Dispersion Relations of Periodic Quantum Graphs

Alan Talmage
Washington University

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Abstract

We present methods of Kuchment and Post for calculating the dispersion relation of periodic quantum graphs and reformulate them in terms of a matrix-valued function on such graphs. We show how this leads to simpler methods for computing the dispersion relations for many periodic quantum graphs. We also reduce computing the dispersion relation for an undirected Cayley graph of a group of the form $G = H \times \mathbb{Z}^n$, where H is any finite graph together with a set of generators to finding the eigenvalues of the adjacency matrix of the undirected Cayley graph of H.

1 Introduction

Quantum graphs are of interest in a number of different fields of mathematics and physics. Primarily studied for their applications to crystal lattices ([1]), they are also used in quantum chaos ([3]), scattering ([4]), the Riemann hypothesis ([5]), and much more. In this paper we begin with the methods of [1], simplify the computations, and generalize them to more general classes of periodic quantum graphs.

Section 2 works through the computational methods of [1] and reformulates them in a simpler and more general way. Section 3 proves results that follow for graphs having certain symmetries. Section 4 shows how a certain set of Cayley graphs yield quantum graphs whose spectra are easy to compute. Section 5 gives examples of these computations applied to several specific graphs.

2 Computing the Dispersion Relation

In this section we present methods of Kuchment and Post from [1] to compute the dispersion relation of certain quantum graphs. The purpose of this section is to isolate the portion of their work that is relevant to this paper, and present it in a simplified format.

We begin by making the following assumptions:

1. G is an equilateral undirected metric graph with a finite fundamental domain M such that G can be obtained from M by translation by a group of translations isomorphic to some $\mathbb{Z}^n$.

2. G is a quantum graph under the Schrödinger Hamiltonian H with potential q and Neumann boundary conditions at each vertex v:

    (a) f is continuous at v

    (b) $\sum_{e \in E(v)} f'_e(v) = 0$, i.e. the flux of f through the vertex v is zero.

3. Each edge of G is assumed to have length 1, and is identified with the closed unit interval $[0, 1]$ (where the direction is assigned arbitrarily).

4. The potential q is required to satisfy $q(x) = q(1 - x)$ on each edge in G.

We now use the idea from [1] that the analysis of the spectrum of a quantum graph can be split into two essentially separate parts: the analysis on a single edge, which does not depend on the graph structure, and thus does not concern us here, and the analysis on the graph structure, which is independent of the potential (which is why we need only the symmetry condition of the potential here). Specifically, we can use the following result ([1], [2]):

Theorem 2.1. *The spectrum of H is the range of the dispersion relation $\theta \mapsto \lambda_j(\theta)$, where the $\lambda_j(\theta)$ are the points in the (purely discrete) spectrum of the Bloch Hamiltonian H^θ, which is obtained by restricting H to M and adding the cyclic boundary conditions*

$$u(x + p_1\overrightarrow{e_1} + p_2\overrightarrow{e_2} + \ldots + p_n\overrightarrow{e_n}) = e^{i(p_1\theta_1+\ldots+p_n\theta_n)}u(x)$$

where $\overrightarrow{e_1}, \ldots, \overrightarrow{e_n}$ are the translational symmetries of G.

We can now compute the dispersion relation of H by computing the spectrum of H^θ. Since the spectrum of H^θ is known to be purely discrete, this means we have to solve the eigenvalue problem

$$H^\theta u = \lambda u$$

It is known (see [1]) that on any edge, we can express any such u in terms of a basis φ_0, φ_1, which are linearly independent solutions of

$$-\varphi'' + q_0\varphi = \lambda\varphi$$

where q_0 is the restriction of the potential q to this edge, such that $\varphi_0(0) = 1$, $\varphi_0(1) = 0$, $\varphi_1(0) = 0$, and $\varphi_1(1) = 1$. The symmetry of the potential q_0 gives

$$\varphi_1'(1) = -\varphi_0'(0)$$

and

$$\varphi_0'(1) = -\varphi_1'(0)$$

We will now put a restriction on the structure of the graph under study to be able to prove our results. We require that we can choose a basis $\overrightarrow{e_1}, \overrightarrow{e_2}, \ldots, \overrightarrow{e_n}$ for the symmetry group of G such that M is only connected to its n translates $\overrightarrow{e_1}M, \ldots, \overrightarrow{e_n}M$. Unlike the previous assumptions, this is not necessary for the analysis. However, it defines the class of graphs which we can study here.

Let $v_1, v_2, \ldots, v_m$ be the vertices of M, let v_i^k be the vertex v_i translated by $\overrightarrow{e_k}$, and let a_{ij^k} be the edge connecting v_i to v_j^k, if it exists. For clarity, we will use the convention that $v_i^0 = v_i$, and that v_i^{-k} is the vertex v_i translated by $-\overrightarrow{e_k}$, and we define $\theta_{-k} = -\theta_k$. We can now express any solution u of the eigenvalue problem as follows: On each edge a_{ij^k},

$$u_{a_{ij^k}} = u(v_i)\varphi_0 + e^{i\theta_k} u(v_j)\varphi_1$$

Note that defining u in this way on each edge automatically satisfies the eigenvalue equation and the continuity condition at each vertex. We can now express the remaining Neumann vertex condition in terms of the values $u(v_1), u(v_2), \ldots, u(v_m)$. At vertex v_i, we have

$$\sum_{v_j^k \sim v_i} u'_{a_{ij^k}}(0) = 0$$

But

$$u'_{a_{ij^k}} = u(v_i)\varphi'_0 + e^{i\theta_k} u(v_j)\varphi'_1$$

so we have

$$0 = \sum_{v_j^k \sim v_i} u(v_i)\varphi'_0(0) + e^{i\theta_k} u(v_j)\varphi'_1(0) = \sum_{v_j^k \sim v_i} -u(v_i)\varphi'_1(1) + e^{i\theta_k} u(v_j)\varphi'_1(0)$$

We now define the quotient

$$\eta(\lambda) = \frac{\varphi'_1(1)}{\varphi'_1(0)}$$

Aside: As is shown in [1], the dispersion relation will differ from η by a constant factor. However, since η is the result that concerns us here, will will abuse the nomenclature mildly and refer to η as the dispersion relation.

Expressing the Neumann condition in terms of η yields

$$0 = \sum_{v_j^k \sim v_i} -u(v_i)\eta + e^{i\theta_k} u(v_j)$$

We now have a set of linear equations in terms of $u(v_1), \ldots, u(v_m)$. To solve the eigenvalue problem, η must make the determinant of the matrix of coefficients of these equations equal to zero. Let S be this matrix, and observe that $S = (s_{ij})$ is defined by

$$s_{ij} = -\delta_{ij} \deg(v_i)\eta + \sum_{v_i^k \sim v_j} e^{i\theta_k}$$

The dispersion relation η for any periodic quantum graph can now be computed by solving the equation

$$\det(S) = 0$$

3 Special Cases

First, let us make a few observations about the structure of S that will shed some light on certain types of periodic quantum graphs. The most immediate observation is that we can break S down as

$$S = T - \eta D$$

where $T = (t_{ij})$ is defined by

$$t_{ij} = \sum_{v_i^k \sim v_j} e^{i\theta_k}$$

and $D = (d_{ij})$ is the diagonal matrix defined by

$$d_{ij} = \delta_{ij} \deg(v_i)$$

This observation leads to a few special types of graphs whose dispersion relations will be easy to compute.

Theorem 3.1. *If all vertices of G have degree d, then the dispersion relation is given by $\eta = \frac{\lambda_T}{d}$, where λ_T is any eigenvalue of T.*

Proof. If all vertices of G have degree d, then $D = dI$, so

$$S = T - \eta dI$$

In this case, $\det(S) = 0$ reduces to

$$\det(T - \eta dI) = 0$$

which is equivalent to ηd being an eigenvalue of T. Thus in the case of a graph of constant degree, if λ_T is any eigenvalue of T, the values of η are

$$\eta = \frac{\lambda_T}{d}$$

□

Theorem 3.2. *If $G = M \times \mathbb{Z}^n$, and A is the adjacency matrix of M, then*

$$S = A + \left(\sum_{k=1}^{n} 2\cos\theta_k \right) I - \eta D$$

Proof. If $G = M \times \mathbb{Z}^n$, then $v_i^n \sim v_j \iff i = j$. Thus $T = R + A$, where

$$a_{ij} = \chi(v_i \sim v_j)$$

is the adjacency matrix of M, and R is diagonal with

$$r_{ii} = \sum_{k=1}^{n} e^{i\theta_k} + e^{-i\theta_k} = \sum_{k=1}^{n} 2\cos\theta_k$$

Thus we have

$$S = A + \left(\sum_{k=1}^{n} 2\cos\theta_k \right) I - \eta D$$

□

Theorem 3.3. *If $G = M \times \mathbb{Z}^n$ and every vertex of G has degree d, then*

$$S = \left(\sum_{k=1}^{n} 2\cos\theta_k - \eta d \right) I + A$$

and if λ_A is an eigenvalue of A,

$$\eta = \frac{1}{d} \left(\lambda_A + \sum_{k=1}^{n} 2\cos\theta_k \right)$$

Proof. This follows immediately from the two previous results. □

Specifically, this result states that a graph of this form has all branches of its dispersion relation differ only by adding a constant. This means that the intersection of any two branches will either be empty or consist of the entire branch. Note that this means that no graph of this form can have a conical singularity in its dispersion relation (a point that is a local minimum of one branch and a local maximum of another), as the hexagonal lattice is shown to have in [1].

4 Undirected Cayley Graphs

Before we compute η for specific graphs, we want to be able to catalog graphs in terms of their underlying structure more efficiently. One set of graphs whose underlying structure is easy to see is Cayley graphs, so we present the following result on the dispersion relation for periodic quantum graphs formed from Cayley graphs.

Theorem 4.1. *Let H be any finite group, together with a set E of generators, where E is closed under the operation $g \mapsto g^{-1}$. Let M be the undirected Cayley graph of H with these generators. Then the branches of the dispersion relation η for the Cayley graph of $G = H \times \mathbb{Z}^n$ with generating set consisting of E and the generators ± 1 in each copy of $\mathbb{Z}^n$ will be*

$$\eta = \frac{1}{d}\left(\lambda_H + \sum_{k=1}^{n} 2\cos\theta_k\right)$$

where λ_H is an eigenvalue of the adjacency matrix of M.

Proof. This follows directly from Theorem 3.3 and the fact that each vertex of a Cayley graph will have degree equal to the number of generators used. □

Note: The condition requiring the set of generators to be closed under taking inverses is necessary to obtain an undirected Cayley graph.

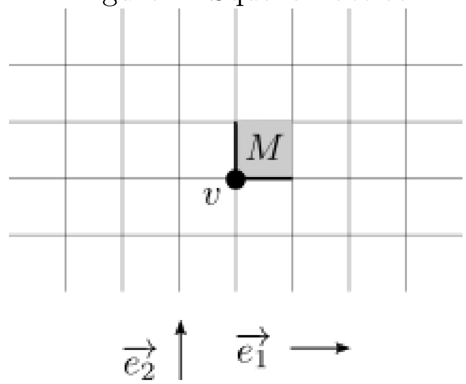
From the standpoint of someone interested in finding graphs with unique properties in their dispersion relations, this is a negative result in that it shows that the approach of looking at periodic Cayley graphs will only yield a certain type of dispersion relation.

5 Examples

We will now use these methods to compute η explicitly for some graphs. This shows how the methods are used, and also how they streamline the computational process (see for comparison the computation of η for the hexagonal lattice in [1]).

The square lattice ($\mathbb{Z}^2$):

Figure 1: Square Lattice



In this case, the fundamental domain M consists of a single point, so S is the 1×1 matrix

$$S = \left(e^{i\theta_1} + e^{-i\theta_1} + e^{i\theta_2} + e^{-i\theta_2} - 4\eta\right) = (2\cos(\theta_1) + 2\cos(\theta_2) - 4\eta)$$

Thus

$$\eta = \frac{\cos(\theta_1) + \cos(\theta_2)}{2}$$

Note that this is a case of Theorem 3.3.

The general cubical lattice ($\mathbb{Z}^n$):

Theorem 3.3 applies to the cubical lattice in any dimension, so we have

$$S = \left(\sum_{k=1}^{n} 2\cos(\theta_k) - (2n)\eta\right)$$

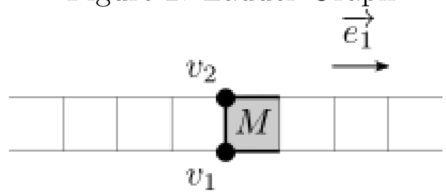
which gives

$$\eta = \frac{1}{n}\sum_{k=1}^{n} \cos(\theta_k)$$

The "ladder graph" ($\mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}$):

This graph is useful as an example of Theorem 3.3 which is more complicated than the square lattice, but is still easy enough to compute the spectrum by hand without it.

Figure 2: Ladder Graph



$$S = \begin{pmatrix} 2\cos(\theta) - 3\eta & 1 \\ 1 & 2\cos(\theta) - 3\eta \end{pmatrix}$$

$$\det(S) = (2\cos(\theta) - 3\eta)^2 - 1 = 0$$

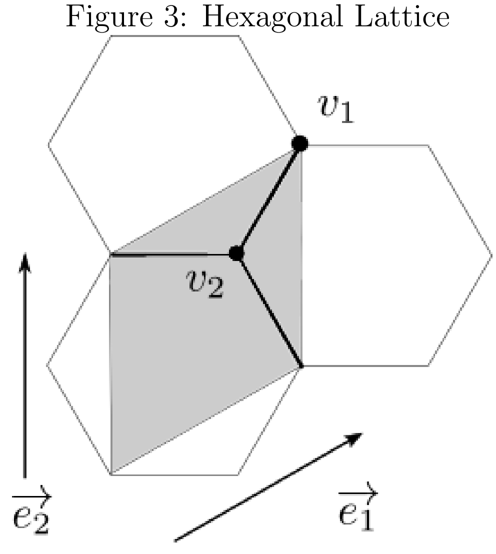
$$2\cos(\theta) - 3\eta = \pm 1$$

$$\eta = \frac{2\cos(\theta) \pm 1}{3}$$

The hexagonal lattice:

To show how the method of using the matrix S to compute η works even in cases not covered by Theorem 3.2, and to show that this method agrees with the method of [1], we consider the hexagonal lattice.

Figure 3: Hexagonal Lattice



$$S = \begin{pmatrix} -3\eta & 1 + e^{-i\theta_1} + e^{-i\theta_2} \\ 1 + e^{i\theta_1} + e^{i\theta_2} & -3\eta \end{pmatrix}$$

$$\det(S) = 9\eta^2 - (1 + e^{-i\theta_1} + e^{-i\theta_2})(1 + e^{i\theta_1} + e^{i\theta_2}) = 0$$

$$\eta = \pm\sqrt{\frac{1}{9}|1 + e^{i\theta_1} + e^{i\theta_2}|^2} = \pm\frac{1}{3}|1 + e^{i\theta_1} + e^{i\theta_2}|$$

which agrees with Lemma 3.1 of [1].

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