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Explicitly Solvable Cases of One-Dimensional Quantum Chaos

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We identify a set of quantum graphs with unique and precisely defined spectral properties called *regular quantum graphs*. Although chaotic in their classical limit with positive topological entropy, regular quantum graphs are explicitly solvable. The proof is constructive: we present exact, convergent periodic orbit expansions for individual energy levels, thus obtaining an analytical solution for the spectrum of regular quantum graphs that is complete, explicit, and exact.

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A quantum graph [1–8] is a network of vertices and bonds with a quantum particle moving along its bonds. An example of a graph with five vertices and seven bonds is shown in Fig. 1. The wave function and the energy levels of a quantum particle on a graph are defined by the corresponding one-dimensional Schrödinger equation. Despite the apparent simplicity of the system, quantum graphs have proven to be a rich source of physical insight. From the mathematical point of view, the spectral properties of Schrödinger operators on graphs are highly nontrivial and have been widely investigated in the mathematical literature [1–4]. Quantum graphs and networks have also been used to model various phenomena in different branches of physics and chemistry for more than 30 years. The most recent physical development appeared in a series of publications [5–8], where quantum graphs were studied in the context of quantum chaos.

It is easy to see that the behavior of a particle on a quantum graph is very complex. Each time the particle encounters a vertex V_i of the graph, it can scatter with different probabilities in the forward or backward directions along any of the bonds emanating from the vertex. A simple physical analog of this system is a beam of light traveling along a network of optical fibers. At every joint of the fibers the light waves scatter in such a way that the total energy flux is conserved.

As a result of the multiple scattering possibilities at the vertices, the dynamics of a classical particle on a graph is very complex and the number of possible periodic orbits traced by the particle increases exponentially with their lengths. Consequently the topological entropy of the particle is positive and, since the phase space of the system is bounded, the dynamics of the particle is mixing [6]. The classical chaoticity notwithstanding, it was shown that several important spectral characteristics of quantum graphs, such as the density of states and the spectral staircase, can be obtained exactly in terms of periodic orbit expansion series [5–7].

The “wiring” of a quantum graph, i.e., the arrangement of bonds and vertices, is called the topology of the quantum graph. For any given graph topology there exists a wide variety of possible quantum graphs. The vertices, for instance, may be realized as simple hubs that redistribute

the quantum flux into various channels, or we may place δ function potentials of various strengths at the vertices, or there may even be potential functions on the bonds. Because of this flexibility we anticipate that the topology of a quantum graph alone does not uniquely specify the graph’s spectral properties. We conjecture that there are several different types of quantum graphs, all chaotic in their classical limit, but each exhibiting unique and precisely defined spectral characteristics.

We start a rigorous classification of quantum graphs by defining *regular quantum graphs*. Although, generically, their classical limit is chaotic, we show that their spectrum is explicitly solvable analytically, state by state, via explicit periodic orbit expansions. This result is backed up by rigorous mathematical proofs [9] whose basic elements are presented below. To our knowledge this is the first time that the spectrum of a quantum chaotic system is obtained *exactly* and *explicitly*. In addition regular quantum graphs show a spectral gap at small energy spacings and a cutoff at large spacings. Both the size of the gap and the location of the cutoff are computed analytically.

Regular quantum graphs are different from a class of quantum graphs described in the literature [5–7] whose level spacing distributions, to a good approximation, exhibit features of the Gaussian orthogonal (unitary)

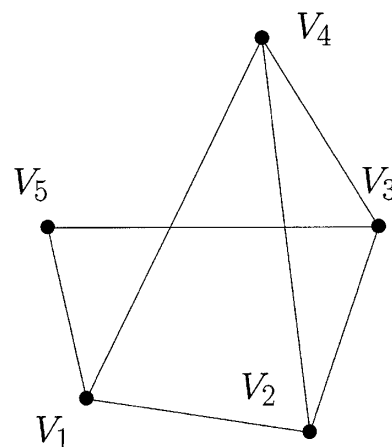


FIG. 1. A generic (quantum) graph with five vertices and seven bonds.

ensemble [10,11]. Thus there are at least two different types of quantum graphs with distinct spectral properties.

The periodic orbits of graphs are defined as the periodic connected sequences of bonds B_{ij} . Denoting by $k(x)$ the local wave number (momentum) of the particle, each bond contributes

$$S_{ij} = \int_{B_{ij}} k(x) dx \quad (1)$$

to the total action of a path traced by the particle. It turns out that the information contained in the totality of all the possible classical periodic orbits often allows one to reconstruct *exactly* certain quantities of a purely quantum nature. For example, according to recent results [4–7], the exact periodic orbit expansion for the density of states can be written as

$$\begin{aligned} \rho(k) &\equiv \sum_{j=1}^{\infty} \delta(k - k_j) \\ &= \bar{\rho}(k) + \frac{1}{\pi} \operatorname{Re} \sum_p T_p \sum_{\nu=1}^{\infty} A_p^\nu e^{i\nu S_p(k)}. \end{aligned} \quad (2)$$

Here $\bar{\rho}(k)$ is the average density of states, ν is the repetition index, $T_p = \partial S_p(k)/\partial k$, and S_p, A_p are, correspondingly, the action and the weight factor of the prime periodic orbit labeled by p . We assume in what follows that the system is scaling [12–17]. This means that the actions of the periodic orbits are proportional to the wave number,

$$S_p(k) = S_p^0 k, \quad (3)$$

where S_p^0 , a constant, is the reduced action. In this case $T_p = S_p^0$ and A_p are k -independent constants. We define the total reduced action S_0 of the graph, $S_0 = (\int k(x) dx)/k$, where the integral is extended over all of the bonds of the graph. The scaling assumption is not an artificial restriction. It occurs, for instance, in atomic physics where scaled spectroscopy is now a common experimental technique [17]. In addition, scaling quantum systems of this type are the analogs of certain electromagnetic ray-splitting systems, flat metal cavities partially filled with a dielectric substance such as Teflon [13–15].

The formal description of a quantum graph system proceeds as follows [5–7]. On a bond B_{ij} connecting the vertices V_i and V_j , the wave function of a quantum particle is defined by the one-dimensional Schrödinger equation which may include potentials on the bonds [16]. At every vertex V_i the wave function satisfies the usual boundary conditions of continuity and flux conservation. The consistency of the boundary conditions at every vertex of the graph naturally yields the global quantization conditions that determine the momentum eigenvalues k_n . A simple and elegant method based on the scattering quantization approach was presented in [5–7], where the quantization condition is given in the form

$$\det[1 - S(k)] = 0. \quad (4)$$

Here $S(k)$ is the scattering matrix [5], which can be expressed explicitly in terms of the connectivity matrix [5] of the graph. It can be shown that the modulus of the complex function (4) is a trigonometric function of the form

$$\cos(S_0 k - \pi \gamma_0) - \Phi(k) = 0, \quad (5)$$

where

$$\Phi(k) = \sum_i a_i \cos(S_i k - \pi \gamma_i). \quad (6)$$

In the scaling case the a_i are constants and $S_i < S_0$ are certain combinations of the reduced bond actions. In general the functions γ_0 and γ_i are bounded and tend to constant values for $k \rightarrow \infty$. In the scaling case they are k -independent constants.

In order to proceed we define regular quantum graphs. A regular quantum graph fulfils the condition

$$\alpha = \sum_i |a_i| < 1. \quad (7)$$

It is convenient for the following discussion to assume $\alpha > 0$, i.e., we exclude trivial graphs with $\alpha = 0$. They are regular quantum graphs whose spectrum can be obtained trivially. For regular quantum graphs, Eq. (5) can be solved formally for the momentum eigenvalues k_n . We obtain the following implicit solution for the roots of this quasiperiodic function:

$$\begin{aligned} k_n &= \frac{\pi}{S_0} [n + \mu + \gamma_0] \\ &+ \frac{1}{S_0} \begin{cases} \arccos(\Phi_n), & \text{for } n + \mu \text{ even,} \\ \pi - \arccos(\Phi_n), & \text{for } n + \mu \text{ odd,} \end{cases} \end{aligned} \quad (8)$$

where $\Phi_n = \Phi(k_n)$ and $\mu \in Z$, a fixed integer, is to be chosen such that k_1 is the first non-negative solution of (5). Because of (7), the boundedness of the trigonometric functions in (6) and the properties of the arccos function, the second term of (8) is bounded away from 0 and π/S_0 and assumes only values between u and $\pi/S_0 - u$, where $0 < u = \arccos(\alpha)/S_0 < \pi/2S_0$. Thus, for regular graphs the points

$$\hat{k}_n = \frac{\pi}{S_0} (n + \mu + \gamma_0 + 1), \quad n = 1, 2, \dots, \quad (9)$$

are not roots of (4). They serve as separators between root number n and root number $n + 1$. In fact (8) implies even more: the existence of finite-width “root-free zones” $F_n = (\hat{k}_n - u, \hat{k}_n + u)$ surrounding every separating point \hat{k}_n , where no roots of (4) can be found. Thus, roots of (4) can only be found in the “root zones” $R_n = [\hat{k}_{n-1} + u, \hat{k}_n - u]$, subsets of the root cells $I_n = [\hat{k}_{n-1}, \hat{k}_n]$. Since S_0 is the largest action in (5) and (6), it can be shown [9] that k_n is the *only* root in R_n . Therefore, in summary, there is exactly one root k_n inside $R_n \subset I_n$, and this root is bounded

away from the separating points \hat{k}_{n-1} and \hat{k}_n by a finite amount u .

The spectral properties of regular graphs discussed above allow us to draw several important conclusions. (i) Since there is exactly one root k_n of (4) in I_n , this proves rigorously that the number of roots of (4) smaller than k grows like $\bar{N}(k) \sim S_0 k / \pi$ (Weyl's law). (ii) The existence of the root-free zones F_n gives rise to a spectral gap of finite width $g = 2u$ in the nearest neighbor spacing distribution of regular quantum graphs, i.e., no level spacings smaller than g are ever found. This, for instance, precludes the possibility of degenerate eigenvalues. (iii) The existence of the separating points (9) together with the root-free zones imply the existence of a spectral cut at $c = 2(\pi/S_0 - u)$, i.e., no level spacings greater than c are ever found. (iv) The existence of the separating points (9) and the root-free zones F_n are the key for obtaining an explicit and exact periodic orbit expansion for every root of (4).

The properties (ii) and (iii) indicate that the spectral statistics of regular quantum graphs is not Wignerian. Although in many cases the spectral statistics of classically chaotic systems is well described by the three universal random matrix ensembles [10,11,18], the non-Wignerian spectral statistics of regular quantum graphs is not a contradiction to their classical chaoticity. Many quantum systems are known and are described in the literature (see, e.g., [19]) whose classical mechanics is completely chaotic, but their level spacing statistics deviates substantially from the expected universal behavior.

Multiplying both sides of (2) by k , integrating from \hat{k}_{n-1} to \hat{k}_n and using the fact that k_n and only $k_n \in I_n$, we obtain

$$k_n = \hat{k}_n - \frac{\pi}{2S_0} - \frac{1}{\pi} \operatorname{Re} \sum_p \sum_{\nu=1}^{\infty} A_p^\nu \frac{e^{i\nu S_p^0 \hat{k}_n}}{\nu} \times \left\{ (1 - e^{-i\nu\omega_p}) \left(i\hat{k}_n - \frac{1}{\nu S_p^0} \right) + \frac{i\pi}{S_0} e^{-i\nu\omega_p} \right\}, \quad (10)$$

where $\omega_p = \pi S_p^0 / S_0$. Since all the quantities on the right-hand side of (10) are known, this formula provides an explicit representation of the roots k_n of the spectral equation (4) in terms of the geometric characteristics of the graph. To our knowledge, this is the first time that the energy levels of a chaotic system are expressed explicitly in terms of a periodic orbit expansion. Previously, explicit formulas for individual energy levels were known only for integrable systems. In the context of periodic orbit theory, the energy levels of integrable systems are given by the Einstein-Brillouin-Keller (EBK) formula [18]. However, apart from a few exceptional cases [20], EBK quantization is only of semiclassical accuracy.

For a generic chaotic system the energy levels can only be obtained indirectly as the singularities of the periodic orbit expansion of the density of states (Gutzwiller's formula [18]), an implicit method which, in general, is only of semiclassical accuracy. Formula (10), on the other hand, shows that for regular quantum graphs every quantum level can be obtained *individually, explicitly, and exactly* in terms of classical parameters.

In order to demonstrate that the class of regular quantum graphs is not empty we present an explicit example: the one-dimensional step potential shown in Fig. 2(a) [21]. With

$$U_0 = \lambda E \quad (11)$$

we turn it into a scaling system. Physically this potential is realized for a rectangular microwave cavity partially loaded with a dielectric substance [13–15]. The scaling step potential is equivalent to the scaling three-vertex chain graph shown in Fig. 2(b), with two bonds $L_1 = b$ and $L_2 = \beta(1 - b)$, $\beta = \sqrt{1 - \lambda}$. In this case the spectral equation (4) is given by

$$\sin(Lk) - r \sin[(L_1 - L_2)k] = 0, \quad (12)$$

where $L = L_1 + L_2$, and $r = (1 - \beta)/(1 + \beta)$ is the reflection coefficient at the vertex V_2 between the two bonds. For a given prime periodic orbit p , such as the ones shown in Fig. 2, the coefficients A_p in (10) are given by [16]

$$A_p = (-1)^{\chi(p)} r^{\sigma(p)} (1 - r^2)^{\tau(p)/2}, \quad (13)$$

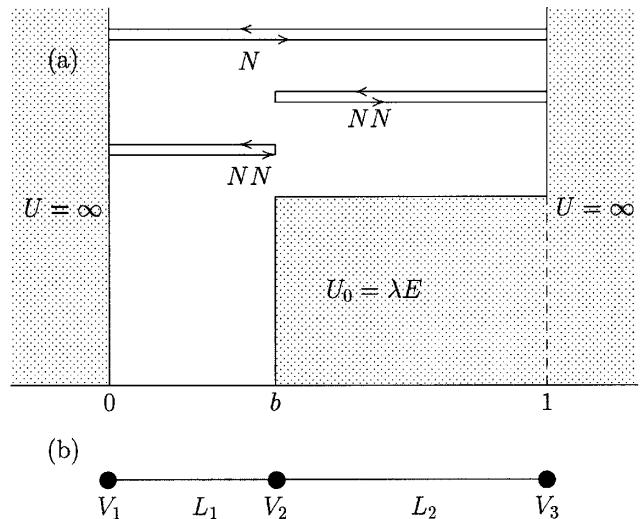


FIG. 2. (a) Simple step potential, a basic problem in one-dimensional quantum mechanics. Also shown are examples of Newtonian (“ N ”) and non-Newtonian (“ NN ”) periodic orbits used in the periodic orbit expansion of its energy eigenvalues (see text). (b) Three-vertex chain graph corresponding to the step potential above.

where $\sigma(p)$ and $\tau(p)$ are, correspondingly, the number of reflections off the vertex V_2 and transmissions through it. Since the reflection amplitude at V_2 may be positive or negative depending on whether the particle scatters from the right or from the left, the factor $(-1)^{\chi(p)}$ is needed to keep track of how many times it appears with a minus sign. Moreover χ keeps track of how many times the particle scatters off the walls of the potential, since each scattering event from the walls gives rise to a minus sign in the wave function. Using (13) we obtain the explicit form (10) of the eigenvalues for a quantum particle in the step potential in terms of classical Newtonian and non-Newtonian [13] periodic orbits.

In order to illustrate the validity of (10) we computed k_1 , k_{10} , and k_{100} including all Newtonian and non-Newtonian periodic orbits that experience up to ten scattering events. We chose $b = 0.3$ (see Fig. 2) and $\lambda = 1/2$ [see (11)]. We obtain $k_1^{(10)} = 4.1161$, $k_{10}^{(10)} = 39.2866$, and $k_{100}^{(10)} = 394.9477$. This can be compared with the exact k values given by $k_1 = 4.107149$, $k_{10} = 39.305209$, and $k_{100} = 394.964713$. In order to illustrate convergence to the exact eigenvalues, we also computed k_1 , k_{10} , and k_{100} including all periodic orbits that experience up to 40 scattering events. This amounts to including more than 100 000 periodic orbits and results in $k_1^{(40)} = 4.105130$, $k_{10}^{(40)} = 39.305212$, and $k_{100}^{(40)} = 394.964555$. This result indicates that the convergence of (10) is not destroyed by keeping more and longer periodic orbits.

Additional examples of regular graphs are provided by the scaling “Manhattan potentials.” These potentials are obvious generalizations of the step potential shown in Fig. 2(a) to piecewise constant potentials where the potential heights scale with the energy. Furthermore we checked explicitly that linear chain graphs with scaling δ function potentials at the vertices provide more examples of regular quantum graphs. In this case the strengths of the δ function potentials scale linearly with the momentum.

The key physical feature of these one-dimensional quantum systems, which permits the exact periodic orbit expansion (10) for the eigenvalues, is the rigidity of their spectra. For integrable systems, spectral rigidity is due to the “geometrical rigidity” of the periodic orbits, confined to integrable tori. In the case of quantum graphs, the geometrical structure of the periodic orbits is much more complicated. The complexity of the expansion (10) compared to the EBK formula reflects the geometrical complexity of the periodic orbits.

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