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LETTER TO THE EDITOR

Green function approach for general quantum graphs

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Abstract

We present a recursive prescription to calculate the exact Green function for general quantum graphs. For the closed case, the expression for the poles of G—which gives the individual eigenstates—has the structure of a semiclassical formula, where the sum over the periodic orbit is already performed. As applications we discuss eigenstate localization for a three-arm closed star and filter-like mechanisms for transmission throughout an open trident graph.

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A graph is a network of M connected vertices V, figure 1. Each V_m is attached to N_m arms of length ℓ_{mn} $(n = 1, \ldots, N_m)$. If both ends (just one end) of an arm are fixed to vertices it is called a bond (semi-infinite lead). There are no leads in closed graphs. Along any arm, $\psi(x)$ is defined uniquely from a 1D Schrödinger equation. The total wavefunction is given by such piecewise solutions properly matched at the vertices [1].

For a long time quantum graphs have been used in the description of real systems [2]. Indeed, electron transport in organic molecules [3], such as proteins and polymers, may follow one-dimensional pathways (the bonds) changing from one path to other due to scattering centres (the vertices). Under certain conditions [4], charge transport in solids is also well described by one-dimensional dynamics, as in polymer films [5]. Moreover, such dynamics can be branched, examples being [6]: disordered superconductors, superlattices, quantum wires and mesoscopic networks. From a more fundamental point of view, quantum graphs have also become important tools for studying different aspects in quantum mechanics. For instance, band spectrum properties of lattices [7], the relation between periodic-orbit theory and Anderson localization [8] and chaotic and diffusive behaviour in scattering [9, 10]. Surprisingly, they even have provided exact solvable models in quantum chaos [11].

The countless possibilities in the construction of quantum graphs make difficult the use of a single framework to solve them. In fact, a general prescription should be applied to:

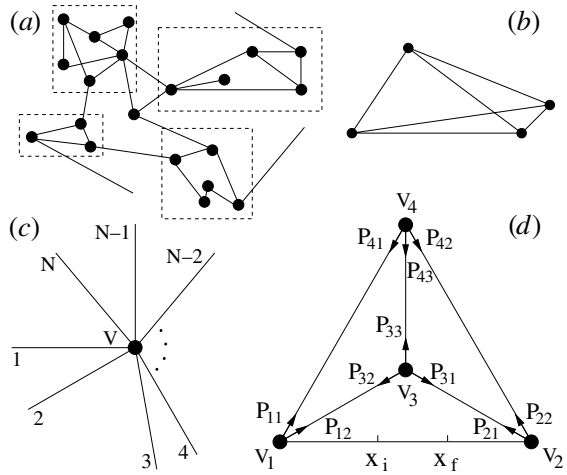

Figure 1. Examples of open (*a*) and closed (*b*) quantum graphs. (*c*) A single vertex V connected to N arms. (*d*) A planar representation of the quantum graph in (*b*) (the bond lengths are not shown to scale). P_{mn} represents the whole class of possible paths which leave the vertex m along the bond n.

(i) both closed and open cases, given the spectrum eigenstates for the former and the scattering states for the latter; (ii) any kind of structure and connectivity of the bonds and (iii) any type of boundary condition (BC) on the vertices, allowing the case of different BCs in each V_m. Furthermore, the method should: (iv) be implemented through some sort of hierarchy or recursive procedure, in order to handle networks with large numbers of bonds and vertices; and (v) work for dressed graphs, i.e., when there is a potential $U_{mn}(x)$ along each bond. Here we report a way to obtain the exact Green function for a general quantum graph. One difficulty in doing so is to make the appropriate matches of the different BCs at each vertex across the whole network. This problem is overcome by applying a recursive construction recently used to derive G for a 1D lattice of very general point-like scatterers [12]. Our approach can be regarded as a factorization method, used in different contexts in the literature (see, e.g., [13, 14]). We mention that the Green function for quantum graphs has been considered in a recent nice work [10]. However, there the most general case of energy-dependent scattering matrices for each vertex is not discussed and a schematic way is not presented to regroup the multi-scattering contributions to G, which is very important if one wishes to analyse larger graphs. This contribution also fulfils this gap. For simplicity we consider the case of free propagation along the bonds. At the end we comment briefly on how to extend our results to some classes of dressed graphs. As examples we discuss exact semiclassical-like formulae for individual energy levels, eigenstate localization and BC-dependent scattering properties.

The most general BC at a vertex of a quantum graph (consistent with flux conservation [7]) can be determined through self-adjoint extension techniques [15]. Indeed, at V_m we define [13]: $\Psi_m = (\psi_{m1}, \psi_{m2}, \ldots, \psi_{mN_m})^{\mathrm{T}}$ and $\Psi'_m = \left(\psi'_{m1}, \psi'_{m2}, \ldots, \psi'_{mN_m}\right)^T$. The BC is specified by $N_m \times N_m$ matrices A_m and B_m, where $A_m\Psi_m = B_m\Psi'_m$. We ensure self-adjointeness of the Hamiltonian operator by imposing current conservation $\Psi_m^\dagger\Psi'_m = \Psi'^{\dagger}_m\Psi_m$. As shown in [13], the general solution for this problem leads to $A_m B_m^\dagger = B_m^\dagger A_m$, resulting in a set of N_m^2 independent real parameters to characterize the BC at V_m.

Consider now a graph with a single vertex V attached to N arms, figure 1(*c*). The scattering solution for a plane wave of energy $E = k^2$ incoming from the arm j is given

by $\psi_n(x;k) = \delta_{nj}\exp[-\mathrm{i}kx] + S_{nj}(k)\exp[\mathrm{i}\,kx]$, for $n = 1,\ldots,N$. Here, $S_{nn} = R_n$ can be interpreted as the reflection coefficient in arm n and $S_{nj} = T_{nj}$ as the transmission coefficient from arm j to arm n. Norm preservation implies $SS^\dagger = S^\dagger S = \mathbf{1}$. Also, from the symmetries of the Schrödinger equation for real potentials we have [16] $S^\dagger(k) = S(-k)$. These properties lead to

$$\begin{aligned} &R_n(k) = R_n^*(-k) \qquad && R_nT_{jn}^* + R_j^*T_{nj} + \sum_{i\neq n,\,j} T_{ni}T_{ji}^* = 0 \\ &T_{nj}(k) = T_{jn}^*(-k) \qquad && R_nR_n^* + \sum_{j\neq n} T_{nj}T_{nj}^* = 1 \end{aligned} \tag{1}$$

which are a natural generalization of the usual relations for the scattering coefficients of a point scatterer on the line [12, 16]. If one also requires time-reversal invariance then $T_{nj} = T_{jn}$. As shown in [13, 17], S is given uniquely from the matrices A and B. Thus, the quantum amplitudes R and T (which satisfy (1)) can be obtained from the N^2 real parameters of the BC. In other words, a vertex with the most general boundary conditions consistent with the flux conservation is completely characterized by its scattering amplitudes.

From the results in [12, 18] we can readily write down the exact Green function for the graph in figure 1(*c*) as ($\hbar = 2\mu = 1$, x_f in the arm n and x_i in the arm l)

$$G_{nl} = \frac{1}{2\mathrm{i}k}\{\delta_{nl}\exp[\mathrm{i}k|x_f - x_i|] + S_{nl}(k)\exp[\mathrm{i}k(x_f + x_i)]\}. \tag{2}$$

For a general open or closed quantum graph with M vertices we can obtain its Green function by using a multiple scattering approach introduced in [18] and further developed in [12, 19] (for a parallel with oriented classical signal flow graphs, see [20]). The exact G is given by $G(x_f, x_i; k) = (2\mathrm{i}k)^{-1}\sum_{\mathrm{s.p.}} W_{\mathrm{s.p.}}\exp[\mathrm{i}S_{\mathrm{s.p.}}(x_f, x_i; k)]$. The sum is performed over all possible scattering paths (s.p.) starting at x_i and ending at x_f. For each s.p., the classical action is obtained from the free propagation along the successive arms composing the path, or $S_{\mathrm{s.p.}} = kL_{\mathrm{s.p.}}$, with $L_{\mathrm{s.p.}}$ being the s.p. total length. The amplitude (or weight) $W_{\mathrm{s.p.}}$ is given by the product of the quantum coefficients gained each time the particle is scattered off a given vertex along the way. For instance, suppose a s.p. which gets to V_m from the arm n, then if it follows an arm j, W gains a factor $T_{jn}^{(m)}$, on the other hand, if it turns back to the arm n, W gains a factor $R_n^{(m)}$. To obtain the Green function we have to classify and to sum up over all the scattering trajectories. The idea is to regroup infinite sets of trajectories into classes [21]. As shown [18], this simplifies the calculations enormously, and so one can obtain G in a closed expression independently of the form of the individual reflection and transmission coefficients at the vertices.

As an example, consider the tetrahedron [22] in figure 1(*b*). Once leaving a vertex m along the arm n, there are infinite possibilities of different paths for the particle due to multiple scattering. We denote by P_{mn} all the contributions of this class to G, figure 1(*d*). Thus, G can be written as a sum over a finite number of classes, instead over infinite individual s.p. [12, 18, 19, 21]. The P are not independent and are obtained from a system of algebraic equations relating each other, e.g., $P_{11} = \exp[\mathrm{i}k\ell_{11}]\{R_1^{(4)}P_{41} + T_{31}^{(4)}P_{43} + T_{21}^{(4)}P_{42}\}$. The system is easily determined and solved. For the end points in the same bond as shown in figure 1(*d*) and assuming $x = 0$ at V_1 and $x = \ell$ at V_2, we have [$g = g_1g_2 - \mathcal{R}_1\mathcal{R}_2\exp[2\mathrm{i}k\ell]$, $g_j = 1 - \mathcal{T}_j\exp[\mathrm{i}k\ell]$)]

$$\begin{aligned} G = \frac{1}{2\mathrm{i}kg}\{&(1 - \mathcal{T}_1\exp[\mathrm{i}k\ell])\exp[\mathrm{i}k(x_f - x_i)] + \mathcal{R}_1\exp[\mathrm{i}k(x_f + x_i)] \\ &+ (\mathcal{T}_2 + (\mathcal{R}_1\mathcal{R}_2 - \mathcal{T}_1\mathcal{T}_2)\exp[\mathrm{i}k\ell])\exp[\mathrm{i}k(\ell - x_f + x_i)] \\ &+ \mathcal{R}_2\exp[\mathrm{i}k(2\ell - x_f - x_i)]\}. \end{aligned} \tag{3}$$

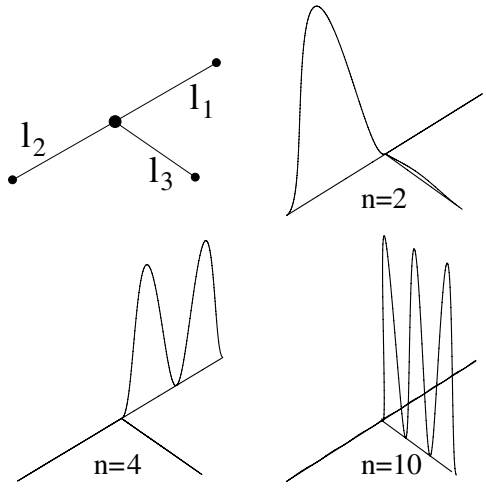

Figure 2. 3-star graph, with $\ell_1 = 1.4, \ell_2 = 1.1, \ell_3 = 1$. Here (see text) $d = 1, c = 1/b = 150, a = 2$. The first 14 states and then some others up to $n = 40$ strongly localize in one of the arms. Three typical examples are shown.

The above coefficients have a simple interpretation [12]: $\mathcal{T}_{1(2)}$ $[\mathcal{R}_{1(2)}]$ is the *total* probability amplitude for the particle to get into the vertex $V_{1(2)}$, to suffer multiple scattering, and then to come out from the vertex $V_{2(1)}$ $[V_{1(2)}]$. The expressions for $\mathcal{R}$ and $\mathcal{T}$ depend on the individual scattering amplitudes at the V_m and are very lengthy in the general case. For example, consider all V_m with the same BC, the so-called δ interaction [7]: $\psi_{mj}(V_m) = \psi_{mn}(V_m) = \psi_m(V_m)$ (for any n, j) and $\sum_j \psi'_{mj}(V_m) = \gamma\psi_m(V_m)$. Then, the individual reflection (transmission) amplitudes of the vertices are all equal, given by $R = (\gamma - (N-2)\,\mathrm{i}k)/(N\mathrm{i}k - \gamma)$ $(T = 2\mathrm{i}k/(N\mathrm{i}k - \gamma))$, where $N = 3$. If also all bonds are of the same length ℓ, we have $\mathcal{T}_1 = \mathcal{T}_2 = \mathcal{T}$ and $\mathcal{R}_1 = \mathcal{R}_2 = \mathcal{R}$, with $\mathcal{T} = T^2 \exp[2\mathrm{i}k\ell]\{(R+T)(1 - R\exp[\mathrm{i}k\ell]) + 2T^2\exp[\mathrm{i}k\ell]\}/f$, $\mathcal{R} = -\{R - R^2\exp[\mathrm{i}k\ell] + (T^3 - 2R^2T - R^3)\exp[2\mathrm{i}k\ell] + (R^4 + 2R^3T - 2R^2T^2 - 3RT^3 + 2T^4)\exp[3\mathrm{i}k\ell]\}/f$ and $f = 2\mathrm{i}k[1 - R\exp[\mathrm{i}k\ell] - (R+T)^2\exp[2\mathrm{i}k\ell] - (2T^3 + RT^2 - 2R^2T - R^3)\exp[3\mathrm{i}k\ell]]$.

The eigenvalues are the poles of G, given from $g = 0$. At first sight it is not clear that g has the structure of a periodic-orbit sum. However, by using $(1-z)^{-1} = 1 + z + z^2 + \cdots$ for all terms of $1/g = (g_1g_2)^{-1}\{1 - \mathcal{R}_1\mathcal{R}_2\exp[2\mathrm{i}k\ell]/(g_1g_2)\}^{-1}$, one sees that g^{-1} is written as the sum of all possible periodic orbits on the tetrahedron. This result is true for any kind of quantum graph discussed here. So, in general the individual eigenvalues and the density of states $\rho(E) = -(1/\pi)\,\mathrm{Im}[\int \mathrm{d}x\, G(x, x; k)]$ are given exactly by such expansions, extending the already known cases in the literature [8, 10, 11, 22]. However, in our case the sum is always already performed.

The regrouping procedure is quite useful for more complicated topologies. For instance, for the graph in figure 1(*a*) we can prescribe to a block of vertices (indicated by dashed boxes) classes of paths representing all the possible s.p. going into and coming out of that block through specific arms. Within each block further divisions can be made, and so on. This substitutes the problem of solving a large graph by one of solving a few smaller. In particular, the calculation is drastically simplified if the blocks have some kind of regularity as for periodic graphs.

One advantage of our approach is that we can derive a formula for the eigenstates of a quantum graph in a very general way. For a given BC, we need just to substitute the

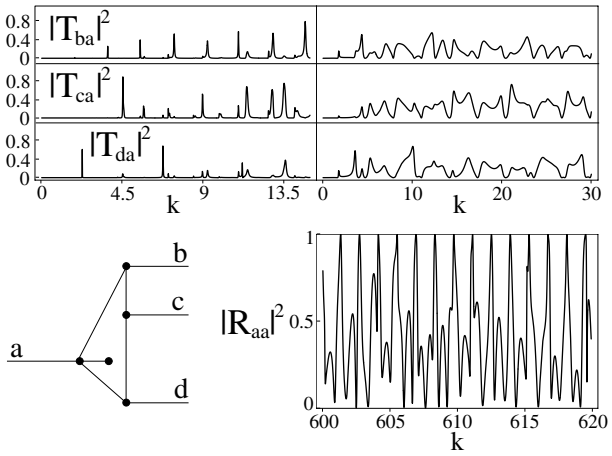

Figure 3. The scattering probabilities for the trident open quantum graph. For the peaked $|T|^2$ we have Dirichlet BC for V_i, $\gamma_a = 50$, $\gamma_b = \gamma_d = 100$, $\gamma_c = 20$, $\ell_{ab} = \sqrt{2}$, $\ell_{ad} = \sqrt{3}$, $\ell_{ai} = \sqrt{5}$, $\ell_{bc} = 0.95\sqrt{5}$ and $\ell_{cd} = \sqrt{5}$. For the oscillating $|T|^2$ we have Neumann BC for V_i, all γ equal to 10, $\ell_{ab} = 1$, $\ell_{ad} = 5/6$, $\ell_{ai} = 1$, $\ell_{bc} = 1/2$ and $\ell_{cd} = 2/3$. $|R_{aa}|^2$ is plotted for the first set of parameters for large values of k.

appropriate individual R and T into the final expression. Consider, for instance, the star graph [23] in figure 2. For arbitrary BC we can quite easily obtain an equation given its eigenvalues. Here we find that *state* localization can take place in this example if appropriate BCs are chosen. Indeed, in our 3-star graph we assume for the central vertex the following BC [15]: $\psi_1 = \psi_2$, $\psi_3 = a\psi_1 + b(\psi_1' + \psi_2')$, $\psi_3' = c\psi_1 + d(\psi_1' + \psi_2')$, with $ad - bc = 1$. For the ending vertices we consider Dirichlet BC. The eigenstates are calculated from the residues of G at the poles (which in this simple case can also be obtained from the Schrödinger equation, given the same result as it should be). In figure 2 we plot $|\psi_n|^2$ for three different states. The probability for the particle to stay at arm 2 is about 95% for $n = 2$, for $n = 4$ it is 99% in arm 1 and for $n = 10$ it is 99% in arm 3.

For open graphs we can identify from G the total scattering amplitudes. Suppose the trident graph of figure 3. The final expression for $G(x_f, x_i)$, with both end points located at any two leads, is very similar to (2). Indeed, if x_i is in the lead a and x_f in b (with the origin of the leads assumed to be at the corresponding vertices), then $G = T_{ba} \exp[\mathrm{i}k(x_i + x_f)]/(2\mathrm{i}k)$. Thus, $|T_{ba}(k)|^2$, which depends on the transmission and reflection amplitudes of each vertex as well as on the lengths of all inner bonds, is the total probability for a particle of wave number k incident from the lead a to be transmitted to the lead b. As an explicit example we consider that for all the vertices connected to the leads, the BCs are of the already discussed δ type. For the only inner vertex V_i, we assume either Neumann or Dirichlet BC. In figure 3 we show the results for two sets of parameters. The strong influence of the BCs on the dynamics becomes evident. In the first set we have very narrow peaks (for k not too large) in the transmission, thus the quantum graphs act like a *filter* for the incident wave. The particle can pass throughout the graph only for very specific values of k. Such values also determine in which lead the particle will come out, as a kind of channel selecting device. On the other hand, for the second set the transmission probabilities oscillate, showing a broader distribution among the different leads. We also show the reflection probability for the first set of parameters for large values of k. Differently from the reflection probability for the usual potential barriers in 1D,

which goes to zero for high energies, reflection can be close to 1 even for very high incident momentum k. This is just a consequence of interference effects due to the inner structure of the graph.

In summary, we have discussed a constructive approach to obtain the exact Green function for general quantum graphs. It is a useful tool for studying the rich dynamics which take place in those systems, as illustrated by some examples. For the dressed case, i.e., when there are potentials $U_{jn}(x)$ along the arms, we observe that if such potentials decay at least exponentially, one can obtain very good analytical approximations for G by using the same method [19]. The difference is that now, in the construction of the $W_{\text{s.p.}}$, one needs to include the transmission and reflection coefficients of the U. The potentials must also be taken into account in the calculations of the $S_{\text{s.p.}}$ (see [19] for details). Finally, one can easily incorporate the case of a magnetic field on each arm, represented by a vector potential A_{jn}, by adding to the action terms linear on the A_{jn} (see [9, 22]).

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