Leading Off-Diagonal Correction to the Form Factor of Large Graphs

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Using periodic-orbit theory beyond the diagonal approximation we investigate the form factor, $K(\tau)$, of a generic quantum graph with mixing classical dynamics and time-reversal symmetry. We calculate the contribution from pairs of self-intersecting orbits that differ from each other only in the orientation of a single loop. In the limit of large graphs, these pairs produce a contribution $-2\tau^2$ to the form factor which agrees with random-matrix theory.

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One of the fundamental open questions in the quantum theory of classically chaotic systems is whether the fluctuations in the spectra follow the predictions of random-matrix theory (RMT) [1] and, if so, precisely under which conditions. An interesting spectral statistics to consider is the form factor $K(\tau)$, which is the Fourier transform of the spectral two-point correlation function and depends on a dimensionless time τ measured in units of the Heisenberg time. We will concentrate on systems with time-reversal symmetry, the appropriate ensemble of random matrices is the Gaussian orthogonal ensemble (GOE), and the corresponding form factor is [2]

$$K_{\mathrm{GOE}}(\tau) = 2\tau - \tau\log(1+2\tau) \qquad (0 \le \tau \le 1)$$
$$= 2\tau - 2\tau^2 + O(\tau^3). \tag{1}$$

There is ample numerical evidence [2] for the conjecture that, in the semiclassical limit, Eq. (1) correctly describes the spectral fluctuations of any "typical" system with chaotic classical limit, but there is no complete analytical theory. A natural starting point for such a theory is the Gutzwiller trace formula [3] expressing the spectral density in terms of classical periodic orbits (POs). However, until recently, the only method for dealing with the resulting double sum over POs was Berry's diagonal approximation [4] which rests on the assumption that classical POs are uncorrelated unless related by exact symmetries. This can be justified only in the limit $\tau \to 0$, and the diagonal approximation results in the leading-order term 2τ but fails to reproduce any higher-order corrections in Eq. (1).

The analogy to diagrammatic perturbation theory for disordered systems suggests that the leading correction to the diagonal approximation is related to correlations between pairs of orbits which differ only in one self-intersection [5,6] (see Fig. 1). These correlations were recently calculated for certain Riemannian surfaces with constant negative curvature [7,8], and they were found to reproduce the $-2\tau^2$ term in Eq. (1).

In this Letter, we study the contribution from self-intersecting orbits in a very different class of systems: quantum graphs [9]. In these systems, two-point correlation functions can be expressed as combinatorial sums and therefore allow a treatment with fundamentally different analytical tools [10–12]. Our result can be summarized as follows. The contributions to the form factor from self-intersecting orbit pairs differing in the orientation of a single loop are calculated analytically. We find that they add to $-2\tau^2$ if correlations in the *classical* dynamics of the graph decay sufficiently fast [Eq. (4) below]. The role of the unitarity of the quantum dynamics is particularly transparent in our derivation, and classical information enters only via the Frobenius-Perron operator—a concept which is not specific to system or representation. However, the most important aspect in which our result extends Refs. [7,8] is that it applies to *generic* graphs and not only to uniformly hyperbolic systems where all POs share the same Lyapunov exponent.

We consider a graph with N vertices and B directed bonds. The quantum dynamics on the graph is defined by the energy dependent unitary bond-scattering matrix S,

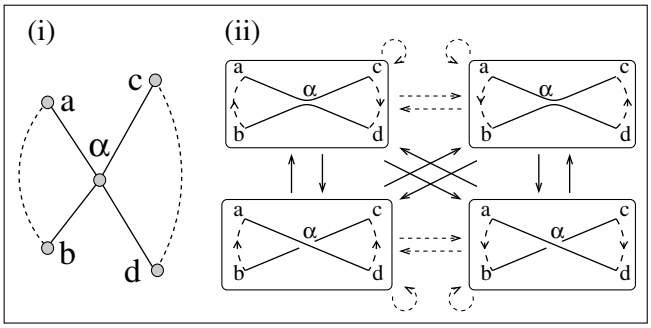

FIG. 1. In (i) we show two loops on a graph intersecting at a vertex α. The dashed arcs indicate trajectories between vertices a,b and c,d, respectively. They may contain intermediate vertices which are not necessarily pairwise different. In (ii) we show all orbits which traverse each of the loops exactly once. Dashed arrows between orbits indicate pairs that were counted in the diagonal approximation. Solid arrows indicate pairs missed by the diagonal approximation but counted by our method.

which can be interpreted as the discrete time-evolution operator on the B dimensional Hilbert space of directed bonds. The matrix element $S_{m'l,lm} = \sigma^{(l)}_{m'm} e^{ikL_{ml}}$ prescribes a transition amplitude from bond $m \to l$ to bond $l \to m'$. This amplitude consists of a phase kL_{ml}, where L_{ml} is the length of the bond $m \to l$, accumulated during the free propagation with wave number k from vertex m to vertex l, and an element of the unitary vertex-scattering matrix $\sigma^{(l)}$ describing the vertex l [9]. Matrix elements which do not correspond to any bond-to-bond transitions are zero. Solely for the purpose of a transparent presentation, we assume that for each pair of vertices m, l there is at most one directed bond $m \to l$. To ensure the invariance of the system under time reversal, we require the matrices $\sigma^{(l)}$ to be symmetric and $L_{ml} = L_{lm}$ for all pairs of connected vertices l, m. Otherwise different bond lengths are assumed rationally independent.

The form factor of a graph can be defined as [10]

$$K^{(B)}(\tau) = B^{-1} \langle |\mathrm{tr} S^t(k)|^2 \rangle_k \,, \tag{2}$$

where $\tau = t/B$, and the average is over the wave number $\langle \cdot \rangle_k = \lim_{\kappa\to\infty} \kappa^{-1} \int_0^\kappa dk(\cdot)$. We will be interested in the limiting behavior $K(\tau) = \lim_{B\to\infty} K^{(B)}(\tau)$, i.e., we first fix τ and consider larger and larger graphs, a procedure corresponding to the semiclassical limit. Then we look at the expansion of $K(\tau)$ around $\tau = 0$.

Associated with the unitary matrix S is the doubly stochastic matrix M with $M_{m'l,lm} = |S_{m'l,lm}|^2 = |\sigma^{(l)}_{m'm}|^2$. This matrix defines a Markov chain on the graph which represents the classical analogue of our quantum system [9,13]. M can be considered as the Frobenius-Perron operator of this discrete classical dynamics. Physically, $[M^t]_{m'l',ml}$ is the classical probability to get from bond $(l \to m)$ to bond $(l' \to m')$ in t steps. We will assume the Markov chain to be mixing (and consequently also ergodic), such that any initial distribution approaches for a long time an equidistribution over all bonds,

$$\lim_{t\to\infty} M^t_{m'l',ml} = \frac{1}{B} \,, \tag{3}$$

for all pairs of bonds $m \to l$, $m' \to l'$. Equation (3) is satisfied if the eigenvalue unity of M, corresponding to the invariant equidistribution, is the only eigenvalue on the unit circle while all others are inside. For a given finite graph this is a very weak condition. However, we consider a family of graphs for which the limits of large graphs $N \to \infty$ (and, as a consequence, $B \to \infty$) and large times $t \to \infty$ are connected by $t/B = \tau$ being constant: The size of the graph sets the time scale for the decay of classical correlations. Therefore we make Eq. (3) more precise and require as a *sufficient* condition for the results to be derived below:

$$\lim_{B\to\infty} B^2 N^3(B) \max \left| M^{\tau B}_{m'l',ml} - \frac{1}{B} \right| = 0 \,. \tag{4}$$

This is only slightly stronger than the recent conjecture by Tanner [14], that RMT behavior results in graphs if the spectral gap between unity and the magnitude of the next biggest eigenvalue vanishes slower than the inverse matrix size $1/B$. At the end of this Letter, we give two examples, in which equidistribution is approached at least exponentially fast as $B \to \infty$, such that our results do apply.

Expanding the trace of the matrix powers in Eq. (2) and performing the average over k, we can represent the form factor in terms of pairs of returning trajectories p, q on the graph which share the same length $K^{(B)}(\tau) = B^{-1} \sum_{p,q} A_p A^*_q \delta_{L_p,L_q}$ [9,10]. Here p, q denote sequences of t vertices $p = [p_1, \ldots, p_t]$, such that for any i there is a bond $p_i \to p_{i+1}$. The length of the corresponding trajectory is $L_p = L_{p_1 p_2} + L_{p_2 p_3} + \cdots + L_{p_t p_1}$ and the amplitude is $A_p = \sigma^{(p_1)}_{p_t,p_2} \sigma^{(p_2)}_{p_1,p_3} \cdots \sigma^{(p_t)}_{p_{t-1},p_1}$. If the trajectories p, q share the same length, then any pair of cyclic permutations of p, q will do so as well. All returning trajectories p related by cyclic permutations form an equivalence class P which represents a periodic orbit. As $t \to \infty$, only an exponentially small fraction of the set of orbits are multiple repetitions of shorter orbits; ignoring these, we write the form factor as a double sum over POs:

$$K^{(B)}(\tau) = \frac{t^2}{B} \sum_{P,Q} A_P A^*_Q \delta_{L_P,L_Q} \,. \tag{5}$$

Because of the rational independence of different bond lengths, all contributions to Eq. (5) come from pairs of POs which make the same number of transitions between any given pair of vertices m, l (i.e., $m \to l$ or $l \to m$). In particular, the pairs P, P and $P, \overline{P}$, where the bar denotes the time reversal, contribute to (5) for any P since time-reversal symmetry implies $L_P = L_{\overline{P}}$ (and $A_P = A_{\overline{P}}$). These contributions are collected in the diagonal approximation to the form factor,

$$K^{(B)}_{\mathrm{diag}}(\tau) = \frac{t^2}{B} \sum_P (|A_P|^2 + A_P A^*_{\overline{P}}) \to 2\tau \,, \tag{6}$$

which reproduces the linear term in Eq. (1). To evaluate the sum (6) we used that according to Eq. (3) $\sum_P |A_P|^2 = t^{-1} \mathrm{tr} M^t \to t^{-1}$. We also neglected self-retracing orbits $P = \overline{P}$, since they represent an exponentially small fraction as $t \to \infty$.

It is the purpose of this Letter to go beyond the diagonal approximation and investigate the contribution of pairs of orbits which differ from each other at one self-intersection. This is illustrated by Fig. 1: 1(i) is the example of two loops intersecting at a vertex α; 1(ii) shows the four orbits which traverse each of the two loops once and thus have the same length. The arrows between these orbits indicate the possible pairs whose contribution should be counted in (5); the dashed arrows correspond to pairs already counted in the diagonal approximation and the solid arrows to those that we have to sum here.

The two orbits in any pair that is of interest to us differ in the orientation along one of the cycles from vertex α to α. To count such pairs we define a "standard" symbolic code for the orbits of the pair $P = [p_1, p_2, \ldots, p_t] = [\alpha, l_1, \alpha, l_2]$ and $Q = [\alpha, l_1, \alpha, \overline{l_2}]$, where $l_1 = [p_2, \ldots, p_{t'-1}]$ and $l_2 = [p_{t'+1}, \ldots, p_t]$ represent sequences of $t' - 2$ and $t - t'$ vertices, respectively, and $\overline{l_2} = [p_t, \ldots, p_{t'+1}]$ stands for the reversal of the sequence l_2. Alternatively, a pair can also be specified by the code of orbit P and the position t' of the second occurrence of α. For example, the standard code for the pair of the top right and the bottom right orbits of Fig. 1(ii) is $P = [\alpha, a, \ldots, b, \alpha, d, \ldots, c]$ and $Q = [\alpha, a, \ldots, b, \alpha, c, \ldots, d]$. We stress that the orbit P will in general contain more than one self-intersection. It is the pair P, Q which singles out the particular one at α. Nevertheless, the code for the pair P, Q is not yet unique. For example, the pair shown in Fig. 2(i) has two possible codes:

$$P = [\alpha, \beta, a, b, \beta, \alpha, c, d],$$
$$Q = [\alpha, \beta, a, b, \beta, \alpha, d, c],$$

or

$$P = [\beta, a, b, \beta, \alpha, c, d, \alpha],$$
$$Q = [\beta, a, b, \beta, \alpha, d, c, \alpha],$$

with $t' = 6$ and $t' = 4$, respectively (remember that cyclic permutations of the code are irrelevant). To avoid this ambiguity we require (a) $p_{t'+1} \neq p_t$ for the standard code which excludes the second of the two representations shown and requires $c \neq d$ for the first one to be valid. Moreover, we assume (b) $l_1 \neq \overline{l}_1$ since otherwise $Q = \overline{P}$ such that the orbit pair was already counted in the diagonal approximation. Augmented with the conditions (a) and (b), the standard code is a unique representation of all orbit pairs we have to count. Thus we have the contribution of such orbits to the form factor,

$$K_1^{(B)}(\tau) = \frac{t^2}{B} \sum_{t'=4}^{t-2} {\sum_P}' (1 - \delta_{cd}) A_P A_Q^*, \qquad (7)$$

where the sum is over $P = [\alpha, a, p_3, \ldots, b, \alpha, c, \ldots, d]$ (in analogy to the notation of Fig. 1, we write a, b, c, d for $p_2, p_{t'-1}, p_{t'+1}, p_t$). This sum is subject to the restriction $l_1 \neq \overline{l_1}$ indicated by a prime and also to all restrictions implied by the connectivity of the graph (for some sequence of vertices P there might be no orbit).

Now we compute the contribution $A_P A_Q^*$ of an orbit pair P, Q. The amplitude A_Q differs from A_P due only to the vertex-scattering matrix elements picked up at the self-intersection point α. P gets a contribution $\sigma_{da}^{(\alpha)} \sigma_{bc}^{(\alpha)}$ from the two encounters of vertex α, while Q has the combination of adjacent vertices exchanged $\sigma_{ca}^{(\alpha)} \sigma_{bd}^{(\alpha)}$. Thus,

$$A_P A_Q^* = |A_{l_1}|^2 |A_{l_2}|^2 \sigma_{da}^{(\alpha)} \sigma_{bc}^{(\alpha)} \sigma_{ca}^{(\alpha)*} \sigma_{bd}^{(\alpha)*}, \qquad (8)$$

where A_{l_i} is equal to the product of matrices σ over the sequence l_i. After inserting this result into Eq. (7), we can sum over the variables $p_3, \ldots, p_{t'-2}$ and get $\sum_{p_3,\ldots,p_{t'-2}} |A_{l_1}|^2 = M^{t'-2}_{\alpha a, b\alpha}$. After a similar summation over $p_{t'+2}, \ldots, p_{t-1}$, we obtain

$$K_1^{(B)}(\tau) = \frac{t^2}{B} \sum_{t'=4}^{t-2} \sum_{\alpha,a,b,c,d} M^{t'-2}_{\alpha a, b\alpha} M^{t-t'}_{\alpha c, d\alpha} (1 - \delta_{cd}) \times \sigma_{da}^{(\alpha)} \sigma_{bc}^{(\alpha)} \sigma_{ca}^{(\alpha)*} \sigma_{bd}^{(\alpha)*} - K_{1,\mathrm{srt}}^{(B)}(\tau). \qquad (9)$$

Performing an unrestricted summation over $p_3, \ldots, p_{t'-2}$, we lost track of the condition $l_1 \neq \overline{l_1}$, therefore the contribution from such self-retracing orbits is removed by subtracting $K_{1,\mathrm{srt}}^{(B)}(\tau)$, which will be calculated below.

Note that for large t in Eq. (9) either $t' - 2$ or $t - t'$ will be large for any t'. Thus, we partition the sum over t' into two intervals, $\sum_{t'=4}^{t-2} = \sum_{t'=4}^{[t/2]} + \sum_{t'=[t/2]+1}^{t-2}$, where $[\cdot]$ stands for the integer part. We use Eq. (3) to argue that, in the first interval $M^{t-t'} = 1/B$, while in the second interval $M^{t'-2} = 1/B$. Calling $K_{1,\mathrm{S(L)}}$ the contribution of the interval with small (large) t', we have $K_1 = K_{1,\mathrm{S}} + K_{1,\mathrm{L}} - K_{1,\mathrm{srt}}$. Substituting $M^{t'-2}_{\alpha a, b\alpha} = 1/B$ into $K_{1,\mathrm{L}}$, we evaluate the sum over a and use the unitary of $\sigma^{(\alpha)}$ to show that $K_{1,\mathrm{L}} = 0$. There are corrections to this result due to the deviation from equidistribution of $M^{t'-2}$. However, so long as the stronger mixing condition given by Eq. (4) holds, these corrections can be shown to vanish as $N \to \infty$. To show this we use the unitarity of σ and the fact that all matrix elements of $M^{t-t'}$ are bounded from above by unity.

For $K_{1,\mathrm{S}}$ we set $M^{t-t'}_{\alpha c, d\alpha} = 1/B$, then the sum over c can be written as $\sum_c \sigma_{bc}^{(\alpha)} \sigma_{ca}^{(\alpha)*} (1 - \delta_{cd}) = \delta_{ab} - \sigma_{bd}^{(\alpha)} \sigma_{da}^{(\alpha)*}$, since the matrix $\sigma^{(\alpha)}$ is both unitary and symmetric. Hence, $K_{1,\mathrm{S}}$ simplifies to

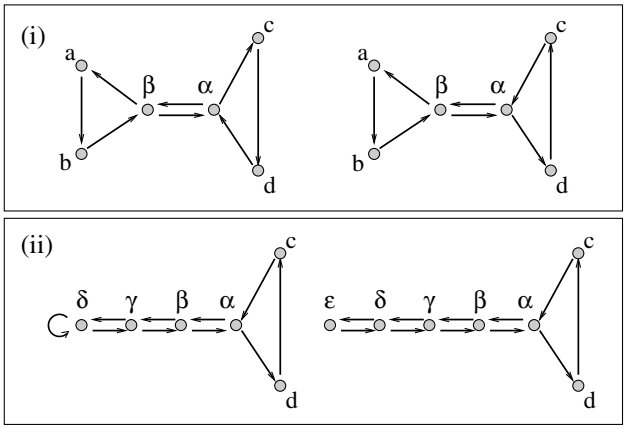

FIG. 2. Two conditions make the standard code unique: (i) If the vertex separating the two loops is ambiguous, we choose it such that the length of the loop with unchanged orientation is maximal, e.g., in the top pair of orbits, we take α. (ii) The loop with unchanged orientation must not be time-reversal invariant (self-retracing), e.g., the bottom orbits are excluded.

$$K_{1,\mathrm{S}}^{(B)} = \frac{t^2}{B^2}\sum_{t'=4}^{[t/2]}\Bigg(\sum_{\alpha,a,d} M_{\alpha a,a\alpha}^{t'-2}|\sigma_{da}^{(\alpha)}|^2 - \sum_{\alpha,a,b,d} M_{\alpha a,b\alpha}^{t'-2}|\sigma_{da}^{(\alpha)}|^2|\sigma_{bd}^{(\alpha)}|^2\Bigg). \tag{10}$$

In the first sum inside the brackets we can sum $|\sigma_{da}^{(\alpha)}|^2$ over d to produce one. In the second sum we substitute $|\sigma_{da}^{(\alpha)}|^2 = M_{d\alpha,\alpha a}$ and $|\sigma_{bd}^{(\alpha)}|^2 = M_{b\alpha,\alpha d}$ and then use $\sum_{a,b} M_{d\alpha,\alpha a}M_{\alpha a,b\alpha}^{t'-2}M_{b\alpha,\alpha d} = M_{d\alpha,\alpha d}^{t'}$. We arrive at

$$K_{1,\mathrm{S}}^{(B)} = \frac{t^2}{B^2}\sum_{t'=4}^{[t/2]}\sum_{a,b}(M_{ab,ba}^{t'-2} - M_{ab,ba}^{t'}) = \frac{t^2}{B^2}\sum_{a,b}(M^2 + M^3 - M^{[t/2]-1} - M^{[t/2]})_{ab,ba}\,. \tag{11}$$

Finally we compute the contribution of $K_{1,\mathrm{srt}}^{(B)}(\tau)$ to Eq. (9) from orbits with $l_1 = \overline{l_1}$ [Fig. 2(ii)]. Such orbits can be described as follows: To the left of vertex γ they must have the same structure as one of the orbits in Fig. 2(ii). To the right of γ they can take any path which comes back to γ (with the exception of *completely* self-retracing paths which are exponentially few in number and can therefore be ignored). The sum over all these configurations to the right of γ yields $M_{\delta\gamma,\gamma\delta}^{t-2}$ or $M_{\delta\gamma,\gamma\delta}^{t-3}$ for even or odd t', respectively. The contribution of the transitions from γ to the left can also be expressed in classical terms, resulting in

$$K_{1,\mathrm{srt}}^{(B)} = \frac{t^2}{B}\sum_{\gamma,\delta}(M_{\gamma\delta,\delta\gamma}^2 M_{\delta\gamma,\gamma\delta}^{t-2} + M_{\gamma\delta,\delta\gamma}^3 M_{\delta\gamma,\gamma\delta}^{t-3}). \tag{12}$$

Matrix elements of large powers of M can again be approximated by B^{-1} both above and in Eq. (11). Then we see that the first two terms in Eq. (11) are exactly canceled by $K_{1,\mathrm{srt}}^{(B)}(\tau)$. The remaining terms in Eq. (11) give our main result:

$$K_1(\tau) = -2\tau^2. \tag{13}$$

Equations (6) and (13) show that the contributions to the form factor of the orbits discussed here precisely reproduce the first two terms of the RMT result, Eq. (1). Note, however, that we have not discussed whether other correlated orbits could produce contributions of the same or lower order. This, we believe, can be shown by considering more and more complicated pairs of orbits, eventually deriving a complete expansion of the form factor in powers of τ.

Finally, we briefly discuss two specific models, to which Eq. (13) applies. We consider complete graphs with N vertices and $B = N^2$ directed bonds connecting every pair of vertices including a bond from a vertex to itself. The first model we consider has "discrete Fourier transform" (DFT) boundary conditions at each vertex [14]. The second has Neumann boundary conditions [9]:

$$\sigma_{mn}^{(l)} = \begin{cases} N^{-1/2}e^{2\pi i mn/N}/\sqrt{N} & \text{(DFT)} \\ 2N^{-1} - \delta_{mn} & \text{(Neumann)}\,. \end{cases} \tag{14}$$

The DFT graph is a uniformly hyperbolic model: The weights of all classical orbits with the same length are equal. We have $M_{ab,cd}^t \equiv 1/N^2$ for $t > 1$, i.e., all correlations vanish immediately and Eq. (3) is an identity. For the Neumann graph, which is not uniformly hyperbolic, the situation is more complicated: Here we have $M_{ab,cd}^{2T} = F_T(a,c)F_T(b,d)/N^2$ and $M_{ab,cd}^{2T+1} = F_{T+1}(a,d)F_T(b,c)/N^2$ with $F_t(a,b) = 1 + (\delta_{ab}N - 1)(1 - 4/N)^t$, but substituting $t = N^2\tau$ and using $(1 - 4/N)^N \to e^{-4}$ as $N \to \infty$ it is easy to see that M^t converges for large graphs exponentially fast to equidistribution.

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