Quantum ergodicity on graphs

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We investigate the equidistribution of the eigenfunctions on quantum graphs in the high-energy limit. Our main result is an estimate of the deviations from equidistribution for large well-connected graphs. We use an exact field-theoretic expression in terms of a variant of the supersymmetric nonlinear $\sigma$-model. Our estimate is based on a saddle-point analysis of this expression and leads to a criterion for when equidistribution emerges asymptotically in the limit of large graphs. Our theory predicts a rate of convergence that is a significant refinement of previous estimates, long-assumed to be valid for quantum chaotic systems, agreeing with them in some situations but not all. We discuss specific examples for which the theory is tested numerically.

PACS numbers: 05.45.Mt,03.65.Sq,11.10.Lm

Quantum graphs may be viewed as networks of quantum wires or waveguides and are standard models for large molecules and complex quantum systems. Since the seminal paper [1] of Kottos and Smilansky, they have become a paradigm for quantum chaos and universal interference effects which can be observed in the statistics of their spectra and of their eigenfunctions (see [2] for a recent review). Kottos and Smilansky showed (numerically) that the spectral statistics for a large class of quantum graphs follow the predictions of the Gaussian random-matrix (RM) ensembles up to deviations which become smaller when the size of the graph increases. They also derived an exact trace formula, analogous to Gutzwiller’s trace formula which is a semiclassical approximation for classically chaotic systems. Subsequently it was found that some special graphs, namely star graphs, exhibit intermediate spectral statistics which correspond to RM statistics in the spectrum of quantum chaotic systems. General conjectures for this rate have been put forward based on heuristic semiclassical arguments, RM theory, the random wave model and periodic orbit theory [3]. Surprisingly, establishing when quantum graphs are quantum ergodic has proved to be a significant problem. The issue is subtle: Neumann star graphs are known not to be quantum ergodic (even though their classical dynamics is ergodic) [4], but quantum ergodicity has been proved for a family of graphs constructed from certain one-dimensional maps [5]. Applying the field-theoretical approach of Gnutzmann and Altland [6] enables us to tackle the quantum ergodicity problem for graphs, yielding a criterion for when quantum ergodicity can be expected for sequences of graphs in the limit as the size tends to infinity and, most significantly, an explicit estimate of the rate at which the limit is approached. Interestingly, in some situations this estimate coincides with the expression conjectured in [8], but in others it differs from it in a fundamental way.

In the scattering approach a quantum graph can be defined by a pair $(G, S)$, where $G$ is a metric graph with $B$ bonds of finite lengths $L_b > 0$ (and coordinates $0 < x_b < L_b$), and $S$ is a $2B \times 2B$ unitary matrix that will be discussed below. We assume that the graph is simple (at most one bond between any two vertices and no loops) and connected, and that the bond lengths are incommensurate (rationally independent) and all in some fixed interval $0 < L_{\text{min}} < L_b < L_{\text{max}}$. Let us define the $2B$ double indices $\alpha = (b, d)$ for directed bonds where $b = 1, \ldots, B$ refers to the bond and $d = \pm 1$ to the two directions on each bond (the lower case Greek letters $\alpha$ and $\gamma$ will be used to denote directed bonds throughout). The matrix $S_{\alpha, \alpha'}$ contains the probability amplitudes for a particle to be scattered from $\alpha' = (b', d')$ to $\alpha = (b, d)$. If the end of $\alpha'$ and beginning of $\alpha$ are different vertices then $S_{\alpha, \alpha'} = 0$. We assume that all scattering amplitudes in $S$ are energy-independent. A graph is time-reversal invariant if the scattering matrix obeys $S = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} S^T \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ such that the scattering amplitudes for the processes $(b, d) \to (b', d')$ and $(b', -d') \to (b, -d)$ coincide. The quantum dynamics consists in the propagation of one-dimensional waves on the bonds of $G$, with scattering at the vertices encoded.
by $S$. The complete quantum dynamics is then encapsulated in the quantum map defined by the unitary matrix $\U(k) = T(k)S$ where the diagonal matrix $T(k) = e^{ikL}$, with $L = \text{diag}(L_1, \ldots, L_B)$, contains the phase factors for propagation with wavenumber $k > 0$ from one end of a bond to the other. $\U(k)$ describes the succession of scattering at a vertex and propagation to the next vertex of a wave function $\Psi(x) \equiv \{\psi_b(x_b)\}$ on the graph, where the wave function is expressed in terms of $2B$ complex amplitudes $a_{b,d}$ (which we will combine into a $2B$-dimensional vector $\mathbf{a}$) of plane waves such that $\psi_b(x_b) = \frac{1}{\sqrt{N}} \left( a_{b,1} e^{ikx} + a_{b,-1} e^{-ikx} \right)$ ($N$ is a normalization constant). The quantization condition on a graph implies that the quantum map does not change the wave function: $\U(k)\mathbf{a} = \mathbf{a}$. Equivalently $\U(k)$ has an eigenvalue unity -- a condition that is satisfied for a discrete set of wave numbers $k_n$ which form the spectrum. Eigenstates will be denoted by $\Psi_n$ and the corresponding coefficients by the vector $\mathbf{a}_n$.

The classical counterpart of the quantum graph $(G,S)$ is a Markov process on the directed bonds of $G$ which is obtained by replacing the quantum scattering amplitudes by the classical probabilities $M_{a,a'} = |U_{a,a'}(k)|^2 = |S_{a,a'}|^2$. The bistochastic matrix $M$ does not depend on the wave number and propagates probability distributions on the directed bonds [1, 2]. For a connected graph the classical map $M$ is generically mixing (i.e. $\lim_{n \to \infty} (M^n)_{a,a'} = \frac{1}{2^B}$) [11] and always ergodic in the stochastic sense. The spectrum of $M$ is confined to lie on or within the unit circle with (exactly) one eigenvalue unity which corresponds to equidistribution on the bonds. We write the eigenvalues of $M$ as $1 - m_i$ with $m_i > 0$ and $\text{Rem}_i > 0$ for $i = 2, \ldots, 2B$ -- this notation anticipates the interpretation of the quantities $m_i$ as masses in a field-theoretic setting: massive modes correspond to decaying modes of the classical map while the invariant measure is massless. The classical spectral gap $\Delta_g = \min_{i=2 \ldots 2B} |m_i|$ determines the slowest decay rate in the (time averaged) classical dynamics. It will turn out that a simple criterion for quantum ergodicity can be expressed in terms of the spectral gap $\Delta_g$, while a more detailed criterion uses the full set of masses in an eigenstate $\Psi_n$. Note, that the topology of a graph influences the spectrum, e.g. any graph which can be cut into two disconnected components of similar size by just erasing one bond has a small gap which is at most of order $1/B$.

Our concern here is to determine how the probability density associated with the eigenstate $\Psi_n$ is spread over $G$ as $k_n \to \infty$. Let us introduce observables that are constant on each bond. These can be represented by real diagonal $2B \times 2B$ matrices $V = \text{diag}(V_1, \ldots, V_B)$. The expectation value of the observable $V$ in an eigenstate $\Psi_n$ is given by

$$\langle V \rangle_n = \sum_b V_b \int_0^{L_b} dx_b |\psi_b(x_b)|^2 = \frac{\langle a_n | V | a_n \rangle}{\langle a_n | a_n \rangle} + \mathcal{O}(k^{-1}).$$

With the spectral counting function $N(k) = \sum_n \theta(k - k_n) \sim \frac{L}{2\pi} k$ the spectral average of the expectation value of the observable $V$ is given by the metric average over the graph

$$A_V = \lim_{k \to \infty} \frac{1}{N(K)} \sum_{k_n \leq K} \langle V \rangle_n = \frac{\text{tr} LV}{\text{tr} L}. \quad (1)$$

This statement is known as the local Weyl law and can be recovered for any finite graphs straightforwardly, e.g. by the periodic-orbit approach developed in [1]. For a uniformly distributed eigenstate the coefficients $a_n$ are all of equal modulus such that the expectation value $\langle V \rangle_n$ coincides with the spectral mean for any observable $V$.

Quantum unique ergodicity is the statement that such uniform distributions are obtained in the high energy limit of any subsequence of states $\Psi_{n_i}$ with $n_{i+1} > n_i$, i.e. one has $\lim_{i \to \infty} \langle V \rangle_{n_i} = A_V$. This property turns out to be too strong for graphs and cannot be expected to be realized because it is known that sequences of states exist that are scarred by short periodic orbits [3, 12]. The less strong property of quantum ergodicity can be defined by the vanishing of the variance

$$F_V = \left( \lim_{k \to \infty} \frac{1}{N(K)} \sum_{k_n \leq K} \langle V \rangle_n^2 \right) - A_V^2, \quad (2)$$

i.e. $F_V = 0$ for all observables $V$. This implies the existence of subsequences of eigenstates of density one for which $\lim_{i \to \infty} \langle V \rangle_{n_i} = A_V$. It will be seen later, see [4], that $F_V$ in general does not vanish for a finite graph. Indeed one may expect, as for spectral statistics, that quantum ergodicity can only be attained in the limit $B \to \infty$. One therefore considers a sequence $\{(G_l, S_l)\}$ of quantum graphs having increasing numbers of bonds $B_{l+1} > B_l$. For each $l$, one defines $A_{V_l}$ and $F_{V_l}$ by formulas (1) and (2) applied to $(G_l, S_l)$. One still has to specify the acceptable sequences $\{V_l\}$ of observables. For these it is natural to require the existence of $\lim_{l \to \infty} A_{V_l}$ and a bound from above for $|V_l|$, e.g. $\|V_l\|_2$. Then a sequence $\{(G_l, S_l)\}$ is said to be asymptotically quantum ergodic if $F_{V_l} \to 0$ as $l \to \infty$ for any acceptable sequence of observables $\{V_l\}$. In order to avoid cumbersome notation, we will separately work on a single quantum graph $(G_l, S_l)$ of the sequence and drop the index $l$. Without loss of generality we will also assume $A_{V_l} = 0$.

Our aim is to show that a large class of such sequences exhibit asymptotic quantum ergodicity and to give explicit conditions which distinguish between ergodic and non-ergodic sequences. In the course of our derivation we will also obtain an estimate of $F_V$ for large (but finite) quantum graphs. While previous attempts have largely relied on periodic-orbit theory we will here employ a field-theoretic approach. In order to implement our approach
let us first introduce
\[
\tilde{F}_V = \lim_{k \to \infty} \frac{1}{N(K)} \sum_{k < K} \langle V \rangle^2 \frac{2 B(a_n | L | a_n)}{\text{tr } L}
\]
\[
= \frac{4 B}{(\text{tr } L)^2} \sum_{\alpha, \alpha'} \langle V \rangle^2 \alpha_a L_\alpha \alpha_a \alpha' \xi_{\alpha \alpha'},
\]
which vanishes asymptotically if and only if \( F_V \) vanishes (note that we assume \( A_V = 0 \)). For all practical purposes, \( F_V \) and \( \tilde{F}_V \) are the same for a large graph. In \( \xi \) we have implicitly defined \( \xi_{\alpha \alpha'} \), which will be the central quantity of interest. It can be expressed as
\[
\xi_{\alpha \alpha'} = \lim_{\epsilon \to 0^+} \epsilon \frac{d^2}{dj_+ dj_-} k \langle U_\alpha(k) \rangle \xi_{\alpha \alpha'},
\]
\[
= \frac{\langle \text{det}(U_\alpha(k) + j_+ E_{\alpha}^\alpha) \text{det}(U_\alpha(k)^\dagger + j_- E_{\alpha}^{\alpha'}) \rangle}{\langle \text{det}(U_\alpha(k)) \rangle \langle \text{det}(U_\alpha(k)^\dagger) \rangle}
\]
(4)
where \( \langle \ldots \rangle_k \) is taken over graphs where the integral over \( k \) in (4) can be replaced exactly by an integral over \( B \) independent phases for incommensurate bond lengths the integral over \( k \) in (4) can be replaced exactly by an integral over \( B \) independent phases for incommensurate bond lengths the integral over \( k \) in (4) can be replaced exactly by an integral over \( B \) independent phases. For broken time-reversal symmetry the \( \sigma \)-model for the graph leads to the exact expression
\[
\xi_{\alpha \alpha'} = \frac{d^2}{dj_+ dj_-} k \langle U_\alpha(k) \rangle \xi_{\alpha \alpha'},
\]
\[
= \int d(Z, \tilde{Z}) \text{sdet}(1 - Z \tilde{Z}) \text{sdet}^{-1}(1 - Z S_\alpha \tilde{Z} S_\alpha).
\]
Here \( Z = \text{diag}(Z_1, \ldots, Z_B) \) and \( \tilde{Z} = \text{diag}(\tilde{Z}_1, \ldots, \tilde{Z}_B) \) are \( 4B \times 4B \) block-diagonal supermatrices where each block is a \( 4 \times 4 \) matrix \( Z_{b,dd',ss'} \) (\( d = \pm 1 \) is the direction index and \( s = B, F \) refers to bosonic and fermionic sectors of the supermatrix, see [4] for further details). The matrices \( S_\alpha = (1 - j_+ E_{\alpha}^\alpha P_{FF}) S \) and \( S_\alpha^\dagger = S_\alpha^\dagger (1 - j_- E_{\alpha}^{\alpha'} P_{FF}) \) (where \( P_{FF} \) is the projector onto the fermionic sector) contain the scattering amplitudes and source terms \( \propto j_\pm \). For time-reversal symmetric graphs an exact \( \sigma \)-model can be derived with slightly more technical effort. The result looks formally similar to [5] with the superdeterminants replaced by their square roots and with the dimension of the matrices doubled (see [4]). Here we will give explicit formulae only for broken time-reversal symmetry but will state the final results also for the time-reversal invariant case. More details will be given elsewhere [13].

We calculate the integral over \( Z \) and \( \tilde{Z} \) in a saddle-point approach (writing \( \text{sdet}^{\pm 1}(1 - Z \tilde{Z} B) = \exp(\pm \text{st } \log((1 - Z \tilde{Z} B))) \) where the saddle-point analysis is performed at \( j_\pm = 0 \). The saddle-point equations lead to a mean-field solution \( Z_{b,dd',ss'} = Y_{s's'dd'} \), \( \tilde{Z}_{b,dd',ss'} = \tilde{Y}_{s's'dd'} \) where the \( 2 \times 2 \) matrices \( Y \) and \( \tilde{Y} \) span the saddle-point manifold. Note that the dependence of the integrand in (4) on the scattering matrix \( S \) of the graph drops out for mean-field configurations so that these give a universal contribution to \( \xi_{\alpha \alpha'} \). Configurations orthogonal to the saddle-point manifold are taken into account in a Gaussian approximation — here, crucially, the system dependence does not drop out. There is a direct correspondence between the modes of the classical map \( M \) and the field configurations. Equidistribution on the graph corresponds to the unique eigenvalue unity of \( M \) on one side and to the mean-field configuration on the other side. This is the massless mode which is calculated exactly in our approach. The decaying modes of the classical map correspond to the (massive) configurations of the supermatrices \( Z \) and \( \tilde{Z} \) which are orthogonal to the saddle-point manifold. The contribution of the massive modes (and their coupling to the mean-field mode) are only taken into account approximately. This goes beyond the diagonal approximation in a periodic-orbit approach to \( \xi_{\alpha \alpha'} \), which is equivalent to a Gaussian approximation of all modes in the field-theoretic approach and which actually diverges like \( 1/e \) for the quantity we are interested in (further details will be published elsewhere [13]).

The contributions from the mean-field configurations and the Gaussian fluctuations turn out to be additive [10] and thus we may write the fluctuations as \( \tilde{F}_V = F^\text{meanfield}_V + F^\text{Gauss}_V \). An explicit calculation yields
\[
F^\text{meanfield}_V = \beta \frac{\text{tr } L^2 V^2}{(\text{tr } L)^2}
\]
for the universal contribution. Here \( \beta = 1 \) for broken time-reversal invariance and \( \beta = 2 \) for time-reversal invariant graphs. The integration over the Gaussian fluctuation yields
\[
F^\text{Gauss}_V = \frac{2}{(\text{tr } L)^2} \text{tr} \frac{M}{1 - M} L^2 V^2
\]
where the trace is over all massive modes such that the unit eigenvalue of \( M \) is excluded.

Equations (6) and (7) are our main results. Crucially, (7) shows that the behavior of \( \tilde{F}_V \) for large graphs depends on the spectrum of the classical map \( M \). Slowly decaying classical modes with eigenvalues near 1 give rise to large deviations from universality in the rate of quantum ergodicity. This does not conform to expectations based on the conjectures in [8], which correspond to ignoring the Gaussian fluctuations.

In the remainder we discuss the different behaviors that sequences of quantum graph may exhibit depending on the spectral properties of \( M \) and on the range of validity of equations (6) and (7). The dependence of
which makes it hard to estimate the error. Especially if we restrict ourselves to the most simple generic choice, the spectral gap remains finite as $B \to \infty$ is correct we do not expect the Gaussian approximation to give the exact asymptotic result if $\tilde{F}_V$ is dominated by the massive contributions. We have checked numerically the validity of the saddle-point approximation for two sequences of complete graphs with different scattering matrices; see Fig. 1. In the first sequence we have used discrete Fourier transform (DFT) matrices at each vertex. In order to break time-reversal invariance we also added magnetic fields. In this case $\tilde{F}_V^{\text{meanfield}} \gg \tilde{F}_V^{\text{Gauss}} \approx 0$ and the numerics show perfect agreement. In the second sequence we have used a scattering matrix which is equivalent to the so-called Neumann (or Kirchhoff) boundary conditions at each vertex. These strongly enhance backscattering which leads to a large number of small masses. As one may expect, the saddle-point approximation is far from perfect in this case but still gives a reasonable estimate of the rate.

We would like to thank Uzy Smilansky for invaluable discussions.

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[16] Note that for $j_b \neq 0$ the saddle-point manifold becomes coupled to the Gaussian fluctuations. This coupling turns out to be essential to obtain a contribution to $\xi_{\alpha_1}^{\alpha_2}$ in the limit $\epsilon \to 0$. The details will be discussed in [13].