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Explicit analytical solution for scaling quantum graphs

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We show that scaling quantum graphs with arbitrary topology are explicitly analytically solvable. This is surprising since quantum graphs are excellent models of quantum chaos and quantum chaotic systems are not usually explicitly analytically solvable.

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Explicitly solvable systems are rare. Many have become textbook classics, such as the harmonic oscillator and the hydrogen atom. It is therefore always a noteworthy event when another explicitly solvable system is discovered. The purpose of this paper is to add an important class of explicitly solvable quantum systems to this set: quantum graphs. A quantum graph consists of a quantum particle that moves on a quasi-one-dimensional network. An example of such a network is shown in Fig. 1. It consists of seven vertices connected by seven bonds. In physical applications the bonds b of the network are equipped with a local coordinate $0 \leqslant x_b \leqslant 1$ and potentials $V(x_b) = V_0 v(x_b)$, while the vertices, possibly equipped with δ-function potentials $W_0 \delta(x_b)$, serve to redistribute the quantum flux on the network according to preset rules. Thus the spectrum of a quantum graph is obtained by solving the one-dimensional Schrödinger equation of the quantum particle moving on the bonds of the quantum graph subjected to the boundary conditions of continuity and flux conservation at the vertices. A host of related wave systems, such as networks of acoustic pipes or thin dielectric-filled microwave waveguides can be modeled in analogy with quantum graphs. Therefore one might think of these quasi-one-dimensional networks collectively as wave graphs.

Quantum graphs have a long history in theoretical chemistry [1], chemical physics [2,3] mathematics [4,5], mathematical physics [6] superconductivity [7], and mesoscopic [8–10] and general physics [11,12]. A recent review on quantum graphs [13] lists close to 200 papers related to the subject. Due to their usefulness in areas ranging from molecular chemistry to nanotechnology, quantum graphs are an emerging field with many promising applications [13].

Quantum graphs have recently been studied as models of quantum chaos [13–17]. It may therefore come as a surprise that a large and important subset of quantum graphs, scaling quantum graphs, is explicitly solvable in the form $E_n = f(n)$, where n is an integer, E_n are the energy levels of the graph, and f is a function explicitly constructed below. Scaling quantum graphs satisfy $V_0 = v_0 E$ and $W_0 = w_0 \sqrt{E}$, where v_0 and w_0 are constants. Because of the quantum chaos connection it already caused quite a stir when about a year ago explicit solutions of a special class of scaling quantum graphs were discovered [18,19]. This is so, because for any given n the associated energy level E_n is individually computable, without knowledge of the other quantum levels. While in the case of the quantum graphs studied in Refs. [18,19] one might shrug off the existence of explicit solutions by pointing to their special, nongeneric nature, this is now no longer possible. Thus the results reported in this paper are a substantial, qualitative step forward with profound implications for quantum graph theory and quantum chaos. Focusing on scaling quantum graphs, excluding graphs with tunneling and bound states for convenience (tunneling and bound states are discussed in Ref. [20]), we will show below that these quantum graphs, no matter how complex their topology, are explicitly solvable analytically. We emphasize that *scaling* quantum graphs [18,19] represent a huge class of graphs, far larger than and *including* the standard quantum graphs with $V(x_b) \equiv 0$ [13–17]. The class of quantum graphs for which we prove the existence of explicit solutions comprise quantum graphs with arbitrary topology, arbitrary scaling potentials on their bonds, and arbitrary scaling δ functions on their vertices.

The computation of energy eigenvalues of a given quantum graph is straightforward. In analogy with other simple quantum problems, all we have to do is to solve the Schrödinger equation on the graph subjected to a suitable set of boundary conditions at the vertices of the graph, for instance, Dirichlet boundary conditions on the dead-end vertices (examples are the vertices V_1 and V_7 in Fig. 1), and the condition of quantum flux conservation on all internal vertices. Implementing these boundary conditions yields a system of coupled linear equations. In the usual way this system is nontrivially solvable only if its secular determinant vanishes.

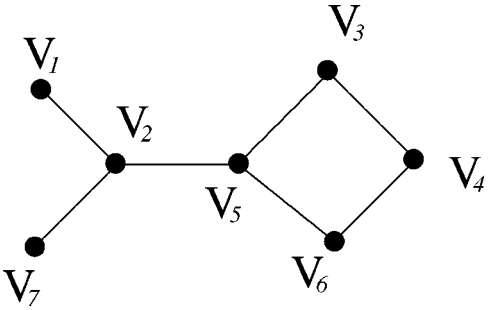

FIG. 1. Sample graph with seven bonds and seven vertices. It is turned into a quantum graph by introducing a local coordinate system on the graph bonds, defining physical potentials on the vertices and bonds, defining a Schrödinger operator on the bonds, and defining boundary conditions at the vertices. Thus, quantum graph =mathematical graph+physical dressing.

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The secular determinant vanishes only at the energy eigenvalues E_n, defining the spectrum of the quantum graph. Therefore this determinant is called the *spectral determinant*. For scaling quantum graphs it has the form [18,19]

$$g^{(0)}(k)=\cos(S_0k+\varphi_0)-\Phi(k), \tag{1}$$

where $\Phi(k)=\Sigma_{j=1}^{N}a_j\cos(S_jk+\varphi_j)$, S_0, $S_j>0$, φ_0, φ_j, a_j are constants, and $k=\sqrt{E}$ is the wave number of the quantum particle. The form (1) is expected on physical grounds: The action the quantum particle accumulates when it travels along the bonds is given by $\sigma=\int k\,dx$. Its optical analog is the optical path length. Assigning an optical path length, or, better, an *optical bond length* σ_b to every bond b, the spectral determinant of a quantum graph is determined by all possible sums and differences of optical bond lengths. The largest quantity we can form this way is the sum of all optical bond lengths. This is the quantity S_0 in the spectral determinant (1). It is also known as the *action length* [13–20] of the quantum graph. Because of its importance it has been singled out in the spectral determinant (1). The other possible optical bond length combinations are denoted by S_j in Eq. (1). We denoted their number by N. Since they involve at least one difference of a pair of optical bond lengths, we have $S_j<S_0$ for all j. With the help of the spectral determinant (1) we can now form the spectral equation

$$g^{(0)}(k_n^{(0)})=0. \tag{2}$$

As discussed above, its roots $k_n^{(0)}=\sqrt{E_n}$ are the wave numbers of the eigenenergies E_n of the quantum graph. It was shown in Refs. [18,19] that Eq. (2) is explicitly solvable in the form $k_n^{(0)}=\cdots$ if the condition

$$\sum_{j=1}^{N}|a_j|=\alpha<1 \tag{3}$$

is satisfied, where α is a constant.

The meaning of Eq. (3) is easily explained. Because of Eq. (1) the roots of Eq. (2) are the intersections of a cos function with "frequency" S_0 and the function $\Phi(k)$. Due to the condition (3) it is guaranteed that the amplitude of the slowly ($S_j<S_0$) varying function $\Phi(k)$ never exceeds the amplitude of the cos function and thus intersects the cos function precisely once between any two extrema of the cos function. This situation is illustrated in Fig. 2.

The vast majority of quantum graphs does not satisfy condition (3). Up to now this was believed to be the hedge that makes general quantum graphs resilient against explicit solution. However, there is a way to solve all scaling quantum graphs, even if they do not fulfill Eq. (3). We do this by constructing a sequence of auxiliary functions $g^{(m)}(k)$ such that knowing the roots of $g^{(m)}(k)$ allows us to compute the roots of $g^{(m-1)}(k)$. This sequence terminates at a function $g^{(M)}(k)$ for which the condition (3) is satisfied, and thus allows explicit computation of its roots. Thus, the process of root finding is bootstrapped. Going backwards through this sequence, starting with the roots of $g^{(M)}(k)$, we now are able to obtain the roots of all of the members of the auxiliary

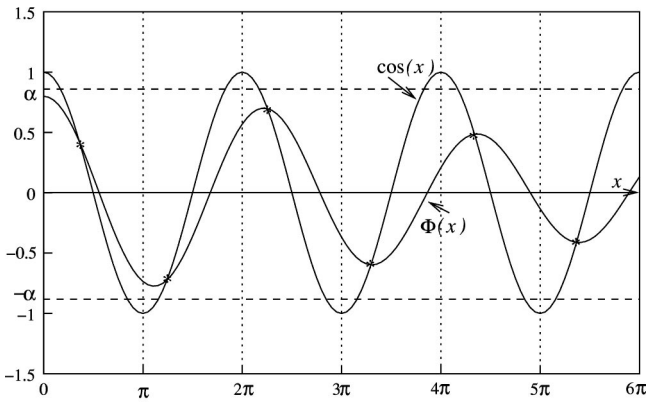

FIG. 2. Illustration of the consequences of condition (3) (see text). A slowly varying function $\Phi(x)$ with bounded amplitude $|\Phi(x)|\leqslant\alpha<1$ intersects the function $\cos(x)$ in precisely one point in each interval $[(n-1)\pi,n\pi]$, $n=1,2,\ldots$.

sequence, in particular, the roots of $g^{(0)}(k)$. The idea is that the roots of $g^{(m)}(k)$ form an interlacing sequence with respect to the roots of $g^{(m-1)}(k)$, i.e., the roots of $g^{(m)}(k)$ separate the roots of $g^{(m-1)}(k)$ from each other. Therefore we refer to the roots of $g^{(m)}(k)$ as *root separators* of the roots of $g^{(m-1)}(k)$.

The mth element of the auxiliary sequence is constructed by taking the mth derivative of Eq. (1) and dividing by S_0^m. We obtain

$$g^{(m)}(k)=\cos(S_0k+\varphi_0+m\pi/2)-\sum_{j=1}^{N}b_j^{(m)}\cos(S_jk+\varphi_j+m\pi/2), \tag{4}$$

where $b_j^{(m)}=a_j(S_j/S_0)^m$. Since $S_j<S_0$, there always exists an M such that $\Sigma_{j=1}^{N}|b_j^{(M)}|=\beta<1$, i.e., for $m=M$ Eq. (4) satisfies the condition (3) and the roots $k_n^{(M)}$ of $g^{(M)}(k)=0$ are explicitly computable [18,19]. Therefore the chain of auxiliary functions terminates at the level M.

Having bootstrapped the roots of Eq. (1) at the level M, we now have to go backwards to the levels $M-1,M-2,\ldots$, until we reach level 0 and possess $k_n^{(0)}$ explicitly. Retracing our steps is indeed possible by making use of the interlacing property of roots discussed above. Suppose we want to compute root number n of $g^{(m)}(k)=0$. Level number $m+1$ supplies us with root separators $\hat{k}_{n-1}^{(m)}$ and $\hat{k}_n^{(m)}$ such that root number n of $g^{(m)}(k)=0$, and only this root, will be found in the interval $[\hat{k}_{n-1}^{(m)},\hat{k}_n^{(m)}]$. Therefore,

$$k_n^{(m)}=\int_{\hat{k}_{n-1}^{(m)}}^{\hat{k}_n^{(m)}}k\,\delta(k-k_n^{(m)})\,dk. \tag{5}$$

This is a formal identity for $k_n^{(m)}$, which can be turned into

an explicit formula for $k_n^{(m)}$ if we use the identity

$$\delta(k-k_n^{(m)})=\left|\frac{d}{dk}g^{(m)}(k)\right|\delta(g^{(m)}(k)), \tag{6}$$

which holds for $\hat{k}_{n-1}^{(m)}<k<\hat{k}_n^{(m)}$. In Eq. (6) we can use any of the standard representations of the δ function, for instance, the Fourier representation

$$\delta(g^{(m)}(k))=\frac{1}{2\pi}\int_{-\infty}^{\infty}\exp[i\xi g^{(m)}(k)]\,d\xi. \tag{7}$$

We are now ready to apply the above root-finding scheme to the level $M-1$ using the known roots on the level M as the root separators $\hat{k}_n^{(M-1)}$ on the level $M-1$. We obtain

$$k_n^{(M-1)}=\int_{\hat{k}_{n-1}^{(M-1)}}^{\hat{k}_n^{(M-1)}}k|g^{(M)}(k)|\,\delta(g^{(M-1)}(k))dk. \tag{8}$$

It is important to realize that due to Eqs. (6) and (7), Eq. (8) is not just a formal solution, but yields $k_n^{(M-1)}$ explicitly, analytically, even numerically, if we wish, to any desired accuracy. This is so since both $g^{(M-1)}(k)$ and the root separators $\hat{k}_n^{(M-1)}$ are known explicitly. It is furthermore important to realize that the ''trick'' (5) does not generally work for other quantum systems, even if their spectral equation $g^{(0)}(k)$ is known. This is so because the root separators $\hat{k}_n^{(m)}$, known and according to the above scheme explicitly constructable in the case of quantum graphs, are not in general known for other quantum systems. Therefore, for more general quantum (chaotic) systems, the missing separators is indeed a hedge, nay a bulwark, which, so far, protects them against explicit solution.

Our retracing process from levels M to $M-1$ can now be continued until we reach level 0. This completes our demonstration that all scaling quantum graphs can be solved analytically.

There is an interesting analogy between our sequence of auxiliary functions (4) and Sturmian sequences for polynomials [21]. With the help of Sturmian sequences the number of roots of a polynomial $P_n(x)$ in an interval $[a,b]$ can be determined. While there are many similarities between Sturmian sequences and our sequence of auxiliary functions, there are also important differences.

(i) Our auxiliary functions are simple derivatives of the spectral determinant (1), while the Sturmian sequence has to be constructed using the Euclidean algorithm for polynomials [21].

(ii) The Sturmian sequence isolates targeted roots of $P_n(x)$ by counting sign changes of the polynomials in the sequence. We isolate roots of the spectral function by an interlacing process which is based hierarchically on the roots of higher-m functions.

(iii) Finally, Sturmian sequences apply to polynomials with a finite number of roots, whereas our method addresses the infinitely many roots of a class of transcendental functions. In this connection we mention that even the two-frequency case, resulting from a simple linear three-vertex graph, is interesting, because it provides the explicit solution of a transcendental function whose roots, so far, could only be determined graphically or numerically.

We stress that the main objective of our paper is to show that scaling quantum graphs are explicitly solvable. This is a conceptual point whose importance cannot be underestimated. However, our method is useful for numerical calculations as well. In the following we address two topics: the computation of targeted eigenvalues and the computation of complete spectra.

(i) In numerical spectral analysis the problem arises to compute long stretches of eigenvalues starting at a very high quantum number. For instance, for a statistical study of the zeros of Riemann's ζ function Odlyzko [22] computed the 10^{20}th zero of the Riemann ζ function and 70 million of its neighbors. Asked to compute the 10^{20}th zero of a scaling quantum graph, we cannot proceed by computing all $10^{20}-1$ zeros preceding the 10^{20}th zero in order to ascertain the correct assignment of the 10^{20}th zero. Even if we assume that we could compute 10^9 zeros per second, corresponding to the processing speed of a powerful contemporary computer, the computation of the 10^{20}th zero would still take 10^{11} sec, corresponding to about 3000 years. This is where our method of root separators comes in. Labeling roots around $n=10^{20}$ on the level M is trivial and requires essentially only the application of modulo operations to accomplish this task. Having determined the root separators $\hat{k}_n^{(M)}$ in the vicinity of $n=10^{20}$ on the level M, we go backwards in our scheme of auxiliary functions to arrive at the root separators $\hat{k}_{n-1}^{(0)}$, $\hat{k}_n^{(0)}$, where $n=10^{20}$. Given the root separators, the root itself is most efficiently computed using simple numerical root-finding methods. Indeed, in this connection, the computation of the root separators $\hat{k}_n^{(m)}$, $m=M,M-1,\ldots,0$ is also most effectively done numerically.

(ii) When computing numerical spectra, the question of completeness of the computed spectra arises. Any numerical method, without analytical input, searches for roots of the spectral equation using a search grid of finite size. Thus, there may always be roots that are closer together than the chosen grid size, independent of what the current grid size is, resulting in missed states. Using our method of auxiliary functions, completeness of spectra for scaling quantum graphs can now be certified since the hierarchical (numerical) computation of root separators allows us to isolate and label any energy eigenvalue of the scaling quantum graph individually.

We note that our methods can be extended to quantum graphs with an infinite number of bonds and vertices as long as $S_j<S_0<\infty$ and $\Sigma_{j=1}^{\infty}|a_j|=\alpha<\infty$. The latter condition guarantees that the function $\Phi(k)$ exists.

Our explicit energy eigenvalues may now be used to determine the spectral statistics [23–25] of the eigenvalues of graph systems. In the context of quantum graphs our results are more fundamental than random matrix theory (RMT) [23–26], which is not a physical theory but a mathematical model of physical systems based on a zero-knowledge assumption without system-specific input. In fact, our energy

eigenvalues may be used to test RMT predictions. We note that in the context of quantum graphs RMT predictions were already tested both numerically [14–17] and analytically [27,28].

In summary, our paper makes the important conceptual point that scaling quantum graphs are explicitly analytically solvable. A spin-off is the possibility of the targeted computation of any selected energy eigenvalue of any given scaling quantum graph.

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