

# Quantum graphs via exercises

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**ABSTRACT.** Studying the spectral theory of Schrödinger operator on metric graphs (also known as “quantum graphs”) is advantageous on its own as well as to demonstrate key concepts of general spectral theory. There are some excellent references for this study such as a book by Berkolaiko and Kuchment (mathematically oriented book), a review by Gnutzmann and Smilansky (review with applications to theoretical physics), and lecture notes by Berkolaiko (elementary lecture notes). Here, we provide a set of questions and exercises which can accompany the reading of these references or an elementary course on quantum graphs. The exercises are taken from courses on quantum graphs which were taught by the authors.

## 1. Basic spectral theory of quantum graphs

### 1.1. $\delta$ -type vertex conditions.

**Background:** The most common vertex conditions of a graph are called Dirichlet and Neumann. Note that the Neumann conditions are also sometimes called Kirchhoff, standard or natural. Nevertheless, we stick to the name Neumann in this note.

For the following set of questions we consider a particle in a box described by the Schrödinger equation

$$-\frac{d^2 f(x)}{dx^2} + V(x)f(x) = k^2 f(x) \quad \text{for } x \in (-l_1, l_2), \quad (1)$$

where  $l_1 > 0$ ,  $l_2 > 0$  and  $V(x)$  is called the electric potential and can be taken for example in  $L^2([-l_1, l_2])$ . We employ here the Dirichlet boundary conditions  $f(-l_1) = 0 = f(l_2)$ , which physically mean that the particle is trapped in an infinite well, whose walls are at  $x = -l_1$  and  $x = l_2$ .

#### Questions:

1. In this question, we choose the potential in (1) to be  $V(x) = \alpha\delta(x)$ , where  $\alpha \in \mathbb{R}$  and  $\delta(x)$  is Dirac’s delta function. By doing so, we extend the original validity of equation (1), since the potential is now considered as a distribution and not merely a function. In order for the action of the  $\delta$  distribution to be well-defined, we must require that  $f$  is continuous at  $x = 0$  with  $f_0 := f(0^+) = f(0^-)$ .

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Show that any eigenfunction  $f$  in (1) satisfies the matching condition

$$\alpha f_0 = f'(0^+) - f'(0^-). \tag{2}$$

*Comment:* Note that the sign of  $\alpha$  determines whether the  $\delta$ -potential is attractive ( $\alpha < 0$ ), repulsive ( $\alpha > 0$ ) or vanishing ( $\alpha = 0$ ).

The relation (2) is called the  $\delta$ -type vertex condition. Indeed, in our example  $x = 0$  may be considered as a graph vertex whose degree is two. If the vertex under consideration is of degree higher than two, then this condition is generalized and takes the form

$$af_0 = \sum_e f|'_e(0), \tag{3}$$

where the sum is taken over all edges adjacent to the considered vertex, and in all the summands the derivative is taken to be directed towards the vertex. In addition, we always require the continuity of the function at the considered vertex, i.e., all adjacent edges agree in the value they obtain at the vertex, and this value equals  $f_0$ .

Note that the Dirichlet and Neumann conditions are obtained as special cases of the  $\delta$ -type vertex condition for some particular values of the parameter ( $\alpha = 0$  for Neumann and  $\alpha \rightarrow \infty$  for Dirichlet).

2. Next, we find the spectrum of the problem above: the interval  $[-l_1, l_2]$  with Dirichlet conditions at the end points,

$$f(-l_1) = f(l_2) = 0, \tag{4}$$

and a  $\delta$ -type vertex condition at  $x = 0$ ,

$$f(0^+) = f(0^-) \tag{5}$$

$$\alpha f_0 = f'(0^+) - f'(0^-). \tag{6}$$

- (a) Show that the non-negative eigenvalues  $k^2$  of the one-dimensional Laplacian,  $-\frac{d^2}{dx^2}$ , with the vertex conditions (4),(5),(6) are given as the zeros of the following function

$$\zeta_\alpha(k) = \alpha + k \cot(kl_1) + k \cot(kl_2). \tag{7}$$

We call such a function, whose zeros provide the graph's eigenvalues, a secular function.

- (b) For an irrational lengths ratio ( $l_1/l_2 \notin \mathbb{Q}$ ) show that there cannot be any eigenfunctions with  $f_0 = 0$ .

Conclude that the poles of the secular function, (7), cannot belong to the spectrum.

- (c) Show that  $\zeta_\alpha(k)$  has only single poles if  $l_1/l_2 \notin \mathbb{Q}$ .

However, if  $l_1/l_2 \in \mathbb{Q}$  there are single and double poles of the secular function. Locate them and show that the double poles belong to the spectrum, while the single poles do not belong to it. This justifies the need of regularization of the secular function

$$\tilde{\zeta}_\alpha(k) = \zeta_\alpha(k) \sin(kl_1) \sin(kl_2). \tag{8}$$

Namely, the zeros of the regularized secular function,  $\tilde{\zeta}_\alpha(k)$ , correspond to the Laplacian eigenvalues (irrespective to the value of  $l_1/l_2$ ).

- (d) Consider an attractive  $\delta$ -potential ( $\alpha < 0$ ). Are there negative eigenvalues among the eigenvalues of the Schrödinger operator? Under what conditions and how many?
- (e) Show that if  $\alpha = 0$  in the problem above, this is equivalent to solving the eigenvalue problem of the Laplacian on the interval,  $[-l_1, l_2]$  with Dirichlet conditions at the boundaries, but with no additional condition at  $x = 0$ .

Conclude that this is the case in general. Namely for any graph, a vertex of degree two with Neumann vertex conditions ( $\alpha = 0$ ) is superfluous, i.e. one can erase the vertex and join the two incident edges to a one single edge such that the lengths add up.

*Hint:* You can read about this in [5, section 2.2]

*Comment:* Equation (7) introduces a secular function which possess poles. The regularization process provides the secular function (8) with no poles. This latter secular function is the more standard one. There is an explicit formula for it (with no need of regularization), which makes it also more convenient to use in proofs and analysis on quantum graphs. See more about that in Section 1.4.

**1.2. From the interval to the star graph.**

**Background:** Consider a star graph which consists of one central vertex which is connected to all other  $V - 1$  vertices. We will enumerate the vertices as  $i = 0, 1, \dots, E$  where  $E = V - 1$  is the total number of edges. The central vertex is privileged to have the index  $i = 0$ . The lengths of the edges are  $\{l_{01}, \dots, l_{0E}\}$ . The restrictions of a function  $f$  to the edges are denoted by  $\{f_{01}, \dots, f_{0E}\}$ . The coordinates along the edges are chosen according to the convention that  $x_{0i} = 0$  at the central vertex and  $x_{0i} = l_{0i}$  at the vertex  $i$ . We will assume Dirichlet boundary conditions at the vertices  $i = 1, \dots, E$ , and a repulsive vertex potential whose strength is  $\alpha_0 \geq 0$  at the central vertex. Namely, the vertex conditions at the boundary vertices are  $\delta$ -type vertex conditions:

$$\forall 1 \leq i \leq E ; f_{0i}(l_{0i}) = 0,$$

and the vertex conditions at the central vertex are

$$\forall 1 \leq i < j \leq E ; f_{0i}(0) = f_{0j}(0) \equiv f_0$$

and

$$\sum_{i=1}^E f'_{0i}(0) = \alpha_0 f_0.$$

Note that the problem considered in section 1.1 is a special case of the problem considered here with  $E = 2$ .

**Questions:**

- 3.** Show that a possible secular function for the graph is

$$\zeta(k) = \frac{\alpha_0}{k} + \sum_{i=1}^E \cot(kl_{0i}). \tag{9}$$

Namely, show that zeros of this function are all eigenvalues of the graph (note that there is not necessarily one to one correspondence - see the next question).

Note that the secular function, (7) in the previous question is a special case of the one above (with  $E = 2$ ).

4. What is the weakest assumption you need to assume in order to have a one to one correspondence between the zeros of the secular function (9) and the graph's eigenvalues?
5. Show that under the assumption you got in the previous question, the graph's spectrum is non degenerate. Namely, that each eigenvalue appears with multiplicity one.
6. Under the same assumption as in questions 4 and 5 show the following interlacing properties:
  - (a) The Dirichlet spectrum ( $\alpha_0 \rightarrow \infty$ ) of the star graph interlaces with the spectrum of the same star graph but with a Neumann vertex condition at the central point ( $\alpha_0 = 0$ ).
  - (b) For any positive value of  $\alpha_0$  the  $n$ -th eigenvalue of the star graph is bounded from below by the  $n$ -th eigenvalue for  $\alpha_0 = 0$  and from above by the  $n$ -th eigenvalue of the Dirichlet spectrum.
  - (c) Similarly to the previous question, which interlacing property holds for the  $n$ -th eigenvalue of the star graph with a negative value of  $\alpha_0$ ?

*Comment:* See [7, theorem 3.1.8] for a general statement on eigenvalue interlacing for quantum graphs.
7. Assume now that  $\alpha = 0$  (Neumann vertex conditions at the center). Consider all star graphs with any number of edges  $E$  and any positive edge lengths  $\{l_{01}, \dots, l_{0E}\}$ , such that the total length of the edges,  $L = \sum_{i=1}^E l_{0i}$  is fixed.
  - (a) What is the supremum of the first eigenvalue among all choices of values for  $E$  and  $\{l_{01}, \dots, l_{0E}\}$  (under the constraint above)? Is this supremum attained (i.e., is it a maximum)?
  - (b) What is the infimum? Is it attained?

*Hint:* The answer can be found in [9].

*Comment:* Similar questions of eigenvalue optimization on graphs and bounds on the eigenvalues are discussed in the recent works [1, 2, 6, 14]

8. *This is a numerical exercise!* Choose any value for the number of edges,  $E$ , and any values for the edge lengths  $\{l_{01}, \dots, l_{0E}\}$ . Plot the secular function for your choice and find its thirteen first zeros.

### 1.3. Secular function - first approach.

#### Question:

9. Consider an arbitrary quantum graph with  $V$  vertices and  $E$  edges. Assume there is an edge connecting vertices 1 and 2 and write the restriction of a function  $f$  to this edge as

$$f_{12}(x_{12}) = A \cos kx_{12} + B \sin kx_{12}.$$

Similarly, write

$$f_{ij}(x_{ij}) = \frac{f_j \sin(kx_{ij}) + f_i \sin(k(l_{ij} - x_{ij}))}{\sin kl_{ij}},$$

for the restriction of  $f$  to an edge connecting vertices  $i, j$  ( $i < j$ ). Using this, obtain a set of homogeneous equations for the coefficients  $A, B, f_i$  ( $i = 1, 2, \dots, V$ ) and derive a secular function that does not have poles at the Dirichlet spectrum of the edge  $e = (1, 2)$ .

*Hint:* There is more than one solution to this - one may also reduce the number of equations (and variables) easily to  $V$  (the number of vertices) without re-introducing poles.

**1.4. Secular function - scattering approach.**

**Background:** One may express the restriction of the eigenfunction to the edge connecting vertices  $i, j$  by

$$f_{ij}(x_{ij}) = a_{ij}^{\text{in}} e^{-ikx_{ij}} + a_{ij}^{\text{out}} e^{ikx_{ij}} \quad (10)$$

where  $a_{ij}^{\text{in}}$  and  $a_{ij}^{\text{out}}$  are some coefficients. If the eigenfunction belongs to the eigenvalue  $k^2$ , we can always choose values to those coefficients, such that expression (10) holds.

For a given vertex  $i$  of degree  $d_i$  we have  $d_i$  coefficients of the type  $a_{ij}^{\text{in}}$  and another  $d_i$  coefficients of the type  $a_{ij}^{\text{out}}$ . Let us collect these into  $d_i$ -dimensional vectors  $\vec{a}^{(i),\text{out}}, \vec{a}^{(i),\text{in}} \in \mathbb{C}^{d_i}$ . The vertex conditions on the vertex  $i$  allow us to express the  $\vec{a}^{(i),\text{out}}$  as a linear transform of the  $\vec{a}^{(i),\text{in}}$

$$\vec{a}^{(i),\text{out}} = \sigma^{(i)}(k) \vec{a}^{(i),\text{in}}. \quad (11)$$

The components of the vectors  $\vec{a}^{(i),\text{out}}, \vec{a}^{(i),\text{in}} \in \mathbb{C}^{d_i}$  have the meaning of incoming and outgoing wave amplitudes;  $\sigma^{(i)}(k)$  is a unitary matrix of size  $d_i \times d_i$  and is called the vertex scattering matrix.

To each quantum graph with  $E$  edges one may associate a unitary matrix  $U(k)$  of dimension  $2E \times 2E$ , known as the graph's *quantum map* or (*discrete*) *quantum evolution operator* that describes the connectivity of the graph, the matching conditions at the vertices and the eigenvalue spectrum of the graph. In Question 12 the quantum map is derived explicitly for a particular graph. The same procedure may be applied to other quantum graphs to find the quantum map.

**Questions:**

- 10. Show that the  $\delta$ -type vertex conditions (i.e., continuity of the eigenfunction at a vertex  $i$  of degree  $d_i$  and ,  $\alpha_i f_i = \sum_{j \in V_i} f'_{ij}(0)$ ) are equivalent to the vertex scattering matrix

$$\sigma_{jj'}^{(i)}(k) = \frac{2}{d_i + i \frac{\alpha_i}{k}} - \delta_{jj'} = \begin{cases} \frac{2}{d_i + i \frac{\alpha_i}{k}} & j \neq j' \\ \frac{2}{d_i + i \frac{\alpha_i}{k}} - 1 & j = j' \end{cases}. \quad (12)$$

- 11. Show that the vertex scattering matrix

$$\sigma^{(i)} = -\mathbf{1}_{d_i} + \frac{2}{v_i + i \frac{\alpha_i}{k}} \mathbb{E}_{d_i}$$

is unitary. Here,  $\mathbb{E}_{d_i}$  is the full  $d_i \times d_i$  matrix with all matrix elements equal to one. You may use  $\mathbb{E}_{d_i}^2 = d_i \mathbb{E}_{v_i}$  and  $\mathbb{E}^* = \mathbb{E}$  where  $\mathbb{E}^*$  denotes the hermitian conjugate of  $\mathbb{E}$ .

- 12. Consider a star graph which consists of three edges. The central vertex is denoted by 0 and supplied with Neumann vertex conditions. The boundary vertices are denoted by 1, 2, 3 and are supplied with Neumann, Dirichlet, Dirichlet conditions, correspondingly. These notations and the edge lengths are shown in Fig. 1.

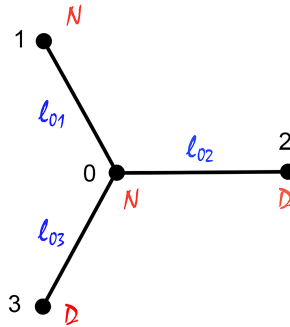


FIGURE 1. A star graph.

In this question you will explicitly build up the quantum map of the graph above by following the given sequence of instructions.

- Write explicitly the scattering matrices,  $\sigma^{(i)}$ , which correspond to each of the vertices 0, 1, 2, 3. You may compare with equation (12) above.
- Write the equation (11) for each of the vertices. Use the explicit matrices which you have found in the previous section and write the components of the vectors  $\vec{a}^{(i),\text{in}}$  and  $\vec{a}^{(i),\text{out}}$  with explicit indices in each case (i.e., write  $a_0^{(2),\text{in}}$ ,  $a_3^{(0),\text{out}}$ , etc.).
- Write (explicitly again) the “big” scattering matrix  $S(k)$  to fit the following set of equations

$$\vec{a}^{\text{out}} = S(k)\vec{a}^{\text{in}},$$

where

$$\vec{a}^{\text{in}} = \begin{pmatrix} a_{10}^{\text{in}} \\ a_{01}^{\text{in}} \\ a_{20}^{\text{in}} \\ a_{02}^{\text{in}} \\ a_{30}^{\text{in}} \\ a_{03}^{\text{in}} \end{pmatrix} \quad \text{and} \quad \vec{a}^{\text{out}} = \begin{pmatrix} a_{01}^{\text{out}} \\ a_{10}^{\text{out}} \\ a_{02}^{\text{out}} \\ a_{20}^{\text{out}} \\ a_{03}^{\text{out}} \\ a_{30}^{\text{out}} \end{pmatrix}.$$

Remember that  $S(k)$  merely consists of the different components of the single vertex scattering matrices  $\sigma^{(i)}(k)$  and zero elements for edges that are not connected to each other. Pay special care to the order of the entries of the vectors above.

- Write the matrix  $T(k)$  such that it fits into the set of equations

$$\vec{a}^{\text{in}} = T(k)\vec{a}^{\text{out}}$$

with  $\vec{a}^{\text{in}}$  and  $\vec{a}^{\text{out}}$  as given above.

*Hint: you may use the fact  $f_{ij}(x) = f_{ji}(l_{ji} - x)$*

- A few tips to check yourself (no need to calculate, just in order to verify your answer).
  - The matrix  $S(k)$  should be  $k$ -independent.
  - The matrix  $S(k)$  should be unitary.
  - The matrix  $T(k)$  should be diagonal.

If you did all the above correctly, the quantum evolution operator is obtained by matrix multiplication of the two matrices,  $U(k) = T(k)S(k)$ .

13. Consider a star graph with Neumann vertex conditions at the central vertex  $i = 0$  and Dirichlet vertex conditions at the boundary vertices  $i = 1, 2, \dots, E$ . Derive the quantum evolution map  $U(k)$  and show that the secular function can be reduced to the form

$$\zeta(k) = \det(\mathbf{1}_{2E} - U(k)) = \det(\mathbf{1}_E + \tilde{T}(2k)\boldsymbol{\sigma}^{(0)}),$$

where  $\boldsymbol{\sigma}^{(0)}$  is the central vertex scattering matrix and  $\tilde{T}(k)$  is a diagonal  $E \times E$  matrix,  $T(k)_{ee'} = \delta_{ee'}e^{ikl_e}$ . You can gain a good intuition for the solution of this question from your solution to the previous question.

14. Show that the following secular function is real

$$\tilde{\zeta}(k) = \sqrt{\det(S^*(k)T^*(k))} \det(\mathbf{1}_{2E} - U(k)). \tag{13}$$

Remember that  $U(k) = T(k)S(k)$  and use the unitarity of  $T(k)$  and  $S(k)$ .

*Comment:* The secular function  $\tilde{\zeta}(k)$  above may even be differentiable in  $k$ , if the complex branch of the square root is appropriately chosen.

## 2. Trace formula and periodic orbits

### 2.1. The trace formula for the spectrum of a unitary matrix.

**Background:** Consider an  $M \times M$  unitary matrix  $U$  with unimodular eigenvalues  $e^{i\theta_\ell}$  for  $\ell = 1, \dots, M$ . One may extend the spectrum of eigenphases  $\theta_\ell$  periodically beyond the interval  $0 \leq \theta < 2\pi$ . The extended spectrum then consists of the numbers

$$\theta_{\ell,n} = \theta_\ell + n2\pi \quad n \in \mathbb{Z}.$$

Assume that  $\theta_\ell \neq 0$  and  $\theta \neq \theta_{\ell,n}$  is real.

**Question:**

15. Consider the spectral counting function

$$N(\theta) = \sum_{n=0}^{\infty} \sum_{\ell=1}^M \vartheta(\theta - \theta_\ell - n2\pi),$$

where  $\vartheta$  is the Heaviside step function. Show that one may write it as the following trace formula.

$$N(\theta) = \frac{M\theta}{2\pi} - \frac{1}{\pi} \text{Im} \log \det(1 - U) + \frac{1}{\pi} \text{Im} \log \det(1 - e^{-i\theta}U).$$

*Comment:* The definition of the spectral counting function may be extended to  $\theta = \theta_{n,\ell}$  such that both expressions (the defining expression and the trace formula) remain consistent. For this one replaces the last term in the trace formula by the limit

$$\frac{1}{\pi} \text{Im} \log \det(1 - e^{-i\theta}U) \mapsto \lim_{\epsilon \rightarrow 0^+} \frac{1}{\pi} \text{Im} \log \det(1 - e^{-i\theta - \epsilon}U)$$

and sets  $\vartheta(0) = 1/2$ . Replacing  $U \mapsto e^{-\epsilon}U$  and considering the limit  $\epsilon \rightarrow 0^+$  also helps to regularize certain expansions that may come up in the proof of the trace formula because the trace formula for finite  $\epsilon > 0$  does not have any singularities for  $\theta$  on the real line.

We strongly recommend plotting the regularized expression for  $N(k)$  with a (small) positive value for  $\epsilon$  for a given unitary matrix  $U$  (which may be chosen diagonal).

*Hint:* There are several ways to perform the derivation. One interesting derivation is based on Poisson summation. This method requires  $\epsilon$ -regularization as mentioned in the comment above.

(a) Write the spectral counting function as

$$N(\theta) = \sum_{n=-\infty}^{\infty} \sum_{\ell=1}^M \vartheta(\theta - \theta_\ell - n2\pi) \vartheta(\theta_\ell + n2\pi).$$

(b) The Poisson summation formula for a smooth function  $f(x)$  which decays sufficiently fast for  $|x| \rightarrow \infty$  (so that all sums and integrals converge absolutely) reads

$$\sum_{n=-\infty}^{\infty} f(n) = \sum_{\nu=-\infty}^{\infty} \int_{-\infty}^{\infty} e^{2\pi i \nu x} f(x) dx .$$

We want to apply it to  $f(x) = \sum_{\ell=1}^M \vartheta(\theta - \theta_\ell - 2\pi x) \vartheta(\theta_\ell + 2\pi x)$  which is not smooth. In this case the Poisson sum is not absolutely convergent but may be regularized by introducing an additional factor  $e^{-\epsilon|\nu|}$  and taking the limit  $\epsilon \rightarrow 0^+$ .

(c) While using the formula above, evaluate separately the  $\nu = 0$  term from the other terms.

(d) Compare this term by term to the expansion

$$\log \det (1 - e^{-i\theta} U) = \text{tr} \log (1 - e^{-i\theta} U) = - \lim_{\epsilon \rightarrow 0^+} \sum_{n=1}^{\infty} \frac{1}{n} e^{-in\theta - n\epsilon} \text{tr} U^n$$

(or the complex conjugate version) in order to perform the sum over  $\nu$  in the Poisson summation.

*Comment:* You may compare this to the trace formula of a quantum graph. Do this by showing that the above formula is equivalent to the one obtained in [11] for quantum graphs if all the edge lengths of the graph are the same. Note that the derivation of the trace formula in this reference uses a different (more general) method.

### 2.2. Periodic orbits.

**Background:** Consider a quantum graph with  $E$  edges of lengths  $l_e$  ( $e = 1, \dots, E$ ) with Neumann matching conditions and let  $U(k)$  be the unitary,  $k$ -dependent  $2E \times 2E$  matrix

$$U(k)_{\alpha'\alpha} = e^{ikl_{\alpha'}} S_{\alpha'\alpha}$$

where  $S_{\alpha'\alpha}$  is the scattering amplitude from the directed edge  $\alpha$  to directed edge  $\alpha'$ .

Note that  $S_{\alpha'\alpha} = 0$  unless the end vertex of the directed edge  $\alpha$  coincides with the start of  $\alpha'$  – one then says that  $\alpha'$  follows  $\alpha$ .

We have

$$\text{tr} U(k)^n = \sum_{\alpha_1, \dots, \alpha_n=1}^{2E} e^{ikl_{\alpha_1}} S_{\alpha_1 \alpha_n} e^{ikl_{\alpha_n}} S_{\alpha_n \alpha_{n-1}} \dots e^{ikl_{\alpha_3}} S_{\alpha_3 \alpha_2} e^{ikl_{\alpha_2}} S_{\alpha_2 \alpha_1} ,$$



where  $\{\alpha_1, \dots, \alpha_n\}$  is a set of  $n$  directed edges of the graph. In the sum above, each term is of the form  $A_\gamma e^{ik\ell_\gamma}$

$$A_\gamma = S_{\alpha_1\alpha_n} S_{\alpha_n\alpha_{n-1}} \dots S_{\alpha_2\alpha_1}$$

$$\ell_\gamma = l_{\alpha_n} + l_{\alpha_{n-1}} + \dots + l_1$$

Here  $\gamma = (\alpha_1, \dots, \alpha_n)$  is a fixed set of summation indices which corresponds to a sequence of directed edges.

Note that  $A_\gamma \neq 0$  only if the edge  $\alpha_{j+1}$  follows the edge  $\alpha_j$  in the graph, for  $j = 1, \dots, n$  (in this context  $\alpha_{n+1} \equiv \alpha_1$ ) – i.e. only if  $\gamma$  is a closed trajectory on the graph. For such a trajectory,  $\ell_\gamma$  is its total length, i.e., the sum of its edge lengths. By definition, the **length spectrum** of the graph is the set of all lengths  $\{\ell_\gamma\}$  of closed trajectories. You can see a few examples of such closed trajectories in Fig. 2.

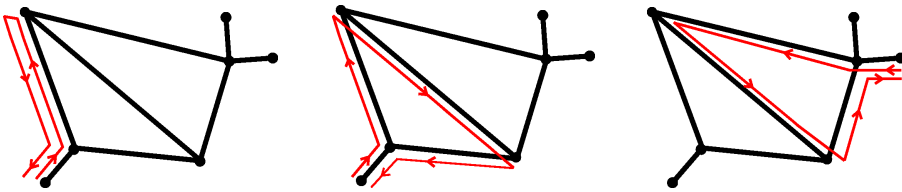


FIGURE 2. Three examples of closed trajectories on a graph.

We now list a few observations and definitions related to periodic orbits.

- Note that any cyclic permutation,  $\gamma'$ , of the indices in the trajectory  $\gamma$  gives a different closed trajectory with the same contribution  $A_{\gamma'} = A_\gamma$  and  $\ell_{\gamma'} = \ell_\gamma$ .
- The equivalence class  $\bar{\gamma} = \overline{\alpha_1 \dots \alpha_n}$  that contains all cyclic permutations of a given closed trajectory  $\gamma = (\alpha_1, \dots, \alpha_n)$  is called a **periodic orbit** with **period**  $n$  on the graph.
- The periodic orbit  $\bar{\gamma} = \overline{\alpha_1 \dots \alpha_n}$  is a **primitive periodic orbit** of primitive period  $n$  if the sequence of indices  $\alpha_1, \dots, \alpha_n$  is not a repetition of a shorter sequence.

All the closed trajectories in Fig. 2 represent primitive periodic orbits.

- If  $\bar{\gamma}$  is a periodic orbit with period  $n$ , then there exists a unique primitive periodic orbit  $\bar{\gamma}_p$  with **primitive period**  $n_p$  such that  $\bar{\gamma}$  is a repetition of  $\bar{\gamma}_p$  and  $n = rn_p$ . Here  $r \geq 1$  is the integer **repetition number** of  $\bar{\gamma}$  and  $n_p$  the **primitive period** of  $\bar{\gamma}$ .
- If  $r = 1$  then  $\bar{\gamma} = \bar{\gamma}_p$  and  $\bar{\gamma}$  is primitive.
- We write  $\bar{\gamma} = \bar{\gamma}_p^r$  for the  $r$ -th repetition of the primitive orbit  $\bar{\gamma}_p$ .

*Comment:* The trace formula of the spectral counting function may be expressed in terms of an infinite sum over the graph's periodic orbits. To answer the following questions, you should read more about that, for example in [7, section 3.7.4] or [11, section 5.2].

**Questions:**

16. Consider the dihedral graphs as given in Fig. 3

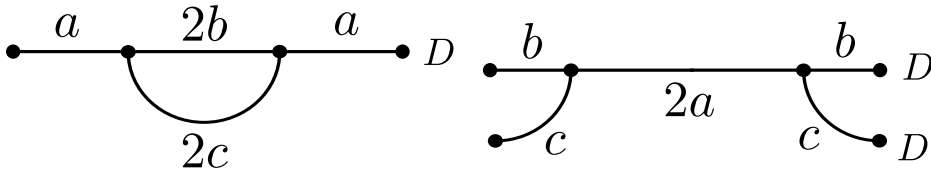


FIGURE 3. Two isospectral quantum graphs. Their edge lengths are indicated by the parameters  $a, b, c$ . The vertices marked with ‘D’ have Dirichlet conditions and all other vertices have Neumann conditions.

It is known that those graphs are isospectral [3]. Solve the following ‘paradox’:

The isospectrality of those graphs means that their spectral counting functions are equal. Hence, the periodic orbit expansions of those counting functions are the same. Therefore, both graphs should have the same set of periodic orbits. Nevertheless, the graph on the left has a periodic orbit of length  $2a$ , whereas the graph on the right does not have such an orbit. How is this possible?

17. This question concerns the tetrahedron graph, i.e. the complete Neumann graph with  $V = 4$  vertices.

- (a) *Warm-up:* Choose two periodic orbits on the graph, such that one of them is primitive and the second is some repetition of the first. For each of those periodic orbits,  $\gamma$ , evaluate the following quantities:
  - (i) The period  $n$  of the orbit.
  - (ii) The length  $\ell_\gamma$  of the orbit (expressed in terms of the graph edge lengths).
  - (iii) The coefficient  $A_\gamma$  which corresponds to the orbit in the periodic orbits expansion (write the explicit number).
  - (iv) The primitive period  $n_p$  and the repetition number  $r$ ?
- (b) Assume that all bond lengths are incommensurate. Go over all periodic orbits of period  $n = 5$  and write their contribution to the length spectrum  $\sigma_\ell$  (expressed in terms of the graph edge lengths). What are the corresponding quantum amplitudes  $A_\gamma$  of those orbits?
- (c) Now assume that all edge lengths are equal. How does your answer to the previous question change?
- (d) The connectivity matrix  $C$  of a simple graph with  $V$  vertices is the real symmetric  $V \times V$  matrix with entries

$$C_{i,j} = \begin{cases} 1 & \text{vertices } i \text{ and } j \text{ are connected by an edge,} \\ 0 & \text{else.} \end{cases}$$

Note that for simple graphs there are no loops, i.e. edges that connect a vertex to itself, so  $\forall i, C_{ii} = 0$ . The connectivity matrix may be used to count the number of trajectories that connect the vertices  $i$  and  $j$  in  $n$  steps – this number is just  $[C^n]_{ji}$ .

Consider the connectivity matrix of the tetrahedron,  $C_{ij} = 1 - \delta_{ij}$ . Show that as  $n \rightarrow \infty$ ,  $[C^n]_{ji} \sim ce^{\alpha n}$  and find  $\alpha$ .

*Hint:* diagonalize  $C$ .

*Comment:* The last question shows that there is an exponential growth in the number of orbits on the graph. This holds in particular for periodic orbits and makes it difficult to use the periodic orbit expansion of the trace formula for spectral computations.

18. In the previous question we counted the number of trajectories between two vertices via the (vertex) connectivity matrix. An alternative approach is based on the  $2E \times 2E$  edge adjacency matrix  $\mathcal{B}$  whose indices correspond to the directed edges where

$$\mathcal{B}_{\alpha\alpha'} = \begin{cases} 1 & \text{if } \alpha \text{ follows } \alpha', \\ 0 & \text{else.} \end{cases}$$

The main difference is that  $[\mathcal{B}^n]_{\alpha\alpha'}$  counts the number of trajectories that start on the directed edge  $\alpha'$  and end after  $n$  steps on the directed edge  $\alpha$ . Both approaches can also be used to count the number of periodic orbits via the traces. We will explore this here for the edge connectivity matrix  $\mathcal{B}$ .

- (a) Show that  $\frac{1}{n} \text{tr } \mathcal{B}^n = \sum_{\gamma: n_\gamma=n} \frac{1}{r_\gamma}$  where the sum is over all periodic orbits of period  $n$ . Conclude that if  $n$  is a prime number then  $\frac{1}{n} \text{tr } \mathcal{B}^n$  is the number of periodic orbits of period  $n$ .
- (b) Derive an expression for the number of periodic orbits of period  $n$  in terms of traces of powers of  $\mathcal{B}$  for
- (i.)  $n = p^j$  where  $p$  is a prime number and  $j \geq 2$  an integer, and
  - (ii.)  $n = p_1 p_2$  where  $p_1$  and  $p_2$  are prime numbers.

Make an educated guess for the general expression when  $n$  has the prime number decomposition  $n = \prod_m p_m^{j_m}$  where  $j_m \geq 0$  is the multiplicity of the  $m$ -th prime.

19. This question demonstrates that given some lengths of periodic orbits of an unknown graph, one can reconstruct the graph.

- (a) Find the graph with the following properties:
- (i.) the total length (sum of all edge lengths) is  $1\frac{5}{6}$ ;
  - (ii.) the lengths of all periodic orbits whose length is not greater than 5 are given by the list

$$\frac{2}{3}, 1\frac{1}{3}, 2, 2\frac{2}{3}, 3, 3\frac{1}{3}, 3\frac{2}{3}, 4, 4\frac{1}{3}, 4\frac{2}{3}, 5.$$

Draw the graph and indicate the edge lengths on the drawing.

- (b) Find the graph with the following properties:
- (i.) the total length is  $5\frac{13}{15}$ ;
  - (ii.) the lengths of all periodic orbits whose length is not greater than 5 are given by the list

$$2, 2\frac{1}{3}, 2\frac{1}{6}, 2\frac{2}{5}, 4, 4\frac{1}{6}, 4\frac{1}{3}, 4\frac{1}{3}, 4\frac{2}{5}, 4\frac{1}{2}, 4\frac{17}{30}, 4\frac{2}{3}, 4\frac{11}{15}, 4\frac{4}{5}, 5.$$

Note that there are two different periodic orbits of length  $4\frac{1}{3}$ . Also, any number which appears only once in the list above indicates that there is exactly one periodic orbit of that length.

What is the graph this time?

- (c) Try to think how to construct a general algorithm for finding the graph out of knowing its total metric length and lengths of all of its periodic orbits.

Assume that the graph is simple (no loops and no multiple edges) and that its edge lengths are incommensurate.

*Hint:* What is the shortest periodic orbit of a graph?

*Another hint:* The answer can be found in [12].

**2.3. The constant term of the trace formula.**

**Background:** The spectral counting function of a quantum graph is

$$N(k) := |\{\lambda \in \mathbb{R} \text{ is an eigenvalue} : \lambda < k^2\}|,$$

where eigenvalues are counted with their multiplicity. One of the forms of the trace formula for the spectral counting function is

$$N(k) = N_0 + \frac{\mathcal{L}}{\pi}k - \lim_{\epsilon \rightarrow 0} \frac{1}{\pi} \text{Im} \log \tilde{\zeta}(k + i\epsilon), \tag{14}$$

where  $\tilde{\zeta}(k)$  is the real secular function given in (13), and  $N_0$  is a constant term. The last two terms in (14) equal to the number of real zeros of  $\tilde{\zeta}$  with absolute value smaller than  $k$ . Those zeros are in one to one correspondence with the graph eigenvalues (including multiplicity), with the exception of  $k = 0$ . The value of  $\tilde{\zeta}$  at  $k = 0$  does not correspond to the multiplicity of the zero eigenvalue and this ‘mismatch’ is compensated by the constant term  $N_0$  in (14).

The expression for this term was originally derived in [16, lemma 1],[17]. Other works related to this subject are [10, 13]. Further reading in [7, section 3.7] and [11, section 5] is recommended.

**Question:**

- 20.** In the following question we derive the value of  $N_0$  for a Neumann graph (all vertex matching conditions are of Neumann aka Kirchhoff type). Initially, assume that the graph has a single connected component. Let  $\vec{E}$  be the space of directed edges on the graph (this space is of dimension  $2E$ , where  $E$  is the number of edges).

- (a) Let  $\omega : \vec{E} \rightarrow \mathbb{C}$  such that

$$\forall (i, j) \in \vec{E} \quad \omega(i, j) = -\omega(j, i)$$

and

$$\forall i \quad \sum_{j \sim i} \omega(i, j) = 0,$$

where  $j \sim i$  means that the vertex  $j$  is adjacent to the vertex  $i$ . All such functions  $\omega : \vec{E} \rightarrow \mathbb{C}$  form a vector space (over  $\mathbb{C}$ ). Prove that the dimension of this space is  $\beta := E - V + 1$ .

*Hint:* Start by considering a tree graph.

- (b) Let  $\vec{a}^{in} \in \mathbb{C}^{2E}$  with entries denoted by  $a_j^{(i),in}$  (for  $i \sim j$ ), such that the following is satisfied

$$\forall i \sim j, i \sim k \quad a_j^{(i),in} + a_i^{(j),in} = a_k^{(i),in} + a_i^{(k),in}$$

and

$$\forall i \quad \sum_{j \sim i} \left( -a_j^{(i),in} + a_i^{(j),in} \right) = 0.$$

Prove that the dimension of the vector space which contains all such solutions  $\vec{a}^{in} \in \mathbb{C}^{2E}$  is  $\beta + 1$ .

- (c) Note that you have shown  $\dim \ker(\mathbf{1} - S) = \beta + 1$ , which implies  $N_0 = \frac{1-\beta}{2}$ . Show that for a Neumann graph with  $C$  (disjoint) connected components, the constant term of the trace formula (14) is  $N_0 = \frac{C-\beta}{2}$ . You can use the generalized definition of  $\beta$ , which is  $\beta := E - V + C$  (this value can be obtained by summing over all the  $\beta$ 's of the different components).

### 3. Further topics

#### 3.1. Quantum to classical correspondence for quantum graphs.

**Background:** In this question we study the classical dynamics of a quantum graph. This will help us to understand in what sense the classical dynamics that corresponds to a quantum graph is 'chaotic'. Remember that the quantum evolution map,  $U(k)$ , contains amplitudes for scattering processes to go from one directed edge to another. We define a corresponding classical map,  $M$ , by replacing the amplitudes  $U(k)_{\alpha\alpha'}$  by

$$M_{\alpha\alpha'} = |U(k)_{\alpha\alpha'}|^2 = |S_{\alpha\alpha'}|^2.$$

Hence,  $M$  is a matrix of dimensions  $2E \times 2E$ , which contains the probabilities for the scattering events.

**Question:**

- 21.** By following the steps below prove that the matrix  $M$  defines a Markov process on the set of directed edges with the stated additional properties.
- (a) Prove that the matrix  $M$  is a *bi-stochastic (doubly stochastic) matrix*. Namely, prove that

$$\sum_{\alpha=1}^{2E} M_{\alpha\alpha'} = \sum_{\alpha'=1}^{2E} M_{\alpha\alpha'} = 1.$$

- (b) Use the bi-stochastic property to verify that the following definition of a Markov process on the directed edges of the graph is well-defined. Let  $P_\alpha(n)$  be the probability to find a particle on the directed edge  $\alpha$ , at some (discrete) time  $n$ . We can then define the probabilities to find the particle on the directed edge  $\alpha$ , at time  $n + 1$ , by

$$P_\alpha(n + 1) = \sum_{\alpha'} M_{\alpha\alpha'} P_{\alpha'}(n)$$

or, in short  $P(n + 1) = MP(n)$ . In particular show that if  $P(n)$  satisfies  $\sum_\alpha P_\alpha(n) = 1$  and  $P(n)_\alpha \geq 0$ , then  $P(n + 1)$  satisfies the same properties. That is if  $P(n)$  is a probability vector then  $P(n + 1)$  is a probability vector.

**Further background:** We next consider the equilibration properties of the Markov process  $P(n + 1) = MP(n)$ . Let  $P^{\text{inv}} = \frac{1}{2E}$  be the equi-distributed probability vector on the graph. For any quantum graph this is an invariant probability vector, i.e.

$$M P^{\text{inv}} = P^{\text{inv}}$$

The classical dynamics which corresponds to a quantum graph is chaotic in the following sense: The Markov process on the graph is called *ergodic* if

$$\lim_{n \rightarrow \infty} \frac{1}{n} \sum_{m=1}^n P(m) = P^{\text{inv}}$$

for every initial probability vector  $P(0)$ . We call a graph dynamically connected<sup>1</sup>, if for any two directed edges  $\alpha$  and  $\alpha'$  there is an integer  $n > 0$  such that  $(M^n)_{\alpha\alpha'} \neq 0$  (i.e one can get from one directed edge to another with a non-vanishing probability in a finite number of steps). Every dynamically connected graph is ergodic. Most graphs are also *mixing* which is the stronger property

$$\lim_{n \rightarrow \infty} P(n) = P^{\text{inv}}$$

for every initial probability vector  $P(0)$ .

**Question:**

**22.** In this question we will characterize ergodicity and mixing in terms of the eigenvalue spectrum of the bi-stochastic matrix  $M$ . The results apply to any bi-stochastic Markov process on a directed graph whether or not there is a corresponding quantum graph such that  $M_{\alpha\alpha'} = |U(k)_{\alpha\alpha'}|^2$  in terms of the quantum map.

- (a) Prove that all the eigenvalues of  $M$  are either on the unit circle or inside it. Namely, if we denote the set of eigenvalues by  $\{\lambda_i\}$ , then  $\forall i; |\lambda_i| \leq 1$ .
- (b) We know that  $M$  has at least one eigenvalue which equals 1 (the corresponding eigenvector is  $P^{\text{inv}}$ ). Let us denote this eigenvalue by  $\lambda_1$  ( $\lambda_1 = 1$ ). Prove that if  $\min_{2 \leq i \leq 2E} (1 - |\lambda_i|) > 0$  then the graph is mixing.

*Hint:* It might be useful to prove the convergence property using the vectors  $L_1$ -norm.

- (c) Using the notation above ( $\lambda_1=1$ ), prove that if  $\min_{2 \leq i \leq 2E} (|1 - \lambda_i|) > 0$  then the graph is ergodic.

*Hint:* Again, use the  $L_1$ -norm .

*Comment:* Note that the conditions above are consistent with the trivial fact that mixing is a stronger notion than ergodicity (namely, that every mixing system is also ergodic which follows directly from the definition).

The quantity  $\Delta := \min_{2 \leq i \leq 2E} (|1 - \lambda_i|)$  is called the spectral gap and it determines the convergence rate of  $\lim_{n \rightarrow \infty} \frac{1}{n} \sum_{m=1}^n P(m)$  (the greater the gap, the quicker is the convergence).

Similarly,  $\tilde{\Delta} := \min_{2 \leq i \leq 2E} (1 - |\lambda_i|)$  determines the convergence rate of  $\lim_{n \rightarrow \infty} P(n)$ .

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<sup>1</sup>In the literature a matrix  $M$  with this property is sometimes called irreducible.

### 3.2. The quadratic form.

**Background:** Consider a quantum graph with the edge and vertex sets,  $\mathcal{E}$  and  $\mathcal{V}$ . We take the operator to be the Laplacian with  $\delta$ -type vertex conditions (see (3)). The quadratic form of this operator is:

$$h[f] := \sum_{e \in \mathcal{E}} \int_0^{l_e} \frac{df}{dx_e} \overline{\frac{dg}{dx_e}} dx_e + \sum_{v \in \mathcal{V}; \alpha_v \neq \infty} \alpha_v f(v) \overline{g(v)},$$

where  $\alpha_v$  is the coupling coefficient of the  $\delta$ -type vertex condition at vertex  $v$ , and  $\alpha_v = \infty$  indicates Dirichlet vertex conditions. The length of the edge  $e$  is denoted by  $l_e$ .

The domain  $D(h)$  of this quadratic form consists of all functions  $f$  on the metric graph that satisfy the following three conditions:

- (i.) for each edge  $e$  the restriction  $f|_e$  belongs to the Sobolov space  $H^1([0, l_e])$ ,
- (ii.)  $f$  is continuous at each vertex, and
- (iii.)  $f(v) = 0$  at each vertex  $v$  for which  $\alpha_v = \infty$ .

The quadratic form is useful for variational characterization of the spectrum. More on this topic is found in [7, section 1.4.3].

**Questions:**

**23.** Consider a Schrödinger operator with a bounded non-negative potential ( $V \geq 0$ ) on a quantum graph,  $H\psi = -\psi'' + V\psi$ . Show that the spectrum of this operator is non-negative if all the vertex conditions are of  $\delta$ -type with non-negative coupling coefficients (i.e.,  $\forall v \in \mathcal{V}; \alpha_v \geq 0$ ). *Hint:* You need to modify the quadratic form given above to fit the case of Schrödinger operator with a potential.

**24.** Prove the following statements:

- (a) Let  $\lambda = \lambda(\alpha)$  be a simple eigenvalue of a graph with  $\delta$ -type vertex condition at a certain vertex  $v$  with the coupling coefficient  $\alpha \neq \infty$ . The operator on this graph is just the Laplacian (no potential). Then

$$\frac{d\lambda}{d\alpha} = |f(v)|^2.$$

- (b) Now, re-parameterize the  $\delta$ -type vertex condition at  $v$  as:

$$\zeta \sum_{e \in E_v} \frac{df}{dx_e}(v) = -f(v),$$

with  $E_v$  denoting the set of edges adjacent to  $v$ . This parametrization allows Dirichlet condition ( $\zeta = 0$ ) and excludes Neumann condition ( $\zeta = \infty$ ). Show that if the simple eigenvalue is now given by  $\lambda = \lambda(\zeta)$  then the derivative is

$$\frac{d\lambda}{d\zeta} = \left| \sum_{e \in E_v} \frac{df}{dx_e}(v) \right|^2.$$

*Hint:* The answer is given in [7, proposition 3.1.6]

### 3.3. From quantum graphs to discrete graphs.

#### Question:

**25.** In this question we consider the spectral connection between quantum graphs and discrete graphs.

- (a) Consider an arbitrary quantum graph with  $V$  vertices and  $E$  edges. Assume that Neumann conditions are imposed at all vertices and that all edges are of the same length,  $l$ . Use the following representation for an eigenfunction with eigenvalue  $k^2$  on the edge  $(i, j)$

$$f_{ij}(x_{ij}) = \frac{f_j \sin(kx_{ij}) + f_i \sin(k(l - x_{ij}))}{\sin(kl)}$$

and the Neumann conditions to obtain a set of  $V$  homogeneous equations for the variables  $f_i$  ( $i = 1, 2, \dots, V$ ).

- (b) Denote by  $\vec{f}$  the vector whose entries are all the  $f_i$  variables. Assume that  $\sin(kl) \neq 0$  and manipulate the linear set of equations you got in the previous section to have the following form

$$A \vec{f} = \cos(kl) \vec{f}.$$

What is the matrix  $A$ ? Note that this matrix describes the underlying discrete graph and this establishes a spectral connection between the discrete and the quantum graph.

- (c) Denote by  $\{\lambda_i\}_{i=1}^V$  the eigenvalues of  $A$ . Express the  $k$ -eigenvalues of the quantum graph (remember that there are infinitely many of those) in terms of the eigenvalues of  $A$ . Are all the eigenvalues of the quantum graph can be obtained in this way? If so, prove it, or otherwise, point on the eigenvalues which are not obtained in this way.

*Comment:* Further reading on the spectral connection between discrete and quantum graphs may be found in [4, 8, 13, 15, 19]. The most general derivation of this connection, treating electric and magnetic potentials as well as  $\delta$ -type vertex conditions appears in [18].

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