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# A relation between the bond scattering matrix and the spectral counting function for quantum graphs

Holger Schanz

ABSTRACT. For finite quantum graphs with standard boundary conditions (continuity and current conservation at the vertices) we derive a simple identity relating the eigenphases of the bond scattering matrix at some given energy and the spectral counting function of the Hamiltonian at the same energy. Using this relation it is possible to compute the counting function without knowledge of the spectrum. Our result may be applied to speed up the numerical calculation of eigenenergies in particular in situations where the level repulsion is weak (e. g. quantum graphs with localized eigenstates).

## 1. Introduction

One important reason why quantum graphs are very convenient and popular model systems is their numerical simplicity. For example, the energy eigenvalues of the Schrödinger operator on a quantum graph can be found by solving a secular equation in the form

$$\det(A(k_n)) = 0 \qquad (n = 1, 2, \dots)\,, \tag{1.1}$$

where $A(k)$ is a finite matrix which is easy to construct. There are various ways to choose this matrix, and the three most important versions have been given by Kottos and Smilansky [**1**]. Namely, one can set

(1) $A_h = h$, where $h$ has a dimension equal to the number of vertices of the graph, $\dim(h) = V$. The matrix $h$ is found when

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the boundary conditions are expressed as a set of linear equations for the amplitudes at the vertices. Thus, for an eigenenergy the vector $|\varphi_n\rangle$ with $h(k_n)\,|\varphi_n\rangle = |0\rangle$ gives the values of the wave function on the vertices (up to normalization).

(2) $A_S = I - S(k)$, where $S(k)$ is the bond scattering matrix with a dimension equal to the number of directed bonds on the graph, $\dim(S) = 2B$. The vector $|a_n\rangle$ solving $S(k_n)\,|a_n\rangle = |a_n\rangle$ gives the amplitudes of the partial waves emanating from the vertices.

(3) $A_{\tilde{S}} = I - \tilde{S}(k)$ where $\tilde{S}$ is the scattering matrix of the graph when it is turned into an auxiliary open system by attaching one or more semi-infinite leads. Its dimension $\dim(\tilde{S}) \geq 1$ is equal to the number of leads and the eigenvectors with eigenvalue one give the amplitude of the eigenstates at the points where the leads are attached.

On first sight the bond scattering matrix may seem to be the least favorable of the above options since its dimension is largest. However, it has properties which can make up for this drawback. For example, the elements of the bond scattering matrix are explicitly known while the calculation of $\tilde{S}(k)$ involves the inversion of $I - S(k)$ [**2**]. In comparison with the vertex matrix $h(k)$, the bond scattering matrix has the advantage that it does not rely on the continuity of the wave function across the vertices and is also applicable to graphs with the more general boundary conditions described in [**3**]. Even for graphs with standard (mixed) boundary conditions [**4**] the vertex matrix is numerically not very convenient since it has as a function of $k$ either poles or spurious zeroes (solutions of Eq. (1.1) which do not correspond to an eigenstate of the graph) [**1**]. Finally, as we shall show in this contribution, the bond scattering matrix has an important numerical advantage which is related to the algorithm for solving Eq. (1.1).

The typical strategy for finding the roots of a highly nonlinear equation such as Eq. (1.1) has two steps: First one tries to find an estimate for a solution. This could be an interval in which a sign change of (the real part of) the secular function occurs, or simply a value where the modulus of this function is relatively small. In the second step one can use iterative methods to improve the accuracy of the solution (or to reject it if the initial guess was wrong). Once a sign change has been detected, it is, for sufficiently well-behaved functions, not a problem to converge to a solution in a few iterations. However, locating a suitable initial guess can be a problem if one needs to be sure that all eigenvalues are found. Then this step requires to compute the secular

function on a grid for which the spacing between neighboring points is much lower than the average distance between eigenvalues. The reason is that eigenvalues can be almost degenerate even if there are no symmetries allowing for exact level crossings. So either one wastes a lot of computer time with a grid that is much too dense, or one wastes a lot of human time searching for missing eigenvalues and filling in the gaps.

We will show how this problem can be avoided if the secular function is based on the bond scattering matrix. The point is that it is possible to calculate directly from the bond scattering matrix $S$ at wave number $k$ the counting function (integrated density of states)

$$N(k) = \{\#n : 0 \leq k_n \leq k\}\,, \tag{1.2}$$

which counts the number of eigenvalues up to $k$. More precisely, we will give in Eq. (3.24) below an identity

$$N(k) = N(\{\theta_\lambda(0)\}, \{\theta_\lambda(k)\}, k) \tag{1.3}$$

which expresses the counting function in terms of the eigenphases $\theta_\lambda$ of the bond scattering matrix at wave numbers 0 and $k$ without any reference to the actual eigenvalues $k_n$. As the function (1.3) involves explicit knowledge of the eigenphases of $S(k)$, it can be calculated only numerically in non-trivial situations. With its help it is possible to perform the root searching for Eq. (1.1) with arbitrarily large grid size without losing any eigenvalues. It is also possible to calculate directly an eigenvalue with given number $m$ without prior calculation of all $k_n < k_m$. Finally, in some statistical applications such as the calculation of the number variance of the energy levels [**5**] it is actually sufficient to know how many levels are in a given energy interval. Then Eq. (1.3) enables one to avoid the calculation of eigenvalues altogether.

In this paper we will construct the function in Eq. (1.3) for the Schrödinger operator on a connected graph with standard (mixed) boundary conditions on all vertices, i.e., we require that the wave function is continuous across all vertices. We begin in the following Section 2 by compiling a few relevant definitions and results from the literature. Section 3 contains the derivation of our main result. Some numerical data will be shown in Section 4, and the application of Eq. (1.3) in the numerical determination of eigenvalues will be discussed. Finally, Section 5 contains some concluding remarks.

## 2. Definitions and notations

Although we essentially follow the definitions given in [**1**] we briefly repeat the formalism in order to be self-contained, and in order to introduce our notation.

*The graph and its eigenstates.* We consider a graph with $V$ vertices which are connected by $B$ undirected bonds. Multiple connections between vertices and loops from a vertex back to itself are allowed. It is assumed that the graph is connected. Each bond $b$ is equivalent to a pair of directed bonds, $b = (d, \hat{d})$. We will use the notation $\alpha(d)$ and $\omega(d)$ to refer to the initial and the final vertex of the directed bond $d$. Thus we have $\alpha(d) = \omega(\hat{d})$, and the valency of a vertex $l$ is given by

$$v_l = \sum_{d=1}^{2B} \delta_{l,\alpha(d)} = \sum_{d=1}^{2B} \delta_{l,\omega(d)} \,. \tag{2.1}$$

The bond lengths are $L_b = L_d = L_{\hat{d}} > 0$ and the total length of the graph is

$$L = \sum_{b=1}^{B} L_b = \frac{1}{2} \sum_{d=1}^{2B} L_d \,. \tag{2.2}$$

With every directed bond $d$ comes a coordinate $x_d \in [0, L_d]$ measuring the distance from the vertex $\alpha(d)$ along the bond $b$ such that $x_d$ and $x_{\hat{d}} = L_d - x_d$ denote the same point on $b$. We study the scaled Schrödinger equation

$$\forall b: \qquad (\Delta + k^2)\psi(x_d) = 0 \tag{2.3}$$

($k = \sqrt{2mE/\hbar^2}$) with the most general boundary conditions compatible with continuity and current conservation at the vertices,

$$\forall i, d \text{ with } \alpha(d) = i: \qquad \psi(x_d = 0) = \phi_i \tag{2.4}$$

and

$$\forall i: \qquad \sum_d \delta_{i,\alpha(d)} \left.\frac{d\psi}{dx_d}\right|_{x_d=0} = \lambda_i \phi_i \qquad (\lambda_i \in [0, \infty]) \,. \tag{2.5}$$

Following [**1**] we distinguish (i) Neumann boundary conditions ($\lambda_i = 0$), (ii) mixed b.c. ($0 < \lambda_i < \infty$) and (iii) Dirichlet b.c. ($\lambda_i = \infty$). Mixed b.c. reduce to Neumann and Dirichlet for $k \to \infty$ and $k \to 0$, respectively. For $k > 0$ the solutions of Eqs. (2.3)-(2.5) have the form

$$\psi_n(x_d) = A_{n,d} \exp(ik_n x_d) + A_{n,\hat{d}} \exp(ik_n x_{\hat{d}}) \,, \tag{2.6}$$

where the $A_{n,d}$ are complex constants which depend on the boundary conditions. The case $k = 0$ will be treated separately in Section 3.

*The bond scattering matrix.* The bond scattering matrix of the graph is defined by

$$S(k) = T(k)\, D(k)\,, \tag{2.7}$$

where $S$, $T$ and $D$ are unitary matrices of dimension $2B$. $T$ is given by

$$\begin{aligned} T_{dd'} &= \delta_{\alpha(d),\,\omega(d')} \left( \frac{2k}{v_{\alpha(d)} k + i\lambda_{\alpha(d)}} - \delta_{\hat{d},d'} \right) \\ &= \delta_{\alpha(d),\,\omega(d')} \left( \frac{1 + e^{-i\omega_{\alpha(d)}}}{v_{\alpha(d)}} - \delta_{\hat{d},d'} \right) \end{aligned} \tag{2.8}$$

with

$$\omega_i(k) = 2 \arctan \frac{\lambda_i}{v_i k}\,. \tag{2.9}$$

This reduces to $\omega_i = 0$ and

$$T^{(\mathrm{Neu})}_{dd'} = \delta_{\alpha(d),\,\omega(d')}\, (2 v^{-1}_{\alpha(d)} - \delta_{\hat{d},d'}) \tag{2.10}$$

for Neumann boundary conditions. $D(k) = \mathrm{diag}[\exp(ikL_d)]$ is a diagonal matrix which contains the phases accumulated along the bonds,

$$D_{dd'}(k) = \exp(ikL_d)\, \delta_{dd'}\,. \tag{2.11}$$

We have $D_{dd'}(0) = I$ and thus $S(0) = T(0)$.

For any given $k$, the bond scattering matrix $S(k)$ can be diagonalized so that

$$S\,|a_\lambda\rangle = z_\lambda\,|a_\lambda\rangle \qquad (\lambda = 1, \ldots, 2B)\,. \tag{2.12}$$

$z_\lambda(k)$ are the unimodular eigenvalues of $S(k)$ and $|a_\lambda(k)\rangle$ the corresponding eigenvectors. Their components will be denoted by $a_{\lambda,d}$ and are normalized according to

$$\sum_d |a_{\lambda,d}|^2 = 1\,. \tag{2.13}$$

We define two types of eigenphases

$$z_\lambda(k) = e^{i\theta_\lambda(k)} = e^{i\tilde{\theta}_\lambda(k)}\,, \tag{2.14}$$

namely

$$-\pi \le \theta_\lambda < +\pi \tag{2.15}$$

and

$$\tilde{\theta}_\lambda(k) = 2\pi m_\lambda(k) + \theta_\lambda(k)\,, \tag{2.16}$$

where $m_\lambda(k)$ is an integer which is chosen such that (i) all $\tilde{\theta}_\lambda(k)$ are continuous as a function of $k$ and (ii) $m_\lambda(0) = 0$. We will assume that the eigenphases are ordered, i.e., $\tilde{\theta}_\lambda \le \tilde{\theta}_{\lambda'}$ for $\lambda \le \lambda'$. Note that the

eigenphases $\theta_\lambda(k)$ can be obtained from a single diagonalization of $S$ at wave number $k$ while this is not the case for $\tilde{\theta}_\lambda(k)$.

The convention Eq. (2.15) has been adopted because it is numerically convenient to have the solutions $\theta_\lambda = 0$ inside the domain of $\theta$ rather than at its ends. For a different choice also our final result Eq. (3.24) below will take a different form.

## 3. The spectral counting function

*Counting function and bond scattering eigenphases.* Let us recall the result of Kottos and Smilansky [**1**] on the relation between the bond scattering matrix Eq. (2.7) and the spectrum of the graph. They showed that $k_n$ is in the spectrum if and only if $S(k_n)$ has an eigenphase $\theta_\lambda(k_n) = 0$, so that $k_n$ is a solution of the secular equation $\det(I - S(k_n)) = 0$. More precisely, from every eigenvector of the bond scattering matrix $|a_\lambda(k_n)\rangle$ with $\theta_\lambda(k_n) = 0$ and $k_n > 0$ one can construct an eigenstate of the Hamiltonian on the graph. This state is given by Eq. (2.6) with constants that are equal to the components of $|a_\lambda\rangle$ up to an overall normalization factor, $A_{n,d} = c\, a_{\lambda,d}(k_n)$. As a consequence of this result we have the identity

$$N(k) = N(0) + \int_\varepsilon^{k+\varepsilon} dk \sum_{\lambda=1}^{2B} \delta(\theta_\lambda)\, \theta'_\lambda(k) \qquad (\varepsilon \to +0)\,. \tag{3.1}$$

It is our goal to get rid of the integration in Eq. (3.1) and to express the counting function in terms of the eigenphases at the limits of integration, 0 and $k$.

*The ground state for mixed b.c.* Special care must be taken at $k = 0$. In general, $S(k = 0)$ has eigenvectors with $\theta_\lambda(0) = 0$ which do not correspond to eigenstates of the graph. They have the property that $a_{\lambda,d} = -a_{\lambda,\hat{d}}$ such that the wave function Eq. (2.6) vanishes everywhere. To understand this in detail we consider Eq. (2.5) and note that for $k = 0$ the wave function must be linear on each bond

$$\forall d: \qquad \psi(x_d) = \phi_{\alpha(d)} + \frac{\phi_{\omega(d)} - \phi_{\alpha(d)}}{L_d}\, x_d\,. \tag{3.2}$$

As mentioned above we restrict the discussion to connected graphs. Then the only solution to this set of equations is the constant ground state for Neumann b.c., $\psi(x_d) = L^{-1/2}$, which corresponds to a constant eigenvector $a_{\lambda_0,d} = 1/\sqrt{2B}$ of the bond scattering matrix. If $\lambda_i > 0$ for some vertex $i$ this state would violate the boundary conditions and also a non-constant piecewise linear solution cannot exist due to the following argument. For such a state there must be one vertex $i$ where

(i) the wave function is minimal[1] ($\forall j: \ \phi_i \leq \phi_j$) and (ii) for at least one vertex $j$ which is connected to $i$ the strict inequality $\phi_i < \phi_j$ holds (otherwise the wave function would be constant). Consequently the sum of derivatives on the r.h.s. of Eq. (2.5) is positive and this equation implies (besides $\lambda_i > 0$) that the *minimal* value of the wave function is *positive*, $\phi_i > 0$. With analoguous reasoning we find that the *maximal* value of the wave function is *negative*. The obvious contradiction rules out any non-constant eigenstates at $k = 0$ and thus we can conclude that $N(0) = 1$ for Neumann b.c. and $N(0) = 0$ otherwise.

*The eigenphases are increasing functions.* As a next step we will show that the eigenvalues of $S(k)$ move clockwise around the unit circle as $k$ increases. This follows from standard first order perturbation theory. We write

$$S(k+\delta k) = S(k) + \frac{dS}{dk}\delta k + O(\delta k^2)\,, \tag{3.3}$$

$$z(k+\delta k) = z(k) + \frac{dz}{dk}\delta k + O(\delta k^2)\,, \tag{3.4}$$

$$|a_\lambda(k+\delta k)\rangle = |a_\lambda(k)\rangle + O(\delta k)\,, \tag{3.5}$$

substitute into Eq. (2.12) keeping only terms of order $\delta k$ and find the well-known result

$$\frac{dz_\lambda}{dk} = \langle a_\lambda|\frac{dS}{dk}|a_\lambda\rangle \tag{3.6}$$

which is equivalent to

$$\frac{d\tilde{\theta}_\lambda}{dk} \ = \ \frac{1}{iz_\lambda}\,\langle a_\lambda|\frac{dS}{dk}|a_\lambda\rangle\,. \tag{3.7}$$

In the case of degenerate eigenphases this remains valid if the $|a_\lambda\rangle$ are chosen as a suitable orthonormal system. For the derivative of $S$ we have

$$\begin{aligned}\frac{dS}{dk} &= \frac{dT}{dk}D + T\frac{dD}{dk} \\ &= \frac{dT}{dk}D + i\,S(k)\,\mathrm{diag}(L_d)\end{aligned} \tag{3.8}$$

[1]For mixed b.c. the wave function can be chosen real. Alternatively, for the sake of this argument, it suffices to consider its real part only.

and from Eq. (3.7)

$$\begin{aligned}\frac{d\tilde{\theta}_\lambda}{dk} &= -i\,\langle a_\lambda|\frac{dT}{dk}D\,S^\dagger|a_\lambda\rangle - i\langle a_\lambda|S^\dagger\, iS\,\mathrm{diag}(L_d)|a_\lambda\rangle \\ &= \langle a_\lambda|\frac{1}{i}\frac{dT}{dk}\,T^\dagger|a_\lambda\rangle + \langle a_\lambda|\mathrm{diag}(L_d)|a_\lambda\rangle\,. \qquad (3.9)\end{aligned}$$

It is obvious that the second term is positive since $L_d > 0$. For Neumann or Dirichlet b.c. the first term vanishes as $T$ does not depend on $k$, and for mixed b.c. we will now show that also the first term is positive. We have

$$\frac{dT_{dd'}}{dk} = \delta_{\alpha(d),\,\omega(d')}\,\frac{1}{iv_{\alpha(d)}}\frac{d\omega_{\alpha(d)}}{dk}\,e^{-i\omega_{\alpha(d)}} \qquad (3.10)$$

and

$$\begin{aligned}\left(\frac{1}{i}\frac{dT}{dk}T^\dagger\right)_{dd''} &= \sum_{d'}\frac{1}{i}\frac{dT_{dd'}}{dk}T^*_{d''d'} \\ &= \sum_{d'}\frac{1}{i}\left[\delta_{\alpha(d),\,\omega(d')}\frac{1}{iv_{\alpha(d)}}\frac{d\omega_{\alpha(d)}}{dk}\,e^{-i\omega_{\alpha(d)}}\right] \\ &\qquad\times\left[\delta_{\alpha(d''),\,\omega(d')}\left(\frac{1+e^{+i\omega_{\alpha(d'')}}}{v_{\alpha(d'')}} - \delta_{\hat{d}'',d'}\right)\right] \\ &= -\delta_{\alpha(d),\alpha(d'')}\frac{1}{v_{\alpha(d)}}\frac{d\omega_{\alpha(d)}}{dk}\,e^{-i\omega_{\alpha(d)}} \\ &\qquad\times\sum_{d'}\delta_{\alpha(d),\,\omega(d')}\left(\frac{1+e^{+i\omega_{\alpha(d)}}}{v_{\alpha(d)}} - \delta_{\hat{d}'',d'}\right) \\ &= -\delta_{\alpha(d),\alpha(d'')}\frac{1}{v_{\alpha(d)}}\frac{d\omega_{\alpha(d)}}{dk}\,e^{-i\omega_{\alpha(d)}}\left(v_{\alpha(d)}\frac{1+e^{+i\omega_{\alpha(d)}}}{v_{\alpha(d)}} - 1\right) \\ &= -\delta_{\alpha(d),\alpha(d'')}\frac{1}{v_{\alpha(d)}}\frac{d\omega_{\alpha(d)}}{dk}\,. \qquad (3.11)\end{aligned}$$

In evaluating the sum we have used Eq. (2.1). Coming back to Eq. (3.9), we have now

$$\begin{aligned}\frac{d\tilde{\theta}_\lambda}{dk} &= -\sum_{dd'}a^*_{\lambda,d'}a_{\lambda,d}\,\delta_{\alpha(d),\alpha(d')}\frac{1}{v_{\alpha(d)}}\frac{d\omega_{\alpha(d)}}{dk} + \sum_d |a_{\lambda,d}|^2\,L_d \\ &= -\sum_{i=1}^{V}\frac{1}{v_i}\frac{d\omega_i}{dk}\sum_{dd'}\delta_{\alpha(d),i}\delta_{\alpha(d'),i}a^*_{\lambda,d'}a_{\lambda,d} + \sum_d |a_{\lambda,d}|^2\,L_d \\ &= -\sum_{i=1}^{V}\frac{1}{v_i}\frac{d\omega_i}{dk}\left|\sum_d \delta_{\alpha(d),i}a_{\lambda,d}\right|^2 + \sum_d |a_{\lambda,d}|^2\,L_d\,. \qquad (3.12)\end{aligned}$$

According to Eq. (2.9), $\omega_i(k)$ is a monotonically decreasing function of $k$ for mixed b.c. while it is constant for Neumann and Dirichlet b.c. Thus the first term is non-negative in general and we can conclude that all phases are strictly increasing functions of $k$,

$$\forall\lambda: \qquad \frac{d\tilde{\theta}_\lambda}{dk} > 0\,. \tag{3.13}$$

*Total phase and counting function.* At given $k$, let us denote by $\Lambda_-$ the number of negative eigenphases $\theta_\lambda < 0$. Since the eigenphases are moving clockwise, $\Lambda_-$ will decrease by one when an eigenphase crosses zero so that an additional eigenvalue is found. On the other hand, $\Lambda_-$ will increase by one whenever an eigenphase reaches $\pi$. According to the definitions in Eqs. (2.15) and (2.16), at these points the eigenphase gets reinjected from below into the spectrum of $S$ and at the same time $m_\lambda(k)$ increases by one. In other words, we have

$$\Lambda_-(k) - \Lambda_-(0) \;=\; \sum_\lambda [m_\lambda(k) - m_\lambda(0)] - [N(k) - N(0)] \tag{3.14}$$

or, using $m_\lambda(0) = 0$,

$$N(k) = N(0) + \Lambda_-(0) - \Lambda_-(k) + M(k) \tag{3.15}$$

with

$$M(k) = \sum_\lambda m_\lambda(k)\,. \tag{3.16}$$

Our final step will be to eliminate $M(k)$ from Eq. (3.15) as it cannot be computed from the numerically available eigenphases $\theta_\lambda(k)$. For this purpose we consider the total phase of the bond scattering matrix

$$\Theta(k) \;=\; \sum_{\lambda=1}^{2B} \theta_\lambda(k)\,, \tag{3.17}$$

$$\tilde{\Theta}(k) \;=\; \sum_{\lambda=1}^{2B} \tilde{\theta}_\lambda(k)\,. \tag{3.18}$$

From Eqs. (2.1), (3.9) and (3.11) and the invariance of the trace of a matrix under basis transformations we have

$$\begin{aligned}\frac{d\tilde{\Theta}}{dk} &= \sum_\lambda \langle a_\lambda | \frac{1}{i}\frac{dT}{dk}T^\dagger | a_\lambda\rangle + \langle a_\lambda | \mathrm{diag}(L_d) | a_\lambda\rangle \\ &= \sum_d \left(\frac{1}{i}\frac{dT}{dk}T^\dagger\right)_{dd} + \sum_d L_d \\ &= -\sum_i \frac{1}{v_i}\frac{d\omega_i}{dk}\sum_d \delta_{\alpha(d),i} \\ &= -\sum_i \frac{d\omega_i}{dk} + 2L \qquad (3.19)\end{aligned}$$

and consequently

$$\tilde{\Theta}(k) - \tilde{\Theta}(0) = -\Omega(k) + \Omega(0) + 2kL \qquad (3.20)$$

with

$$\Omega(k) = \sum_{i=1}^{V} \omega_i(k)\,. \qquad (3.21)$$

According to Eq. (2.9) we have $\Omega(0) = 0$ for Neumann b.c. and $\Omega(0) = V\pi$ for mixed or Dirichlet b.c. Eq. (3.20) had been obtained before in [**1**] up to the offset at $k = 0$ which depends on the precise definition of the phases $\tilde{\theta}_\lambda$.

On the other hand we have

$$\begin{aligned}\tilde{\Theta}(k) &= \sum_{\lambda=1}^{2B}(2\pi m_\lambda(k) + \theta_\lambda(k)) \\ &= 2\pi M(k) + \Theta(k) \qquad (3.22)\end{aligned}$$

and thus

$$M(k) = \frac{\Theta(0) + \Omega(0) - \Theta(k) - \Omega(k) + 2kL}{2\pi}\,. \qquad (3.23)$$

We can now state the identity

(3.24)

$$N(k) = N(0) + \Lambda_-(0) - \Lambda_-(k) + \frac{\Theta(0) + \Omega(0) - \Theta(k) - \Omega(k) + 2kL}{2\pi}$$

which is the main result of this paper. The r.h.s. can be computed from the eigenphases of the bond scattering matrix at the wave numbers 0 and $k$. Namely, the sum of the eigenphases yields $\Theta(k)$ and from the relative location of the phases with respect to $\theta = 0$ we can infer $\Lambda_-(k)$. $N(0)$ and $\Omega(k)$ are explicitly known from the boundary conditions of

the graph. Eq. (3.24) allows one to obtain from this information the spectral counting function of the Hamiltonian on the graph.

## 4. Numerical considerations

We illustrate Eq. (3.24) for a fully connected graph with $V = 4$ vertices (tetrahedron). We plot as a function of $k$ the 12 eigenphases $\theta_\lambda(k)$ of the bond scattering matrix and the counting function $N(k)$. This is done for Neumann and mixed b.c in Figs. 1 and 2, respectively. The counting function has been calculated from Eq. (3.24) without using information about the spectrum of the graph. Indeed we observe jumps by one whenever one of the eigenphases vanishes (dashed vertical lines).

Note that in both cases the graph has several degenerate eigenphases $\theta_\lambda = 0$ at $k = 0$. Due to numerical inaccuracies some of their numerical approximations may be small negative numbers and therefore some care must be taken in the determination of the offset value $\Lambda_-(k = 0)$ (for example, $\Lambda_-(0) = 5$ in Fig. 1). However, this step is easily verified by checking that for sufficiently small $\varepsilon$, $N(\varepsilon)$ equals the known value of $N(0) = 1$ (Neumann) or $N(0) = 0$ (mixed b.c.).

Numerically it may also be a problem to distinguish between $\theta_\lambda \approx -\pi$ or $\theta_\lambda \approx +\pi$ when $z_\lambda \approx -1$. However, the counting function will not be affected by such errors since they leave $\Lambda_-(k)+\Theta(k)/2\pi$ unchanged.

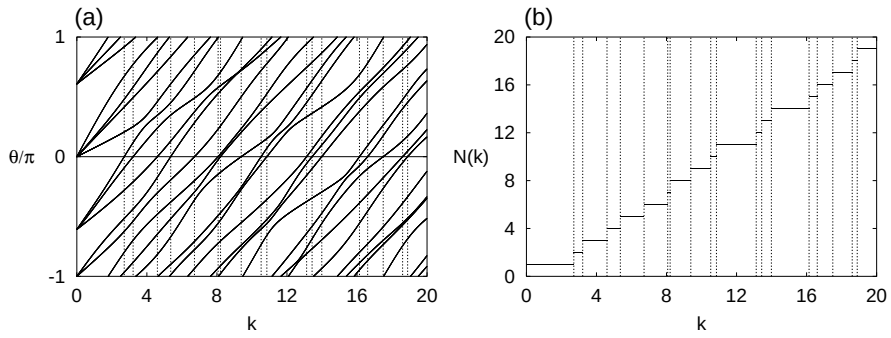


FIGURE 1. (a) The eigenphases of the bond scattering matrix of a fully connected graph with $V = 4$ vertices and Neumann b.c. are shown with bold lines. Eigenenergies of the graph Hamiltonian correspond to wave numbers $k$ where any of these phases vanishes. These values $k_n$ are indicated with vertical dashed lines in (a) and in (b). The spectral counting function as predicted by Eq. (3.24) is shown with a bold line in (b).

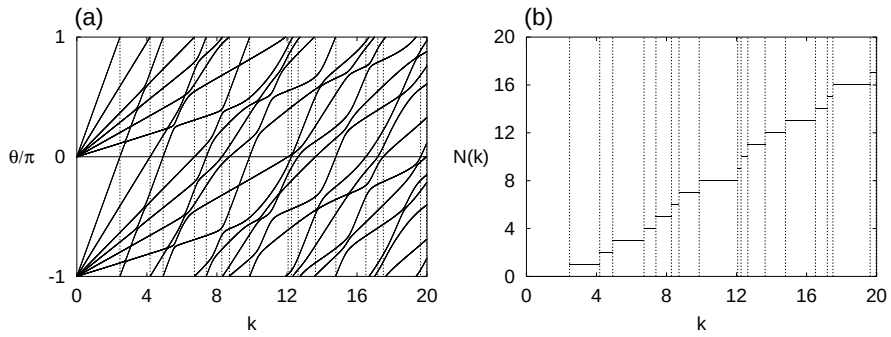


FIGURE 2. As Fig. 1 but with mixed b.c. $\lambda_i = 100$.

In principle it is possible to determine the exact location of the eigenvalues by searching for the points where Eq. (3.24) jumps (exact up to the precision in the diagonalization of $S(k)$). However, this would not be a very efficient strategy. Rather one can use Eq. (3.24) to determine an interval in which exactly one eigenvalue of the graph is contained and then converge to this root using any standard root-searching method and any secular function. In this way the iteration of the solution does not necessarily require additional diagonalizations of the large bond scattering matrix. Note that the direct application of Eq. (3.24) is also not the best strategy in the search for a suitable initial approximation to the eigenvalue $k_n$ since knowledge of the discrete counting function $N(k)$ alone gives no clue how far $k$ is from $k_n$. Rather we can make use of Eq. (3.24) in order to select the particular eigenphase $\theta_{\mu(n,k)}(k)$ which is responsible for the eigenvalue $k_n$. Namely, we have

$$\mu(n,k) = 1 + \Lambda_-(k) + N(k) - n\,, \tag{4.1}$$

where the index $\mu$ refers here to the sorted eigenphases $\theta$ (instead of sorting $\tilde{\theta}_\lambda$). The equation $\theta_{\tilde{\lambda}(n,k)}(k) = 0$ has exactly one real root $k = k_n$ and it is safe to search for this root using a standard routine which will make efficient use of all previously computed function values.

## 5. Summary and discussion

I have presented a non-standard way to calculate the spectral counting function of the Hamiltonian on a quantum graph which does not involve knowledge of any eigenenergies. Instead it suffices to diagonalize the bond scattering matrix at the wave number where the counting function is required. I hope that this result will be of use when one models extended structures which are so complex that even the numerical treatment of the corresponding quantum graph is non-trivial. In fact I

have successfully used Eq. (3.24) in order to speed up the calculation of eigenvalues in connection with a number of previous publications [**6, 7, 8**]. Clearly the problem of nearly degenerate levels, which was avoided in this way, is more relevant for graphs where level repulsion is weak and small spacings have a high probability, e. g. extended graphs with localized states or energy bands [**7, 8**]. At the same time these are the systems for which the difference in the dimensions of the matrices $S(k)$ and $h(k)$ is just a factor which is independent of the graph size (e. g. $2B/V = 4$ for a square lattice). In contrast, for fully connected graphs $S(k)$ has dimension $\sim V^2$ and there is relatively strong level repulsion. Therefore the numerical advantage of using Eq. (3.24) should be lowest in fully connected graphs.

The present paper was restricted to the Schrödinger operator on graphs and to boundary conditions which require continuity of the wave function across the vertices, but it should be possible to obtain an analogue of Eq. (3.24) also for more general situations. In fact the crucial ingredient is a sufficiently accurate estimate of the total phase $\tilde{\Theta}(k)$ of the unitary scattering matrix which is used to formulate the quantization condition. In the present case this is Eq. (3.20), which is an identity. However, in other systems where the semiclassical approximation is not exact one only needs an accuracy which ensures that the *integer* $M(k)$ can be determined without uncertainty. In fact an example for such a situation has been given in the context of the scattering approach to the quantization of the Sinai billiard [**9, 10**]. In general the requirement is that the auxiliary scattering system has only a finite number of trapped primitive periodic orbits since each one of them contributes an oscillatory term to the total phase. In the case which was discussed here the scattering system is a formal one and does not correspond to a physically relevant scattering setup. Therefore we encountered the exceptionally simple situation that there are no trapped periodic orbits at all and $\tilde{\Theta}(k)$ is a smooth function of energy.

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Max Planck Institute for Dynamics und Self-Organization and Institute of Nonlinear Dynamics, University of Göttingen, D-37073 Göttingen, Germany

*E-mail address*: holger@chaos.gwdg.de