Chaotic Scattering on Graphs

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Quantized, compact graphs were shown to be excellent paradigms for quantum chaos in bounded systems. Connecting them with leads to infinity we show that they display all the features which characterize scattering systems with an underlying classical chaotic dynamics. We derive exact expressions for the scattering matrix, and an exact trace formula for the density of resonances, in terms of classical orbits, analogous to the semiclassical theory of chaotic scattering. A statistical analysis of the cross sections and resonance parameters compares well with the predictions of Random Matrix Theory. Hence, this system is proposed as a convenient tool to study the generic behavior of chaotic scattering systems, and their semiclassical description.

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Quantum graphs provide a very useful tool to study bounded quantum systems which are chaotic in the classical limit \[.\] Here, by attaching infinite leads we turn the compact graphs into scattering systems, and show that they display chaotic scattering \[\text{a},\text{b},\text{c},\text{d},\text{e},\text{f},\text{g},\text{h},\text{i},\text{j},\text{k},\text{l},\text{m},\text{n},\text{o},\text{p},\text{q},\text{r},\text{s},\text{t},\text{u},\text{v},\text{w},\text{x},\text{y},\text{z} \]

on the bonds \[b \text{ or leads } i \] the wave function is expressed in terms of counter propagating waves with a wave number \[k\]:

\[
\psi_b = a_b e^{i(k+A_b)x_b} + a_b' e^{i(k+A_b)(L_b-x_b)}
\]

On the leads:
\[
\psi_i = I_i e^{-ikx_i} + O_i e^{ikx_i}, \tag{1}
\]

where the coordinate \(x_b\) on the bond \(b = (i, j)\) takes the value \(0 (L_b)\) at the vertex \(i (j)\) while \(x_i\) measures the distance from the vertex along the lead \(i\).

The amplitudes \(a_b, a_b'\) on the bonds and \(I_i, O_i\) on the leads are determined by matching conditions at the vertices. They are expressed in terms of the \(v_i\) vertex scattering matrices \(\Sigma^{(i)}_{j,j'}\), where \(j, j'\) go over all the \(v_i\) bonds and the lead which emanate from \(i\). The \(\Sigma^{(i)}\) are symmetric unitary matrices, which guarantee current conservation at each vertex by requiring

\[
\begin{pmatrix}
O_i \\
\chi_{i,j_1}^{(i)} \\
\cdots \\
\chi_{i,j_v}^{(i)}
\end{pmatrix}
= \begin{pmatrix}
\rho^{(i)}_{j_1} & \tau^{(i)}_{j_1} & \cdots & \tau^{(i)}_{j_v} \\
\tau^{(i)}_{j_1} & \delta^{(i)}_{j_1,j_1} & \cdots & \delta^{(i)}_{j_1,j_v} \\
\vdots & \vdots & \ddots & \vdots \\
\delta^{(i)}_{j_v,j_1} & \cdots & \delta^{(i)}_{j_v,j_v} & \delta^{(i)}_{j_v,j_v}
\end{pmatrix}
\begin{pmatrix}
I_i \\
c_{j_1,i}^{(i)} \\
\cdots \\
c_{j_v,i}^{(i)}
\end{pmatrix} \tag{2}
\]

where \(c_{j,i}^{(i)} = a_{j,i} e^{i(k+A_{i,j})(L_{i,j})}\). Above, the vertex scattering matrix \(\Sigma^{(i)}\) was written explicitly in terms of the vertex reflection amplitude \(\rho^{(i)}\), the lead-bond transmission amplitudes \(\{\tau^{(i)}\}\), and the \(v_i\) bond-bond transition matrix \(\delta^{(i)}_{j,j'}\), which is sub unitary (\(|\det \delta^{(i)}| < 1\)), due to the coupling to the leads. As an example, for \(v\)-regular graphs \((v = v(i))\) with Neumann matching conditions on the vertices, \(\delta^{(i)}_{j,j'} = \frac{2}{v+1} - \delta_{j,j'}; \tau^{(i)}_{j} = \frac{2}{v+1}; \rho^{(i)} = \frac{2}{v+1} - 1.\) \tag{3}

by boundary conditions on the vertices \(L\). The “vector potentials” \(A_b = -A_j\) are introduced to break time reversal symmetry, and their value may vary from bond to bond. On each of the bonds \(b\) or leads \(i\) the function is expressed in terms of counter propagating waves with a wave number \(k\):

On the bonds:
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\psi_b = a_b e^{i(k+A_b)x_b} + a_b' e^{i(k+A_b)(L_b-x_b)}
\]

On the leads:
\[
\psi_i = I_i e^{-ikx_i} + O_i e^{ikx_i}, \tag{1}
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The amplitudes \(a_b, a_b'\) on the bonds and \(I_i, O_i\) on the leads are determined by matching conditions at the vertices. They are expressed in terms of the \(v_i\) vertex scattering matrices \(\Sigma^{(i)}_{j,j'}\), where \(j, j'\) go over all the \(v_i\) bonds and the lead which emanate from \(i\). The \(\Sigma^{(i)}\) are symmetric unitary matrices, which guarantee current conservation at each vertex by requiring

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\end{pmatrix}
= \begin{pmatrix}
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\tau^{(i)}_{j_1} & \delta^{(i)}_{j_1,j_1} & \cdots & \delta^{(i)}_{j_1,j_v} \\
\vdots & \vdots & \ddots & \vdots \\
\delta^{(i)}_{j_v,j_1} & \cdots & \delta^{(i)}_{j_v,j_v} & \delta^{(i)}_{j_v,j_v}
\end{pmatrix}
\begin{pmatrix}
I_i \\
c_{j_1,i}^{(i)} \\
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\end{pmatrix} \tag{2}
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where \(c_{j,i}^{(i)} = a_{j,i} e^{i(k+A_{i,j})(L_{i,j})}\). Above, the vertex scattering matrix \(\Sigma^{(i)}\) was written explicitly in terms of the vertex reflection amplitude \(\rho^{(i)}\), the lead-bond transmission amplitudes \(\{\tau^{(i)}\}\), and the \(v_i\) bond-bond transition matrix \(\delta^{(i)}_{j,j'}\), which is sub unitary (\(|\det \delta^{(i)}| < 1\)), due to the coupling to the leads. As an example, for \(v\)-regular graphs \((v = v(i))\) with Neumann matching conditions on the vertices, \(\delta^{(i)}_{j,j'} = \frac{2}{v+1} - \delta_{j,j'}; \tau^{(i)}_{j} = \frac{2}{v+1}; \rho^{(i)} = \frac{2}{v+1} - 1.\) \tag{3}
Combining the equations for all the vertices, we obtain the $V \times V$ scattering matrix $S^{(V)}$ which relates the outgoing and incoming amplitudes on the leads,

$$S_{i,j}^{(V)} = \delta_{i,j} \rho^{(i)} + \sum_{p \in P_{i \rightarrow j}} B_p e^{i(k_p + b_p)}$$

(5)

where $P_{i \rightarrow j}$ is the set of the trajectories on $\hat{G}$ which lead from $i$ to $j$. $B_p$ is the amplitude corresponding to a path $p$ whose length and directed length are $l_p = \sum_{b \in P} L_b$ and $b_p = \sum_{b \in P} L_b A_b$ respectively. The scattering amplitude $S_{i,j}^{(V)}$ is a sum of a large number of partial amplitudes, whose complex interference brings about the typical irregular fluctuations of $|S_{i,j}^{(V)}|^2$ as a function of $k$.

The resonances are the (complex) zeros of

$$Z_{\hat{G}}(k) = \det \left( I - \hat{S}(k; A) \right).$$

(6)

The eigenvalues of $\hat{S}$ are in the unit circle, and therefore the resonances appear in the lower half of the complex $k$ plane. Denoting the eigenvalues of $S^{(V)}(k)$ by $e^{i\theta_i(k)}$, we have $S^{(V)}(k) = \exp[i\Theta(k)] = \exp[i \sum_{i=1}^{V} \theta_i(k)]$ is derived from (3) by standard manipulations giving

$$\Theta(k) - \Theta(0) = -2i m \log \det(I - \hat{S}(k; A)) + \mathcal{L} k.$$  

(7)

where $\mathcal{L} = 2 \sum_{b=1}^{B} L_b$ is twice the total length of the bonds of $\hat{G}$. The resonance density $d_R(k)$ (which is proportional to the Wigner delay time) is given by

$$d_R(k) = \frac{1}{2\pi} \frac{|\Theta(k)|}{\tau^2}.$$ 

(8)

where the sum is over the set $P_n$ of primitive periodic orbits whose period $n_p$ is a divisor of $n$, with $r = n/n_p$, $l_p$ and $b_p$ are the length and the directed length, respectively, and the amplitudes $\tilde{A}_p$ are the products of the bond-bond scattering amplitudes $\tilde{b}_{b,b'}$ along the primitive loops. The mean resonance spacing is given by

$$\Delta = \frac{2\pi}{\mathcal{L}}.$$  

FIG. 1. (a) The 5000 resonances of a single realization of a pentagon with $A \neq 0$. The solid line marks the position of the gap $\gamma_{gap}$. (b) The distribution $P(\gamma)$. The solid line is the RMT prediction. The difference $P(\gamma) - P_{CUE}(\gamma)$ is shown in the inset.

The classical dynamics associated with $\hat{G}$ can be easily defined on the bonds, but not on the vertices which are singular points. However, a Liouville description is constructed (see [3]) by considering the evolution of a phase-space density over the $2B$ dimensional space of directed bonds. The corresponding evolution operator consists of the transition probabilities $\tilde{U}_{b,b'}$ between connected bonds $b,b'$, taken from the corresponding quantum evolution operator, $\tilde{U}_{b,b'} = |\tilde{R}_{b,b'}|^2$. Due to scattering to the leads $\sum_{b'} \tilde{U}_{b,b'} < 1$, and the phase-space measure is not preserved, but rather, decays in time. Let $\tilde{p}_b(n)$ denote the probability to occupy the bond $b$ at the (topological) time $n$. The probability to remain on $\hat{G}$ is

$$\tilde{P}(n) \equiv \sum_{b=1}^{2B} \tilde{p}_b(n) = \sum_{b,b'} \tilde{U}_{b,b'} \tilde{p}_b(n-1) \approx e^{-\Gamma_c n} \tilde{P}(0)$$

(9)

where $\exp(-\Gamma_c)$ is the largest eigenvalue of the “leaky” evolution operator $\tilde{U}_{b,b'}$. For the $v$-regular graph [3], the probability to leak to the lead per time step is $\tau^2$, hence, $\Gamma_c \approx (2/(1+v))^2$. The set of trapped trajectories whose occupancy decays exponentially in time is the analogue
of the strange repeller in generic Hamiltonian systems displaying “chaotic scattering”.

The formalism above can be easily modified for graphs where not all the vertices are attached to leads. If \( l \), is not attached, one has to set \( \rho^{(l)} = 1, \tau_j^{(l)} = 0 \) in the definition of \( \Sigma^{(l)} \). The dimension of \( S_{\{V\}} \) is changed accordingly.

For generic graphs, the eigenvalues of the \( \hat{S} \) matrix are strictly inside the unit circle so the resonance widths \( \Gamma_n \equiv -2\Im(m_n) \), are excluded from the domain \( \Gamma_n \geq \Gamma_{\text{gap}} = -2 \log(|\lambda_{\text{max}}|)/L_{\text{max}} \), where \( \lambda_{\text{max}} \) is the largest eigenvalue of \( \hat{S}(0; \Delta) \) and \( L_{\text{max}} \) is the longest bond. The existence of a gap - typical for chaotic scattering - is apparent in Fig. 1a. The form factor for the compact system [12] is displayed “chaotic scattering”.

Another signature of overlapping resonances are the Ericson fluctuations observed in the \( k \) dependence of the scattering cross-sections. They are one of the prominent features which characterize generic chaotic scattering, in the semiclassical limit. A convenient measure for Ericson fluctuations is the autocorrelation function

\[
C(\chi; \nu) = \frac{1}{\Delta \gamma} \sum_{j=j_{\text{min}}}^{j_{\text{max}}} \langle S_{j, j+\nu}^{(V)}(k + \frac{\lambda}{2}) S_{j, j+\nu}^{(V)*}(k - \frac{\lambda}{2}) \rangle_k
\]

where \( \Delta = j_{\text{max}} - j_{\text{min}} + 1 \). Substituting (6) in (11) we split the sum over trajectories into two distinct parts: the contributions of short trajectories are computed explicitly by following the multiple scattering expansion up to trajectories of length \( l_{\text{max}} \). The contribution of longer orbits are approximated by using the diagonal approximation, which results in a Lorentzian with a width \( \gamma_{\text{Er}} \), expected to be well approximated by \( \gamma_{\text{cl}} \). Including explicitly up to \( n = 3 \) scatterings we get,

\[
C(\chi; \nu) \approx G e^{2\lambda t} \frac{\gamma_{\text{Er}}}{\gamma_{\text{Er}} - i\lambda} + \frac{1}{\Delta} \sum_{j=j_{\text{min}}}^{j_{\text{max}}} \left[ \tau^4 e^{i\chi L_{j, j+\nu}} + \tau^4 \rho^2 e^{i\chi L_{j, m+j} + \nu} + \tau^6 \sum_{m \neq j, j+\nu} e^{i\chi(L_{j, m} + L_{m, j+\nu})} \right]
\]

where the constant \( G \) is determined by the normalization condition \( C(\chi = 0; \nu = 1) = 1 \). The interplay between the contributions of long and short periodic orbits is shown in Fig. 3a. For overlapping resonances, the autocorrelation function is well reproduced by the Lorentzian expected from the standard theory of Ericson fluctuations. The

\[
K_R(t) = \int d\chi \ e^{i2\pi \tau \lambda t} (\tilde{d}_R(k + \frac{\lambda}{2}) \tilde{d}_R(k - \frac{\lambda}{2}))_k
\]
other case corresponds to isolated resonances where the contributions of short paths are clearly seen. From each of the various statistical measures of the resonance density and the cross sections fluctuations discussed above, we extracted the effective average $\gamma$, which would fit best the numerical data. In Fig. 3b we compare these numerical values, with the classical expectation, and the predictions of RMT \cite{13}. The results justify the use of the classical estimate for the computation of these quantities especially in the limit $V \to \infty$ for fixed $v/V$ (which is the analogue of the semiclassical limit). In this limit, the RMT and and the classical estimate coincide.

To investigate further the statistical properties of the $S^{(V)}$ matrix, we study the distribution of scaled partial Wigner delay times $T = \frac{\Delta}{2\pi} \frac{\partial \theta_r(k)}{\partial k}$. The resulting distribution for various graphs with $A = 0$ and $A \neq 0$ are shown in Figs. 4a,b respectively, together with the predictions of RMT \cite{13}. An overall agreement is evident. Deviations appear at the short time regime (i.e. short orbits), during which the “chaotic” component due to multiple scattering is not yet fully developed \cite{14}.

To summarize, we presented analytical and numerical results, on the basis of which, we propose quantum graphs as a model for the study of quantum chaotic scattering. Their simplicity enable us to get new understanding on the subject. Because of lack of space we defer the discussion of other results and further comparisons with RMT to a later publication \cite{15}.

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