r}}_0 | \ell_0 \rangle + \sqrt{\epsilon} \left(\lambda_0 \langle \mathbf{\mathfrak{r}}_1 | \ell_0 \rangle + \lambda_0 \langle \mathbf{\mathfrak{r}}_0 | \ell_1 \rangle + \langle \mathbf{\mathfrak{r}}_0 | \mathbf{U}_1 | \ell_0 \rangle \right) | + O(\epsilon) \\ &= \sqrt{\epsilon} |\langle \mathbf{\mathfrak{r}}_0 | \mathbf{U}_1 | \ell_0 \rangle | + O(\epsilon) \end{aligned}$$

By construction, $\langle P|Q\rangle = 0 \Rightarrow \langle \mathfrak{r}|\ell\rangle = 0$, and in the last step this fact is used twice.

First $\langle \mathbf{r}_0 | \ell_0 \rangle = 0$ and second, by theorem 4.6, $\langle \mathbf{r}_0 | \ell_1 \rangle + \langle \mathbf{r}_1 | \ell_0 \rangle = 0$. By assumption, $|\ell_0 \rangle$ and $|\mathbf{r}_0 \rangle$ are adjacent to the hub vertex, $\langle \mathbf{r}_0 | \mathbf{U}_1 | \ell_0 \rangle \neq 0$.

So we now have that $|\mathbf{U}_{12}| = O(\sqrt{\epsilon})$ and $|\mathbf{U}_{11} - \mathbf{U}_{22}| = O(\epsilon)$. It follows that $\sin^2(2\omega) = \left(1 + \left|\frac{\mathbf{U}_{11} - \mathbf{U}_{22}}{2\mathbf{U}_{12}}\right|^2\right)^{-1} = (1 + O(\epsilon))^{-1} \Rightarrow \sin^2(2\omega) = 1$, since ω was originally defined independently of ϵ (e.g., $\cos(\omega) = \langle \ell_0 | V_0^+ \rangle$). So, $\sin(2\omega) = \pm 1$, and since $0 \le \omega \le \frac{\pi}{2}$,

we find that $\omega = \frac{\pi}{4}$. Now **U** takes a much simpler form in the $\{|\ell\rangle, |\mathfrak{r}\rangle\}$ basis:

$$\mathbf{U} = \frac{\lambda_0}{2} \begin{pmatrix} (e^{ip(\epsilon)} + e^{iq(\epsilon)}) & (e^{ip(\epsilon)} - e^{iq(\epsilon)}) \\ (e^{ip(\epsilon)} - e^{iq(\epsilon)}) & (e^{ip(\epsilon)} + e^{iq(\epsilon)}) \end{pmatrix} + O(\epsilon)$$

Since $|e^{ip(\epsilon)} - e^{iq(\epsilon)}| = 2|\mathbf{U}_{12}| = O(\sqrt{\epsilon})$ it follows that $p(\epsilon) - q(\epsilon) = O(\sqrt{\epsilon})$. So,

 $p(\epsilon) = O(\sqrt{\epsilon})$ or $q(\epsilon) = O(\sqrt{\epsilon})$. Without loss of generality, assume that $p(\epsilon) = c\sqrt{\epsilon} + O(\epsilon)$.

In addition,

$$\begin{aligned} \mathbf{U}_{11} &= \langle \ell | \mathbf{U} | \ell \rangle \\ &= \langle \ell_0 | \mathbf{U}_0 | \ell_0 \rangle + \sqrt{\epsilon} \left(\langle \ell_1 | \mathbf{U}_0 | \ell_0 \rangle + \langle \ell_0 | \mathbf{U}_1 | \ell_0 \rangle + \langle \ell_0 | \mathbf{U}_0 | \ell_1 \rangle \right) + O(\epsilon) \\ &= \lambda_0 \langle \ell_0 | \ell_0 \rangle + \sqrt{\epsilon} \left(\lambda_0 \langle \ell_1 | \ell_0 \rangle + 0 + \lambda_0 \langle \ell_0 | \ell_1 \rangle \right) + O(\epsilon) \\ &= \lambda_0 + \lambda_0 \sqrt{\epsilon} \left(\langle \ell_1 | \ell_0 \rangle + \langle \ell_0 | \ell_1 \rangle \right) + O(\epsilon) \\ &= \lambda_0 + O(\epsilon) \\ &\text{Since } \frac{\lambda_0}{2} (e^{ip(\epsilon)} + e^{iq(\epsilon)}) = \lambda_0 + O(\epsilon), \ p(\epsilon) + q(\epsilon) \text{ has no } \sqrt{\epsilon} \text{ term, and therefore } q(\epsilon) = \\ &-c\sqrt{\epsilon} + O(\epsilon). \end{aligned}$$

Clearly, this situation is case iii in the three-case theorem, and since there are only two non-constant eigenvalues, and all eigenvalues that vary by $O(\sqrt{\epsilon})$ are paired with another eigenvalue, these two eigenvalues are paired to each other (and not merely coincidentally
related). So by definition $|P\rangle$ and $|Q\rangle$ are paired eigenvectors. In fact, they are $|V^{\pm}\rangle$.

The reverse implication, that the λ_0 -eigenspace of \mathbf{U}_0 is adjacent to both sides of the hub vertex if there exists paired eigenvectors, is a direct result of theorem 4.7.

A.4 Proofs from section 5 (Tolerances)

With some foresight, define:

$$\begin{cases} |V^{+}(\delta,\epsilon)\rangle = \cos(\omega) |\ell_{0}\rangle + \sin(\omega) |\mathfrak{r}_{0}\rangle + O(\delta,\sqrt{\epsilon}) \\ |V^{-}(\delta,\epsilon)\rangle = -\sin(\omega) |\ell_{0}\rangle + \cos(\omega) |\mathfrak{r}_{0}\rangle + O(\delta,\sqrt{\epsilon}) \end{cases}$$

Theorem. 5.4 The angle between the paired eigenvectors and the active eigenvectors, ω , is to lowest order a function of $\frac{\delta^2}{4c^2\epsilon}$.

Proof The (arbitrary) phase of each of the eigenvectors can be carefully chosen so that each of these amplitudes are real, and so that $0 \le \omega \le \frac{\pi}{2}$.

Define
$$\begin{cases} |\ell\rangle = \cos\left(\omega\right)|V^{+}(\delta,\epsilon)\rangle - \sin\left(\omega\right)|V^{-}(\delta,\epsilon)\rangle \\ |\mathfrak{r}\rangle = \sin\left(\omega\right)|V^{+}(\delta,\epsilon)\rangle + \cos\left(\omega\right)|V^{-}(\delta,\epsilon)\rangle \\ \text{and define} \begin{cases} |V^{+}(\delta,\epsilon)\rangle = \cos\left(\omega\right)|\ell\rangle + \sin\left(\omega\right)|\mathfrak{r}\rangle \\ |V^{-}(\delta,\epsilon)\rangle = -\sin\left(\omega\right)|\ell\rangle + \cos\left(\omega\right)|\mathfrak{r}\rangle \end{cases}. \end{cases}$$

 $|\ell\rangle$ and $|\mathfrak{r}\rangle$ are projections of the corresponding active eigenvectors onto the space spanned by the paired eigenvectors. As such, $Span\{|\ell\rangle, |\mathfrak{r}\rangle\} = Span\{|V^+\rangle, |V^-\rangle\}$ is an invariant subspace of **U**.

$$\begin{split} &\mathbf{U}\begin{pmatrix} |\ell\rangle\\ |\mathfrak{r}\rangle \end{pmatrix} \\ &= \begin{pmatrix} \cos\left(\omega\right) & \sin\left(\omega\right)\\ -\sin\left(\omega\right) & \cos\left(\omega\right) \end{pmatrix} \begin{pmatrix}\lambda^{+} & 0\\ 0 & \lambda^{-} \end{pmatrix} \begin{pmatrix} \cos\left(\omega\right) & -\sin\left(\omega\right)\\ \sin\left(\omega\right) & \cos\left(\omega\right) \end{pmatrix} \begin{pmatrix}|\ell\rangle\\ |\mathfrak{r}\rangle \end{pmatrix} \\ &= \sqrt{\lambda_{\ell}\lambda_{r}} \begin{pmatrix} \cos\left(\omega\right) & \sin\left(\omega\right)\\ -\sin\left(\omega\right) & \cos\left(\omega\right) \end{pmatrix} \begin{pmatrix} e^{ic\sqrt{\epsilon-\epsilon_{0}}} & 0\\ 0 & e^{-ic\sqrt{\epsilon-\epsilon_{0}}} \end{pmatrix} \begin{pmatrix} \cos\left(\omega\right) & -\sin\left(\omega\right)\\ \sin\left(\omega\right) & \cos\left(\omega\right) \end{pmatrix} \begin{pmatrix}|\ell\rangle\\ |\mathfrak{r}\rangle \end{pmatrix} + O(\Delta) \\ &= \sqrt{\lambda_{\ell}\lambda_{r}} \begin{pmatrix} \cos\left(\omega\right) & \sin\left(\omega\right)\\ -\sin\left(\omega\right) & \cos\left(\omega\right) \end{pmatrix} \begin{pmatrix} \cos\left(u\right) e^{ic\sqrt{\epsilon-\epsilon_{0}}} & -\sin\left(u\right) e^{ic\sqrt{\epsilon-\epsilon_{0}}}\\ \sin\left(u\right) e^{-ic\sqrt{\epsilon-\epsilon_{0}}} & \cos\left(u\right) e^{-ic\sqrt{\epsilon-\epsilon_{0}}} \end{pmatrix} \begin{pmatrix}|\ell\rangle\\ |\mathfrak{r}\rangle \end{pmatrix} + O(\Delta) \\ &= \sqrt{\lambda_{\ell}\lambda_{r}} \begin{pmatrix} \cos^{2}\left(\omega\right) e^{ic\sqrt{\epsilon-\epsilon_{0}}} + \sin^{2}\left(\omega\right) e^{-ic\sqrt{\epsilon-\epsilon_{0}}} & -\sin\left(\omega\right) \cos\left(\omega\right) \left(e^{ic\sqrt{\epsilon-\epsilon_{0}}} - e^{-ic\sqrt{\epsilon-\epsilon_{0}}} \right) \\ &-\sin\left(\omega\right) \cos\left(\omega\right) \left(e^{ic\sqrt{\epsilon-\epsilon_{0}}} - e^{-ic\sqrt{\epsilon-\epsilon_{0}}} & -\sin\left(\omega\right) \cos\left(\omega\right) \left(e^{ic\sqrt{\epsilon-\epsilon_{0}}} - e^{-ic\sqrt{\epsilon-\epsilon_{0}}} \right) \\ &-\sin\left(\omega\right) \cos\left(\omega\right) \left(e^{ic\sqrt{\epsilon-\epsilon_{0}}} - e^{-ic\sqrt{\epsilon-\epsilon_{0}}} \right) & \cos^{2}\left(\omega\right) e^{-ic\sqrt{\epsilon-\epsilon_{0}}} \\ &-\sin\left(\omega\right) \sin\left(c\sqrt{\epsilon-\epsilon_{0}}\right) & -i\sin\left(2\omega\right) \sin\left(c\sqrt{\epsilon-\epsilon_{0}}\right) \\ &-i\sin\left(2\omega\right) \sin\left(c\sqrt{\epsilon-\epsilon_{0}}\right) & \cos\left(c\sqrt{\epsilon-\epsilon_{0}}\right) - i\cos\left(2\omega\right) \sin\left(c\sqrt{\epsilon-\epsilon_{0}}\right) \\ &-i\sin\left(2\omega\right) \sin\left(c\sqrt{\epsilon-\epsilon_{0}}\right) & \cos\left(2\omega\right) e^{ic\sqrt{\epsilon-\epsilon_{0}}} - e^{ic\sqrt{\epsilon-\epsilon_{0}}} \right) \end{pmatrix} \begin{pmatrix} |\ell\rangle\\ |\mathfrak{r}\rangle \end{pmatrix} + O(\Delta) \end{split}$$

Where $O(\Delta) = O(\delta^2, \delta\sqrt{\epsilon - \epsilon_0}, \epsilon - \epsilon_0)$. Using the same technique used in the proof of

the Fundamental Pairing theorem we can find an expression for $\omega {:}$

$$\frac{4|\mathbf{U}_{lr}|^2}{|\mathbf{U}_{ll} - \mathbf{U}_{rr}|^2 + 4|\mathbf{U}_{lr}|^2}$$

$$= \frac{4\sin^2(2\omega)\sin^2(c\sqrt{\epsilon - \epsilon_0})}{4\cos^2(2\omega)\sin^2(c\sqrt{\epsilon - \epsilon_0}) + 4\sin^2(2\omega)\sin^2(c\sqrt{\epsilon - \epsilon_0})}$$

$$= \frac{\sin^2(2\omega)\sin^2(c\sqrt{\epsilon - \epsilon_0})}{\sin^2(c\sqrt{\epsilon - \epsilon_0})}$$

$$= \sin^2(2\omega)$$

Once again, to solve for ω we need to find $|\mathbf{U}_{ll} - \mathbf{U}_{rr}|^2$ and $4|\mathbf{U}_{lr}|^2$:

$$\begin{split} |\mathbf{U}_{ll} - \mathbf{U}_{rr}|^{2} \\ &= |\langle \ell | \mathbf{U} | \ell \rangle - \langle \mathbf{r} | \mathbf{U} | \mathbf{r} \rangle|^{2} \\ &= \begin{cases} |\langle \ell_{0} | \mathbf{U}_{0} | \ell_{0} \rangle - \langle \mathbf{r}_{0} | \mathbf{U}_{0} | \mathbf{r}_{0} \rangle + \langle \ell_{1} | \mathbf{U}_{0} | \ell_{0} \rangle - \langle \mathbf{r}_{1} | \mathbf{U}_{0} | \mathbf{r}_{0} \rangle \\ &+ \langle \ell_{0} | \mathbf{U}_{0} | \ell_{1} \rangle - \langle \mathbf{r}_{0} | \mathbf{U}_{0} | \mathbf{r}_{1} \rangle + \langle \ell_{0} | \mathbf{U}_{1} | \ell_{0} \rangle - \langle \mathbf{r}_{0} | \mathbf{U}_{1} | \mathbf{r}_{0} \rangle \\ &+ O(\epsilon)|^{2} \\ &= |\lambda_{l} - \lambda_{r} + \lambda_{l} \langle \ell_{1} | \ell_{0} \rangle - \lambda_{r} \langle \mathbf{r}_{1} | \mathbf{r}_{0} \rangle + \lambda_{l} \langle \ell_{0} | \ell_{1} \rangle - \lambda_{r} \langle \mathbf{r}_{0} | \mathbf{r}_{1} \rangle + 0 - 0 + O(\epsilon)|^{2} \\ &= |\lambda_{l} - \lambda_{r} + \lambda_{l} (\langle \ell_{1} | \ell_{0} \rangle + \langle \ell_{0} | \ell_{1} \rangle) - \lambda_{r} (\langle \mathbf{r}_{1} | \mathbf{r}_{0} \rangle + \langle \mathbf{r}_{0} | \mathbf{r}_{1} \rangle) + O(\epsilon)|^{2} \\ &= |\lambda_{l} - \lambda_{r} + O(\epsilon)|^{2} \\ &= |\lambda_{0} e^{i\frac{\delta}{2}} - \lambda_{0} e^{-i\frac{\delta}{2}} + O(\epsilon)|^{2} \\ &= |2i\lambda_{0} \sin \left(\frac{\delta}{2}\right) + O(\epsilon)|^{2} \\ &= 4 \sin^{2} \left(\frac{\delta}{2}\right) + O(\delta\epsilon, \epsilon^{2}) \end{split}$$

$$\begin{aligned} 4|\mathbf{U}_{lr}|^{2} \\ &= |\langle \ell | \mathbf{U} | \mathbf{r} \rangle|^{2} \\ &= |\langle \ell | \mathbf{U} | \mathbf{r} \rangle|^{2} \\ &= |\langle \ell | \mathbf{U} | \mathbf{r} \rangle|^{2} \\ &= |0 + \lambda_{r} \langle \ell_{1} | \mathbf{r}_{0} \rangle + \langle \ell_{1} | \mathbf{U}_{0} | \mathbf{r}_{0} \rangle + \langle \ell_{0} | \mathbf{U}_{1} | \mathbf{r}_{0} \rangle|^{2} \\ &= |0 + \lambda_{r} \langle \ell_{1} | \mathbf{r}_{0} \rangle + \lambda_{l} \langle \ell_{0} | \mathbf{r}_{1} \rangle + \langle \ell_{0} | \mathbf{U}_{1} | \mathbf{r}_{0} \rangle|^{2} \\ &= |\lambda_{0} \left(e^{i\frac{\delta}{2}} \langle \ell_{1} | \mathbf{r}_{0} \rangle + e^{-i\frac{\delta}{2}} \langle \ell_{0} | \mathbf{r}_{1} \rangle \right) + \langle \ell_{0} | \mathbf{U}_{1} | \mathbf{r}_{0} \rangle|^{2} \\ &= |i\lambda_{0} \sin \left(\frac{\delta}{2}\right) \left(\langle \ell_{1} | \mathbf{r}_{0} \rangle - \langle \ell_{0} | \mathbf{r}_{1} \rangle \right) + \langle \ell_{0} | \mathbf{U}_{1} | \mathbf{r}_{0} \rangle|^{2} \\ &= |i\lambda_{0} \sin \left(\frac{\delta}{2}\right) \left(\langle \ell_{1} | \mathbf{r}_{0} \rangle - \langle \ell_{0} | \mathbf{r}_{1} \rangle \right) |^{2} + 2Re \left[i\lambda_{0} \sin \left(\frac{\delta}{2}\right) \left(\langle \ell_{1} | \mathbf{r}_{0} \rangle - \langle \ell_{0} | \mathbf{r}_{1} \rangle \right) \langle \mathbf{r}_{0} | \mathbf{U}_{1} | \ell_{0} \rangle \right] \\ &+ |\langle \ell_{0} | \mathbf{U}_{1} | \mathbf{r}_{0} \rangle|^{2} \\ &= \sin^{2} \left(\frac{\delta}{2}\right) |\langle \ell_{1} | \mathbf{r}_{0} \rangle - \langle \ell_{0} | \mathbf{r}_{1} \rangle|^{2} + 2Re \left[i\lambda_{0} \sin \left(\frac{\delta}{2}\right) \left(\langle \ell_{1} | \mathbf{r}_{0} \rangle - \langle \ell_{0} | \mathbf{u}_{1} \rangle \right) \langle \mathbf{r}_{0} | \mathbf{U}_{1} | \ell_{0} \rangle \right] + c^{2}\epsilon \\ &= c^{2}\epsilon + O \left(\delta^{2}\epsilon, \delta\epsilon \right) \\ &= c^{2}\epsilon + O \left(\delta \epsilon \right) \end{aligned}$$

Plugging these in to the formula for $\sin^2(2\omega)$,

$$\sin^{2}(2\omega) = \frac{4|\mathbf{U}_{lr}|^{2}}{|\mathbf{U}_{ll} - \mathbf{U}_{rr}|^{2} + 4|\mathbf{U}_{lr}|^{2}}$$

$$= \left(1 + \frac{|\mathbf{U}_{ll} - \mathbf{U}_{rr}|^{2}}{4|\mathbf{U}_{lr}|^{2}}\right)^{-1}$$

$$= \left(1 + \frac{4\sin^{2}\left(\frac{\delta}{2}\right) + O(\delta\epsilon, \epsilon^{2})}{4c^{2}\epsilon + O(\delta\epsilon)}\right)^{-1}$$

$$= \left(1 + \sin^{2}\left(\frac{\delta}{2}\right) \frac{1}{c^{2}\epsilon + O(\delta\epsilon)} + \frac{O(\delta\epsilon, \epsilon^{2})}{c^{2}\epsilon + O(\delta\epsilon)}\right)^{-1}$$

$$= \left(1 + \frac{\sin^{2}\left(\frac{\delta}{2}\right)}{c^{2}\epsilon} \frac{1}{1 + O(\delta)} + \frac{O(\delta, \epsilon)}{1 + O(\delta)}\right)^{-1}$$

$$= \left(1 + \frac{\sin^{2}\left(\frac{\delta}{2}\right)}{c^{2}\epsilon} + O\left(\frac{\delta^{3}}{\epsilon}\right) + O(\delta, \epsilon)\right)^{-1}$$

$$= \left(1 + \frac{\delta^{2}}{4c^{2}\epsilon} + O\left(\frac{\delta^{3}}{\epsilon}, \delta, \epsilon\right)\right)^{-1}$$

Since we have made no statement about how ϵ and δ are related, this cannot be further simplified. However, assuming that both variables are small, we can say that the largest term is $1 + \frac{\delta^2}{4c^2\epsilon}$.

Theorem. 5.5 There is a better than 50% chance of a successful search of the N edges of the hub vertex using the states $|\ell_0\rangle$ and $|\mathfrak{r}_0\rangle$ after $m = \left\lfloor \frac{\pi}{2c}\sqrt{N} \right\rfloor$ iterations of the time step operator, whenever

$$\delta < c\sqrt{\frac{2}{N}} \tag{56}$$

where δ is the difference in phase between the Left and Right eigenvalues, and $c = |\langle \mathfrak{r}_{o} | \mathbf{U} | \ell_{0} \rangle|$.

$$\begin{aligned} &Proof \text{ First, we find an expression for } P(m,t), \\ &P(m,t) \\ &= |\langle \mathbf{t}_0 | \mathbf{U}^m | \ell_0 \rangle|^2 \\ &= |(\sin(\omega) \langle V^+(\delta, \epsilon)| + \cos(\omega) \langle V^-(\delta, \epsilon)|) \mathbf{U}^m (\cos(\omega) | V^+(\delta, \epsilon) \rangle - \sin(\omega) | V^-(\delta, \epsilon) \rangle)|^2 \\ &+ O(\sqrt{\epsilon}, \delta) \\ &= |\sin(\omega) \cos(\omega) (\lambda^+)^m - \sin(\omega) \cos(\omega) (\lambda^-)^m|^2 + O(\sqrt{\epsilon}, \delta) \\ &= |\sin(\omega) \cos(\omega) e^{imc\sqrt{\epsilon-\epsilon_0}} - \sin(\omega) \cos(\omega) e^{-imc\sqrt{\epsilon-\epsilon_0}}|^2 + O(\sqrt{\epsilon}, \delta) \\ &= |\sin(\omega) \cos(\omega)|^2 \left| e^{imc\sqrt{\epsilon-\epsilon_0}} - e^{-imc\sqrt{\epsilon-\epsilon_0}} \right|^2 + O(\sqrt{\epsilon}, \delta) \\ &= |\sin(\omega) \cos(\omega)|^2 \left| e^{imc\sqrt{\epsilon-\epsilon_0}} - e^{-imc\sqrt{\epsilon-\epsilon_0}} \right|^2 + O(\sqrt{\epsilon}, \delta) \\ &= |\sin(\omega) \cos(\omega)|^2 \left| e^{imc\sqrt{(1+t)\epsilon}} - e^{-imc\sqrt{(1+t)\epsilon}} \right|^2 + O(\sqrt{\epsilon}, \delta) \\ &= |\sin^2(2\omega) \sin^2 \left(mc\sqrt{(1+t)\epsilon} \right) + O(\sqrt{\epsilon}, \delta) \\ &= \frac{1}{1+t} \sin^2 \left(mc\sqrt{(1+t)\epsilon} \right) + O(\sqrt{\epsilon}, \delta) \end{aligned}$$

Notice that this is not a function of ϵ , it is a function of $(1 + t)\epsilon$. This raises issues, because we may chose the wrong value of m. $m = \left\lfloor \frac{\pi}{2c\sqrt{\epsilon}} \right\rfloor$ is the value that would be chosen if the graph was assumed to be "correctly tuned", with $\delta = 0$. Knowing only that the "error" between the eigenvalues is small, this value of m is the natural choice.

 $m = \left\lfloor \frac{\pi}{2c\sqrt{(1+t)\epsilon}} \right\rfloor$ is the value of m that should be chosen if δ is known, and is being compensated for. That is, if the exact difference between the eigenvalues is known, then the number of iterations can be adjusted to give a slightly better chance of success.

Taking into account the difference between the eigenvalues, (1, 1)

$$P\left(\left\lfloor \frac{\pi}{2c\sqrt{(1+t)\epsilon}} \right\rfloor\right)$$

= $\frac{1}{1+t}\sin^2\left(\left\lceil \frac{\pi}{2c\sqrt{(1+t)\epsilon}} + O(1) \right\rceil c\sqrt{(1+t)\epsilon}\right) + O(\sqrt{\epsilon})$
= $\frac{1}{1+t}\sin^2\left(\frac{\pi}{2} + O\left(\sqrt{(1+t)\epsilon}\right)\right) + O(\sqrt{\epsilon})$
= $\frac{1}{1+t}\cos^2\left(O\left(\sqrt{(1+t)\epsilon}\right)\right) + O(\sqrt{\epsilon})$
= $\frac{1}{1+t} + O\left((1+t)\epsilon, \sqrt{\epsilon}\right)$
= $\frac{1}{1+t} + O\left(\sqrt{\epsilon}\right)$

And not taking into account the difference δ , but instead assuming that $\delta = 0$,

$$\begin{split} &P\left(\left\lfloor\frac{\pi}{2c\sqrt{\epsilon}}\right\rfloor\right)\\ &=\frac{1}{1+t}\sin^2\left(\left[\frac{\pi}{2c\sqrt{\epsilon}}+O(1)\right]c\sqrt{(1+t)\epsilon}\right)+O\left(\sqrt{\epsilon}\right)\\ &=\frac{1}{1+t}\sin^2\left(\frac{\pi}{2}\sqrt{1+t}+O\left(\sqrt{(1+t)\epsilon}\right)\right)+O\left(\sqrt{\epsilon}\right)\\ &=\frac{1}{1+t}\sin^2\left(\frac{\pi}{2}\sqrt{1+t}\right)+O\left(\sqrt{(1+t)\epsilon},\sqrt{\epsilon}\right)\\ &=\frac{1}{1+t}\sin^2\left(\frac{\pi}{2}\sqrt{1+t}\right)+O\left(\sqrt{\epsilon}\right)\\ &\frac{1}{2}\,<\,\frac{1}{1+t}\sin^2\left(\frac{\pi}{2}\sqrt{1+t}\right)\,\leq\,\frac{1}{1+t} \text{ over the interval } 0\,\leq\,t\,\leq\,\frac{1}{2}. \end{split}$$

 $\frac{1}{2} < \frac{1}{1+t}\sin^2\left(\frac{\pi}{2}\sqrt{1+t}\right) \le \frac{1}{1+t}$ over the interval $0 \le t \le \frac{1}{2}$. This condition can be rewritten,

$$\begin{split} t &\leq \frac{1}{2} \\ \Rightarrow \frac{\delta^2}{4c^2\epsilon} &\leq \frac{1}{2} \\ \Rightarrow \frac{\delta^2 N}{4c^2} &\leq \frac{1}{2} \\ \Rightarrow \delta^2 &\leq \frac{2c^2}{N} \\ \Rightarrow \delta &\leq c\sqrt{\frac{2}{N}} \\ \end{split}$$
This means that $P\left(\left\lfloor \frac{\pi}{2c}\sqrt{N} \right\rfloor\right) > \frac{1}{2}$ whenever $\delta < c\sqrt{\frac{2}{N}}$.



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