

INTEGRABILITY IN 1D QUANTUM CHAOS

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Abstract. Explicit, exact periodic orbit expansions for individual eigenvalues exist for a subclass of quantum networks called regular quantum graphs. We prove that all linear chain graphs have a regular regime.

1. Quantum Networks. As a model of a quantum chaotic system, let us consider a quantum particle that moves on a quasi one-dimensional network. On every bond B_{ij} of the network one may define a potential U_{ij} , which turns the graph into a *dressed* quantum graph [1]. Below we shall consider the case of constant *scaled* bond potentials $U_{ij} = E\lambda_{ij}$, where E is the energy and $0 < \lambda_{ij} < 1$ are real scaling constants. Such potentials will change the action lengths of the bonds and the values of the reflection and transmission amplitudes of the quantum particle at the vertices of the graph. The wave function of the particle is given by

$$\Psi_{ij}(x) = A_{ij}e^{ik_{ij}x_{ij}} + B_{ij}e^{-ik_{ij}x_{ij}}. \quad (1)$$

The scaling assumption allows to avoid unnecessary complications, such as the geometrical restructuring of the periodic orbits for different energies.

The boundary conditions consist of continuity and flux conservation requirements for the wave function Ψ_{ij} across the vertices V_i of the graph [1, 2, 3, 4, 5, 6]. Such boundary conditions produce a spectral determinant $\Delta(k)$, whose zeroes define the spectrum of the problem. Usually, the quantum spectrum determines the energy levels for a given potential. However, for the scaling problems considered here, the scaling constants are given and the potential is determined by the spectrum.

The spectral determinant for the quantum networks is a finite exponential sum,

$$\Delta(k) = 1 + e^{i2(S_0k - \pi\gamma_0)} - \sum_{i=1}^{2N_\Gamma} a_i e^{i2(S_i k - \pi\gamma_i)}, \quad (2)$$

where S_i are constants that can be expressed via the action lengths of the graph bonds and the γ_i are constants. The total length S_0 (the 1D volume) of the graph is the largest frequency that appears in the exponential sum (2), $S_0 > S_i$. The number of terms N_Γ in the sum (2) is finite.

We are interested in studying the roots of $\Delta(k)$. Such functions (for a more general case of a complex argument) were studied from the mathematical perspective in [7], where it was shown that the roots z_n of (2) form an almost periodic set, which is uniformly bounded in the complex plane, i.e. is contained in a stripe of finite width,

$$|\text{Im } z_n| < M < \infty, \quad \Delta(z_n) = 0. \quad (3)$$

Moreover, it was shown that the real parts of the roots have the form

$$\operatorname{Re} z_n = \frac{\pi}{S_0} n + \varphi(n), \quad (4)$$

where $\varphi(n)$ is an almost periodic function, whose frequency set contains linear combinations of the frequencies $\pi S_i/S_0$, with integer coefficients. In [1, 2, 3, 4, 5] these mathematical results were put into the perspective of quantum chaos theory that describes the spectral properties of quantum networks.

2. Quantum Chaos. The spectral problem of quantum networks has a long history (see [8, 9, 10] and the references therein). In fact, the problem of obtaining the energy levels in the step potential

$$V(x) = \begin{cases} 0, & \text{for } 0 \leq x \leq b, \\ V_0, & \text{for } b \leq x \leq L, \\ \infty, & \text{for } x < 0 \text{ or } x > L, \end{cases} \quad (5)$$

is the one that is usually presented following the elementary “infinite square well” problem in many standard quantum mechanics textbooks [11, 12, 13]. However, unlike in the square well problem, the spectral equation for the step potential (5) is not easy to solve analytically. In fact, the only known way to obtain the roots of the spectral equation are numerical or graphical solutions.

The complexity of the spectral equation for the system (5) as well as for a generic quantum network is in fact due to the dynamical complexity of the underlying classical system, which turns out to be chaotic [14].

In the classical limit the quantum graph systems reduce to a classical particle that scatters stochastically at the vertices of the graph (Fig. 3). The scattering probabilities are obtained in the $\hbar = 0$ limit from the quantum-mechanical vertex transition amplitudes $t_{ji,ij}$ [5]. Every time the particle encounters a vertex V_i traveling along the bond B_{ji} , it can reflect back from it with the probability $|t_{ji,ij}|^2$ or pass through to another bond B_{ik} with the transmission probability $|t_{ji,ik}|^2$. After every reflection or transmission (scattering) event, the particle completely loses its memory about the previous stage of its motion.

Using the coefficients $t_{ji,ik}$, it is easy to obtain the probability amplitudes with which a particular periodic orbit is realized. Indeed, if a certain orbit γ reflects $\sigma_i(\gamma)$ times off the vertex V_i and passes through it $\tau_i(\gamma)$ times, then the probability amplitude for such an orbit is

$$A_\gamma = \prod t_{ji,ij}^{\sigma_i(\gamma)} t_{ji,ik}^{\tau_i(\gamma)}, \quad (6)$$

where the product is taken over all the vertices visited by γ . It is usually convenient to distinguish the so-called “primitive” orbits, i.e. the ones that traverse a certain sequence of bonds only once, and the “multiple traversal” orbits. If a certain primitive orbit γ_p with the weight A_p is traversed ν times, then the corresponding amplitude is A_p^ν .

Due to the stochastic scattering, the trajectories of the particle are geometrically very complex and the number of possible orbits (and in particular the periodic orbits), increases exponentially [14]. The number N of the n -bond periodic orbits grows as

$$N \approx \frac{e^{\tau n}}{n}, \quad (7)$$

where the exponential proliferation rate τ depends only on the topology of the graph.

Such behavior mimics closely an important phase space feature of deterministically chaotic systems. Hence quantum networks provide very convenient and simple models for studying various features of quantum systems that correspond to classically chaotic systems in the context of quantum chaos theory.

3. Periodic orbit theory. Let us outline the main attributes of quantum chaos theory [15], applied to quantum networks. In [1] it was shown that for dressed quantum graphs there exists an exact periodic orbit expression for the density of states,

$$\rho(k) = \frac{S_0}{\pi} + \frac{1}{\pi} \operatorname{Re} \sum_p S_p^0 \sum_{\nu=1}^{\infty} A_p^\nu e^{i\pi\nu S_p^0 k}, \quad (8)$$

which generalizes the earlier results obtained in [8, 9]. Here S_p^0 and $A_p(E)$ are correspondingly the action length and the weight factor (6) of the prime periodic orbit labeled by p , ν is the repetition index and S_0 is the total action length of the graph.

Another important characteristic of the spectrum is the spectral staircase function

$$N(k) = \sum_j \Theta(k - k_j), \quad (9)$$

for which there also exists an exact periodic orbit expansion. In accordance with Weyl's law, the average spectral staircase depends linearly on the momentum,

$$\bar{N}(k) = \frac{S_0 k}{\pi} + \bar{N}(0), \quad (10)$$

where S_0 is the total length (1D volume) of the network. This statement implies that the average dependence of the momentum eigenvalues k_n on their index [5] is

$$\bar{k}_n = \frac{\pi}{S_0} \left(n - \bar{N}(0) - \frac{1}{2} \right), \quad (11)$$

which complies with the relationship (4).

Weyl's average (10) of the spectral staircase is the same for all networks with the same action length S_0 . However, different networks vary significantly in how well the average approximates the actual staircase function $N(k)$. It is interesting that there exist certain graphs with a particularly regular behavior of their spectra. For these quantum networks (called regular in [2, 3, 4, 5]), the average spectral staircase (10) pierces every stair-step of $N(k)$. It is clear that for the regular graphs the intersection points \hat{k}_n between the spectral staircase and its average,

$$N(\hat{k}_n) = \bar{N}(\hat{k}_n), \quad (12)$$

occur periodically on the momentum axis [16]. In other words, for such systems there exists exactly one quantum eigenvalue k_n between every two such intersections.

For such graphs one can obtain immediately the exact periodic orbit series representation for the *individual* eigenvalues of the momentum. Indeed, since every

interval $I_n = [\hat{k}_{n-1}, \hat{k}_n]$ contains one delta-peak of $\rho(k)$, the corresponding root k_n can be obtained via

$$k_n = \int_{\hat{k}_{n-1}}^{\hat{k}_n} k\rho(k)dk. \quad (13)$$

Using the periodic orbit expansion for the density of states (8), the integration (13) can be performed explicitly and yields [2, 5]

$$k_n = \frac{\pi}{S_0}n - \frac{2}{\pi} \sum_p \frac{1}{S_p^0} \sum_{\nu=1}^{\infty} \frac{A_p^\nu}{\nu^2} \sin\left(\frac{1}{2}\nu\omega_p\right) \sin(\nu\omega_p n), \quad (14)$$

where $\omega_p = \pi S_p^0/S_0$, and the A_p 's are assumed to be real (no mixed boundary conditions).

The spectral formula (14) provides an explicit harmonic expansion of the function $\varphi(n)$ in (4) for the roots of the spectral determinant of the regular graphs.

It can be shown [6] that the series (14) is convergent. An analytical criterion for the regularity (12) of a given network comes from analyzing the spectral determinant (2). After removing the complex phase of $\Delta(k)$, the spectral equation for quantum graphs can be written as $\cos(S_0 k - \pi\gamma_0) = \Phi(k)$. It was shown in [2, 3, 4, 5, 6], that if the *characteristic function* $\Phi(k)$ of the graph is bounded by 1 for all $k \in R^1$, then the piercing average condition (12) is satisfied [2, 5] and the expansion (14) exists. In terms of the coefficients of (2), $|\Phi(k)| < 1$ is certainly satisfied if

$$\sum_{i=1}^{N_\Gamma} |a_i| < 1. \quad (15)$$

In [2, 3, 4, 5, 6] we called graphs satisfying (15) regular quantum graphs. In general, the regularity condition is satisfied only for a special choice of the potentials (hence the importance of using various "graph dressings") [1, 5].

4. Linear chain graphs. For many network topologies there exist no regular regimes at all [5]. As an example of graphs which can be made regular by an appropriate choice of parameters, let us consider a dressed chain graph (a sequence of 1D square wells), with the vertices positioned at $x = b_0, x = b_1, \dots, x = b_n$ starting at $b_0 = 0$. For every region $b_{i-1} < x < b_i$, the wave function is given by

$$\psi_i(x) = \frac{A_i}{\sqrt{k_i}} e^{ik_i x} + \frac{B_i}{\sqrt{k_i}} e^{-ik_i x}, \quad (16)$$

where $k_i = \sqrt{k^2 - \lambda_i k^2} = \beta_i k$, and where the physically meaningful flux amplitudes $1/\sqrt{k_i}$ are factored out of the arbitrary coefficients A_i and B_i . The boundary conditions at every vertex,

$$\begin{aligned} \frac{A_i}{\sqrt{\beta_i}} e^{ik\beta_i b_i} + \frac{B_i}{\sqrt{\beta_i}} e^{-ik\beta_i b_i} &= \frac{A_{i+1}}{\sqrt{\beta_{i+1}}} e^{ik\beta_{i+1} b_i} + \frac{B_{i+1}}{\sqrt{\beta_{i+1}}} e^{-ik\beta_{i+1} b_i}, \\ A_i \sqrt{\beta_i} e^{ik\beta_i b_i} - B_i \sqrt{\beta_i} e^{-ik\beta_i b_i} &= A_{i+1} \sqrt{\beta_{i+1}} e^{ik\beta_{i+1} b_i} - B_{i+1} \sqrt{\beta_{i+1}} e^{-ik\beta_{i+1} b_i} \end{aligned}$$

can be written in the matrix form

$$M_{i+1,i} \vec{C}_{i+1} = M_{i,i} \vec{C}_i, \quad (17)$$

where

$$M_{ij} \equiv \begin{pmatrix} \frac{1}{\sqrt{\beta_i}} e^{ik\beta_i b_j} & \frac{1}{\sqrt{\beta_i}} e^{-ik\beta_i b_j} \\ \sqrt{\beta_i} e^{ik\beta_i b_j} & -\sqrt{\beta_i} e^{-ik\beta_i b_j} \end{pmatrix}, \quad \vec{C}_i \equiv \begin{pmatrix} A_i \\ B_i \end{pmatrix}.$$

The amplitudes \vec{C}_2 at a vertex V_i can be expressed via the amplitudes at the previous vertex by means of the transfer matrix T_i ,

$$\vec{C}_{i+1} = M_{i+1,i}^{-1} M_{i,i} \vec{C}_i \equiv T_i \vec{C}_i, \quad (18)$$

where

$$T_i = \frac{1}{t_i} \begin{pmatrix} e^{ik(\beta_i - \beta_{i+1})b_i} & r_i e^{-ik(\beta_{i+1} + \beta_i)b_i} \\ r_i e^{ik(\beta_{i+1} + \beta_i)b_i} & e^{ik(\beta_{i+1} - \beta_i)b_i} \end{pmatrix} \quad (19)$$

is unitary, $\det T_i = 1$. Here r_i is the reflection and $t_i = \sqrt{1 - r_i^2}$ is the transmission coefficient,

$$\begin{aligned} r_i &= \frac{\beta_{i+1} - \beta_i}{\beta_{i+1} + \beta_i}, \\ t_i &= \frac{2\sqrt{\beta_i \beta_{i+1}}}{\beta_i + \beta_{i+1}}. \end{aligned}$$

Applying the ‘‘boundary matching’’ equation (18) consecutively to all vertices of the chain yields the equation

$$\vec{C}_n = T \vec{C}_1, \quad (20)$$

where

$$T = T_{n-1} T_{n-2} \dots T_1. \quad (21)$$

Due to the Dirichlet boundary conditions at the end vertices V_0 and V_n of the chain,

$$\vec{C}_1 = \begin{pmatrix} A_1 \\ -A_1 \end{pmatrix}, \quad \vec{C}_n = \begin{pmatrix} A_n e^{-ik_n b_n} \\ -A_n e^{ik_n b_n} \end{pmatrix}, \quad (22)$$

equation (20) can be written in terms of the matrix elements of T only,

$$-e^{ik_n b_n} [t_{11}(k) - t_{12}(k)] = e^{-ik_n b_n} [t_{21}(k) - t_{22}(k)]. \quad (23)$$

Since the spectral equation (23) is linear, the common factor

$$\tau^{-1} = \prod_{i=1}^n t_i^{-1} \quad (24)$$

that multiplies the matrix T (21) cancels out, so that (23) contains only the reflection coefficients r_1, r_2, \dots, r_n , and no transmission coefficients t_i . From the explicit form of T_i it follows that the matrix elements t_{ij} of T ,

$$\left(\prod_{i=1}^n \frac{1}{t_i} \right) \begin{pmatrix} e^{-ik_n b_n} e^{ik S_0} + e^{-ik_n b_n} P(r_i, k) & e^{-ik_n b_n} Q(r_i, k) \\ e^{ik_n b_n} Q^*(r_i, k) & e^{ik_n b_n} e^{-ik S_0} + e^{ik_n b_n} P^*(r_i, k) \end{pmatrix},$$

are certain multivariable polynomials of the variables r_i that may include monomials of all the degrees between 1 and n . Hence the coefficients a_i in the spectral determinant

$$\begin{aligned} \Delta(k) &= e^{2ik_n b_n} (t_{11}(k) - t_{12}(k)) + t_{21}(k) - t_{22}(k) \\ &= 1 + e^{i2(S_0 k - \pi \gamma_0)} - \sum_{i=1}^{2N_\Gamma} a_i e^{i2(S_i k - \pi \gamma_i)}, \end{aligned} \quad (25)$$

are also polynomials in r_i of degree larger or equal to 1.

Hence, by choosing the graph dressing parameters β_i sufficiently close to one another, one can make the coefficients r_i as small as necessary in order to satisfy the regularity condition (15). Hence the regular regime (12) exists for all the linear

chain graphs. Physically this corresponds to the case where the heights of the bond potentials do not differ too much from one another.

As an example, consider the case of a two-bond linear graph with Dirichlet boundary conditions at the end vertices positioned at $x = 0$ and $x = b_2$ [2, 3, 4, 5]. In this case the transfer matrix is

$$T = \frac{1}{t} \begin{pmatrix} e^{ik(\beta_1 - \beta_2)b_1} & r e^{-ik(\beta_1 + \beta_2)b_1} \\ r e^{ik(\beta_1 + \beta_2)b_1} & e^{ik(\beta_2 - \beta_1)b_1} \end{pmatrix}, \quad (26)$$

where r and t are correspondingly the reflection and the transmission coefficients at the middle vertex V_2 . The spectral equation obtained from (26) is

$$\sin [k(\beta_1 b_1 + \beta_2(b_2 - b_1))] + r \sin [k(\beta_1 b_1 - \beta_2(b_2 - b_1))] = 0. \quad (27)$$

Since $r \leq 1$, the condition (15) is satisfied and therefore a two-bond chain graph is always regular [2, 3, 4, 5].

5. Irregular regimes. As a network moves from the regular to the irregular regime, the principle of “one root per interval I_n ” is violated. In the irregular regime certain intervals contain no roots of the spectral equation at all, while others may host two or more roots. The piercing property of the Weyl average [2, 5] also disappears, so in order to separate the intervals that contain exactly one root, one cannot use Weyl’s average and the intersection points (12).

As outlined in [5], in order to repeat the root expansion procedure discussed above, one would need to find some smooth monotonic function $\bar{N}_1(k)$, which pierces every stair of $N(k)$, and find the intersection points $\bar{N}_1(k'_n) = N(k'_n)$. Solving the equation $\bar{N}_1(k'_n) = n$ would lead to the “generalized separators” k'_n , that isolate the roots k_n from each other. Unlike in the regular regime, where the separators k'_n are periodic, the separators k'_n form an almost periodic set [5].

6. Discussion. Since quantum chaos theory deals with non-integrability in the semiclassical regime, the systems it usually addresses are fairly complicated. One of the drawbacks of such complexity is that the various methods used in the theory (such as periodic orbit theory, random matrix theory, etc.) describe the system from quite different perspectives, and the direct connections between these methods are often obscured.

Quantum networks provide a convenient exception to this. For these systems, many essential attributes of quantum chaos theory, and in particular the periodic orbit theory, can be directly established, and the results turn out to be exact. As a result, quantum networks provide a convenient model for testing various phenomenological and approximate methods.

Due to their simplicity, analytical solvability and overall transparency, quantum graphs play the role of the “harmonic oscillator” of the quantum chaos theory.

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