Semiclassical limit of universal parametric density correlations

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Abstract

Reviewing the semiclassical theory for the parametric level density fluctuations, we show that for large parametric changes the density correlation function, after rescaling, becomes universal and coincides with the leading asymptotic term obtained from Random Matrix Theory. The advantage of the semiclassical approach is to provide a simple recipe for the calculation of the non-universal scaling parameter from elements of the underlying classical dynamics specific to the system. We discuss recent improvements of the theory, which introduce a requantization of the smoothed level density.

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I. MOTIVATION

One of the interesting new developments in the study of quantum manifestations of classical chaos concerns parametric correlations. For over a decade, most of the works on quantum chaos concentrated in spectral fluctuations of a fixed Hamiltonian. This large effort led to a solid body of evidence that if a system is chaotic in the classical limit, its quantum spectrum exhibits universal fluctuations which coincide with those of a suitable ensemble of random matrices [1]. There was also some parallel activity in trying to understand the statistical behavior of quantities related to the response of a chaotic Hamiltonian to external perturbations, such as Landau-Zener transitions [2] and energy level curvature [3]. But it was only a few years ago that Szafer, Simons, and Altshuler [4,5] showed that a system whose spectrum follows closely the universal fluctuations predicted by random matrix theory (RMT) will also present universal parametric behavior. More precisely, these authors have concluded that when a chaotic Hamiltonian depends on some external parameter $X$, any correlation function of spectral fluctuations taken at different values of $X$ becomes system-independent after a proper rescaling.

In this paper we study some universal spectral features of a quantum mechanical problem whose Hamiltonian $H$ generates chaotic motion in its classical limit. Considering a parametric dependence of $H$ on $X$, the Schrödinger equation reads

$$H(X)\Psi_\nu(r; X) = E_\nu(X)\Psi_\nu(r; X).$$

(1)

In what follows, the parameter $X$ will be associated with any tunable physical quantity, provided that its variation neither alters significantly the classical dynamics of the system, nor breaks or restores any symmetry. The first condition is easily realized in the semiclassical limit, since classically small parameter variations are responsible for significant level fluctuations. The second condition is not difficult to be satisfied in most cases of practical relevance.

Previous works have concentrated on the level velocity correlation function [4,6]

$$C(X) = \frac{1}{\Delta^2} \left\langle \frac{\partial E_\nu}{\partial X} \left( X - \frac{X}{2} \right) \frac{\partial E_\nu}{\partial X} \left( X + \frac{X}{2} \right) \right\rangle_{X, \nu},$$

(2)

where $\Delta$ denotes the mean level spacing around the state $\nu$. This function, although straightforward to evaluate numerically, is not suitable for any exact or systematic analytical evaluation. We would like to stress that the difficulty is intrinsic to the function, since it requires the precise knowledge of every level as a function of $X$. Therefore, instead of the usual 2-point Green’s function, one would need a combination of arbitrarily high $N$-point Green’s functions, which is very impractical. A few years ago, Berry and Keating [4] proposed a semiclassical approximation based on the density correlation function for $C(X)$. Their result agrees very nicely with the numerical results [2] for the large $X$ limit, indicating that the 2-point Green’s function gives a good asymptotic expansion. For the small $X$ region, their analytical expression gives, as one would expect, very poor results.

For these reasons, in order to study parametric statistics semiclassically, we will rather focus on a formally more amenable quantity, namely, the density correlation function.
\[ K(\Omega, X) = \left\langle \rho^f \left( E - \frac{\Omega}{2}, X - \frac{X}{2} \right) \rho^f \left( E + \frac{\Omega}{2}, X + \frac{X}{2} \right) \right\rangle_{E, X}, \]

(3)

where the fluctuating density \( \rho^f = \rho - \langle \rho \rangle \) is defined in terms of the level density

\[ \rho(E, X) = -\frac{1}{\pi} \text{Im} \sum \frac{1}{E - E_\nu(X) + i0^+}, \]

(4)

and the average density \( \langle \rho \rangle \), or inverse mean level spacing \( 1/\Delta \). Sometimes, in the semiclassical approach, it is convenient to use the cumulative level density, \( N(E) \) defined as \( N(E) = \int_{-\infty}^{E} dE' \rho(E') \), instead of the density itself as we shall see in Section IV.

All statistical measures of spectral fluctuations presuppose a constant average level spacing, which is not guaranteed for general families of Hamiltonians. Indeed, the mean level spacing for smooth Hamiltonians is accurately approximated by the Weyl rule:

\[ N^\text{Weyl}(E, X) \approx V(E, X) / (2\pi\hbar)^d, \]

(5)

\( \Theta \) being the unit step function. It is therefore desirable to work with the “volume spectrum” rather than directly with the energy spectrum, as proposed by Goldberg and collaborators [9]. So as to avoid some technicalities in the classical theory, we will adopt the alternative procedure of defining an “unfolded classical Hamiltonian”

\[ H'(p, q, X) = V \left( H(p, q, X), X \right). \]

(6)

The classical motion is then identical to that of the original Hamiltonian, except for a rescaling in time. Quantizing (3) we obtain levels \( E'_\nu \) that fluctuate with \( X \) about stable mean values \( \nu (2\pi\hbar)^d \), i.e., for the unfolded system, \( \Delta = (2\pi\hbar)^d \). (The primes will be omitted in what follows.)

The paper is organized as follows: In Section II, we present a reminder of the main parametric random matrix results, extracting the relevant asymptotic correlation functions. In Section III the standard semiclassic theory is discussed, putting emphasis on the diagonal approximation and its sequels. In Section IV we discuss the implications for \( K(\Omega, X) \) of the recent proposal of Bogomolny and Keating [10] for requantization of the smoothed level density. We summarize the results and conclude with a general discussion about the range of validity of the semiclassical approach in Section V.

II. REMINDER OF THE RANDOM MATRIX RESULT

The random matrix calculations leading to an exact expression for \( K(\Omega, X) \) have become relatively standard. Several references can serve as introduction to the subject (see, for instance, [11–13]). The detailed derivation of \( K(\Omega, X) \) was first given in Ref. [6] in the context of disordered metallic systems. The technique employed for such continuous systems can be easily adapted to discrete Hamiltonians. It consists in expressing the one-point Green’s function \( G_{jl}(E) = \langle l| (E - H + i0^+)^{-1} |j\rangle \), where \( l \) and \( j \) label arbitrary basis states, in
terms of an integral over $N$ commuting and $N$ anticommuting variables, where $N$ represents the number of basis states, and then directly performing the average over a certain Gaussian ensemble of Hamiltonians, $\{H\}_{N \times N}$. The quartic term thus generated can be decoupled through a Hubbard-Stratonovich transformation at the expense of introducing a graded matrix, also known as a supermatrix. The size and symmetry of this supermatrix depends on the symmetry class of the Hamiltonian and the order of the correlation function in question. For instance, for the Gaussian unitary ensemble (GUE) the calculation of the density correlation function requires an $8 \times 8$ supermatrix transforming according to the group $U(1,1|2)$. After integrating out the commuting and anti-commuting variables, one then has to carry out an integration of an effective action that involves the supermatrix elements. This is usually done in the saddle-point approximation, exploring the condition $N \gg 1$. Notice that this technique greatly simplifies the problem: The $2N$ variables are reduced to a small, workable set. However, we should remark that the apparently straightforward steps just described involve rather difficult mathematical considerations. For the important details the reader should consult the references cited above.

One of the most important conclusions drawn from Refs. [5,6] is the existence of a single quantity controlling the scale of parametric fluctuations of all spectral functions of chaotic Hamiltonians. This result is obtained explicitly in the supersymmetric formulation of the disordered metallic system in the diffusive regime (the so-called zero mode), as well as (but less surprisingly) in RMT when $N \to \infty$. More precisely, if $X$ is the external parameter, the rescaling $x = X/X_c$, where

$$X_c = \left\langle \left[ \frac{1}{\Delta} \frac{dE_\nu(X)}{dX} \right]^2 \right\rangle^{-1/2},$$

eliminates all system dependence in the parametric correlation functions, up to a global prefactor. We will later argue that a similar conclusion can be obtained from a purely semiclassical approach.

We now present the results of Ref. [6] in the rescaled form, assuming also that all energies are expressed in terms of $\Delta$, introducing $\omega = \Omega/\Delta$. In the absence of time-reversal symmetry, the final result for the density correlation function is

$$k_{GUE}(\omega, x) = \frac{1}{2} \Re \int_{-1}^{1} d\lambda \int_{1}^{\infty} d\lambda_1 \exp \left[ -F_{GUE}(\lambda, \lambda_1) \right],$$

where $k = K/\langle \rho \rangle^2$ and the free energy is given by

$$F_{GUE} = \frac{\pi^2 x^2}{2} (\lambda_1^2 - \lambda^2) + i\pi \omega^+ (\lambda - \lambda_1),$$

with $\omega^+ = \omega + i0^+$. The integration in (8) can be carried out explicitly, and gives

$$k_{GUE}(\omega, x) = \frac{1}{4x^2} \Im \left\{ \text{erfc} \left( \frac{\pi x + i\omega/x}{\sqrt{2}} \right) \left[ \text{erfc} \left( \frac{-\omega/x + i\pi x}{\sqrt{2}} \right) - \text{erfc} \left( \frac{-\omega/x - i\pi x}{\sqrt{2}} \right) \right] \right\}.$$

where erfc is the complementary error function [14].
For systems where time-reversal symmetry is preserved, modelled by the Gaussian Orthogonal Ensemble (GOE), the density correlation function is

$$k_{\text{GOE}}(\omega, x) = \text{Re} \int_{-1}^{1} d\lambda \int_{1}^{\infty} d\lambda_1 \int_{1}^{\infty} d\lambda_2 \frac{(1 - \lambda^2)(\lambda - \lambda_1\lambda_2)^2 \exp \left[-F_{\text{GOE}}(\lambda, \lambda_1, \lambda_2)\right]}{(2\lambda_1\lambda_2 - \lambda^2 - \lambda_1^2 - \lambda_2^2 + 1)^2},$$

with the free energy

$$F_{\text{GOE}} = \frac{\pi^2 x^2}{4} (2\lambda_1^2\lambda_2^2 - \lambda_1^2 - \lambda_2^2 - \lambda^2 + 1) + i\pi \omega^+ (\lambda - \lambda_1\lambda_2).$$

In distinction to the previous case, here the triple integral in (11) cannot be expressed in a closed form.

We will now focus on a regime when one either has $x \gg 1$ or $\omega \gg 1$. Considering initially large variations of the external parameter, one finds that the leading contributions to the multiple integrals come from the regions around two points: $\lambda = \lambda_1 = \lambda_2 = 1$ (A) and $\lambda = -\lambda_1 = -\lambda_2 = -1$ (B). In passing, we remark that there exists a mapping of RMT into the problem of many particles interacting by a $1/r^2$ potential in one dimension [15]. In that context, the contribution (A) gives the “hydrodynamical”, $q = 0$ limit of the particle density correlation function, whereas (B) is related to the “Friedel”, $q = 2k_F$ oscillations. Here, (A) is related to the monotonic, non-oscillating decay of the correlation function; (B), on the other hand, yields a series of oscillating terms in $\omega$. To obtain an asymptotic expression for $k(\omega, x)$, we expand the free energies around these points and retain the (linear in $\lambda$’s) lowest-order terms. Performing the exponential integrals (see the Appendix A for details), we find that

$$k_{\text{GUE}}(\omega, x) \approx \frac{1}{2} \frac{\pi^2 \omega^2 - \pi^4 x^4}{(\pi^2 \omega^2 + \pi^4 x^4)^2} + \frac{1}{2} \frac{\cos(2\pi \omega)}{\pi^2 \omega^2 + \pi^4 x^4},$$

and

$$k_{\text{GOE}}(\omega, x) \approx \frac{1}{2} \frac{\pi^2 \omega^2 - \pi^4 x^4/4}{(\pi^2 \omega^2 + \pi^4 x^4/4)^2} + \frac{1}{2} \frac{\cos(2\pi \omega)}{2(\pi^2 \omega^2 + \pi^4 x^4/4)^2}.$$  

The right-hand sides of both equations represent the leading terms of an asymptotic expansion on both $x$ and $\omega$ whenever $|\pi^2 x^2 \beta/2 - i\pi \omega| \gg 1$, with $\beta = 1$ for the GOE and $\beta = 2$ for the GUE. At $x = 0$ one has the usual $1/\omega^2$ decay of the density fluctuations, plus the first oscillating terms. Notice also that the oscillating and non-oscillating terms are held only to their lowest order in $x^{-2}$ and $\omega^{-2}$. For the GOE, this means that we are not showing a non-oscillating term of order $\omega^{-4}$. For the GUE, higher orders terms can be obtained without much effort by recalling (10).

The energy oscillations present in Eqs. (13) and (14) are related to the quantum (discrete) nature of the energy spectrum. For the GUE case they appear even at the lowest order in $\omega^{-2}$; in fact, for $x = 0$, the asymptotic form (13) is actually exact and applies to all $\omega$ scales. For the GOE case, since level repulsion is less pronounced, the oscillations only show up at the next-lowest order, namely, they are weaker corrections to the leading $\omega^{-2}$ decay.

One is tempted to imagine that the $\omega$ oscillations should not be present in a formulation where there is no intrinsic energy level quantization. Indeed, in the following section we
will verify that the semiclassical trace formula (applied in the usual way and based on the assumption that the underlying classical dynamics is chaotic) only yields the monotonic decay of \( k(\omega, x) \). Still, a problem emerges as to whether one can systematically obtain oscillating terms, or any parametric correlation function beyond the asymptotic limit, in a semiclassical framework. This question was partially answered by Bogomolny and Keating [10] when they calculated \( k(\omega, x = 0) \) using an expansion in periodic orbits and forced energy level quantization as an additional constraint. We will get back to this point later.

Another important aspect, often neglected, but particularly relevant to mesoscopic phenomena, is the applicability range of the semiclassical approach used in the study of parametric variations. For this purpose, the calculations below will be carried out with special care.

III. SEMICLASSICAL APPROACH

The fluctuating part of the level density \( \rho^{fl}(E, X) \) can be smoothed over an energy range \( \eta/\hbar \) and expressed, in the semiclassical limit, by the Gutzwiller trace formula [16]

\[
\rho^{fl}(E, X) = \frac{1}{(2\pi\hbar)^2} \left| \sum_{\gamma, r} A_{\gamma r} \left( E + \frac{\Omega}{2}, X + \frac{X}{2} \right) A_{\gamma r} \left( E - \frac{\Omega}{2}, X - \frac{X}{2} \right) \right|
\times \exp \left\{ \frac{i}{\hbar} \left[ rS_\gamma \left( E + \frac{\Omega}{2}, X + \frac{X}{2} \right) - r'S_{\gamma'} \left( E - \frac{\Omega}{2}, X - \frac{X}{2} \right) \right] \right\}_{E, X},
\]

(15)

where \( T_\gamma, M_\gamma, S_\gamma, \) and \( \nu_\gamma \) stand, respectively, for the period, monodromy matrix, action, and Maslov index of a periodic orbit labelled by \( \gamma \). The sum is performed over all primitive orbits \( \gamma \) and their repetitions \( r \) (positive and negative), irrespective of multiplicity due to time-reversal or other symmetries. The smoothing of \( \rho^{fl} \) can be done in other ways than the exponential cutoff introduced in (15). Later on, we shall also cutoff the sum over periodic orbits sharply at a certain period \( T^* \). Both \( \hbar/T^* \) and \( \eta/2\pi \) are always taken larger or equal to \( \Delta \).

Let us write the correlation function \( K(\Omega, X) \) in terms of the semiclassical level density as given by Eq. (15),

\[
K^{sc}(\Omega, X) = \frac{1}{(2\pi\hbar)^2} \left| \sum_{\gamma, r, \gamma', r'} A_{\gamma r} \left( E + \frac{\Omega}{2}, X + \frac{X}{2} \right) A_{\gamma' r'} \left( E - \frac{\Omega}{2}, X - \frac{X}{2} \right) \right|
\times \exp \left\{ \frac{i}{\hbar} \left[ rS_\gamma \left( E + \frac{\Omega}{2}, X + \frac{X}{2} \right) - r'S_{\gamma'} \left( E - \frac{\Omega}{2}, X - \frac{X}{2} \right) \right] \right\}_{E, X},
\]

(16)

where \( A_{\gamma r} = T_\gamma | \det(M_\gamma - I)|^{-1/2} \). In order to further proceed analytically, we restrict the calculations to a regime where classical perturbation theory is applicable. This means that we shall consider variations of \( E \) and \( X \) which classically imply a small change in the actions \( S_\gamma \). Such a change can nonetheless be very large in the scale of \( \hbar \), corresponding to large quantum effects. Under this condition, it is a good approximation to write

\[
S_\gamma \left( E \pm \frac{\Omega}{2}, X \pm \frac{X}{2} \right) = S_\gamma(E, X) \pm \frac{\partial S_\gamma}{\partial E} \frac{\Omega}{2} \pm \frac{\partial S_\gamma}{\partial X} \frac{X}{2} + \cdots
\equiv S_\gamma(E, X) \pm T_\gamma(E, X) \frac{\Omega}{2} \pm Q_\gamma(E, X) \frac{X}{2} + \cdots,
\]

(17)
which defines $Q_\gamma$ as the parametric velocity of the orbit action. The general expression for the parametric variation of the action is presented in Appendix B. In the absence of any dependence on Planck’s constant, one can neglect the energy (or parameter) corrections to $A$, as compared to the strong energy dependence of the exponential term. In this approximation, consider the evaluation of

$$I_{\gamma\gamma'}(T) = \left\langle e^{i\hbar [S_\gamma(E,\vec{X}) - S_{\gamma'}(E,\vec{X})]} \right\rangle_{E,\vec{X}}.$$  \hspace{1cm} (18)

For orbits with period shorter than the Heisenberg time $t_H \equiv \hbar/\Delta$, one does not in general expect to find pairs of orbits $(\gamma, \gamma')$ with actions differing by less than $\hbar$, unless they are symmetry related orbits. As a consequence, upon energy averaging, $I_{\gamma\gamma'}(T < t_H) \approx g_\gamma \delta_{\gamma,\gamma'}$, where $g_\gamma$ is the multiplicity of symmetry-related orbits. (We take here the simplest case where any symmetry holds for all considered parameter values.) This is the essence of the diagonal approximation. On the other hand, due to the exponential proliferation of orbits, for sufficiently long times, i.e., for a small smoothing parameter $\eta$, one enters a regime where there is an abundance of pairs of periodic orbits $(\gamma, \gamma')$ satisfying $S_\gamma - S_{\gamma'} < \hbar$. This situation is expected to occur for time intervals longer than $t_H$ (or, correspondingly, for $E < \Delta$). Under these circumstances, the diagonal approximation is no longer valid. Actually, for such long times even the validity of the trace formula is problematic, so that the unsmoothed energy spectrum should be resummed \[17\]. At this point the necessity of smoothing becomes evident: it keeps the approximations under control.

Restricting ourselves to the range where the diagonal approximation is valid, we have

$$K_{\gamma\gamma}(\Omega, X) = \frac{1}{(2\pi \hbar)^2} \left\langle \sum_{\gamma,\gamma'} g_\gamma |A_{\gamma\gamma'}(E,\vec{X})|^2 \left\{ i \left[ rT_\gamma(E,\vec{X}) \Omega + rQ_\gamma(E,\vec{X}) X \right] - 2\frac{\eta}{\hbar} |r| T_\gamma \right\} \right\rangle_{E,\vec{X}}.$$ \hspace{1cm} (19)

To evaluate the average in (19), we first notice that, in a fully chaotic regime, the proportion of high period orbits that are repetitions of lower periods is exponentially small, so we neglect all $|r| \neq 1$. In the next step we recast (19) as an integral by defining the smooth interpolating functions $A^2(E,\vec{X},t)$ through the relation

$$\int dt A^2(E,\vec{X},t) \sum_\gamma \delta(t - T_\gamma) = \sum_\gamma A^2_\gamma(E,\vec{X}).$$ \hspace{1cm} (20)

Further simplification can be achieved using the uniformity principle over periodic orbits (also known as the Hannay-Ozorio de Almeida sum rule) \[13\]

$$A^2(E,\vec{X},t) \sum_\gamma \delta(t - T_\gamma) \quad \longrightarrow \quad |t| \quad |t| \to \infty.$$ \hspace{1cm} (21)

It is important to notice that this result independs on the “center-of-mass” variables $E$ and $\vec{X}$. We can then evaluate

$$K_{\gamma\gamma}^{\text{sc}}(\Omega, X) = \frac{g}{2(\pi \hbar)^2} \text{Re} \int_\tau^\infty dt |t| e^{i\Omega t/\hbar} \left\langle e^{iQ(E,\vec{X},t)X/\hbar} \right\rangle.$$ \hspace{1cm} (22)
The lower limit $\tau$ is the period of the shortest periodic orbit. Of course it is simplistic to extrapolate the uniformity principle this far, but it is easy to improve the theory by including a few short orbits individually and hence increasing $\tau$.

The average in Eq. (22) is evaluated over periodic orbits with fixed period $t$. In view of the fact that the rest of the integrand oscillates rapidly in time, it is important that the finite range in $E$ and $\mathbf{X}$ allows many orbits with a given large period. There being two parameter families of periodic orbits, one should take $Q_\gamma(E(\mathbf{X}), \mathbf{X}, t)$ and subsequently average only over $\mathbf{X}$, or vice-versa. For the energy correlation with no variation of parameters, there will be isolated periodic orbits of given period in the energy range where the averaging is carried out. Thus, for fixed $\mathbf{X}$, the average in Eq. (22) runs over a large number of periodic orbits with parametric velocity $Q_\gamma(t)$, which may be considered as samples of the probability distribution $P_t(Q)$. The latter is assumed to be Gaussian,

$$P_t(Q) = \frac{1}{\sqrt{2\pi Q^2(t)}} \exp \left[ -\frac{Q^2}{2Q^2(t)} \right],$$

(23)

because our theory involves arbitrary parametric variations $H(X)$. Even if there exist correlations among the actions of the periodic orbits $\gamma(t)$, as postulated by [19], these will in general be broken by the parametric velocities

$$Q_\gamma = \int_0^{T_\gamma} dt \frac{\partial H}{\partial X}(p(t), q(t), X),$$

(24)

evaluated along each orbit. The Gaussian width is a function of $\mathbf{X}$ and $E$ (the center of the energy range), being defined as

$$\overline{Q^2}(t) = \frac{1}{N(t)} \sum_{\gamma(t)} Q^2_\gamma(t),$$

(25)

where $N(t)$ is the number of periodic orbits with period $t$. Note that we take $\overline{Q} = 0$, since the shape of the shell for the unfolded system is affected by $X$, but not its volume, so $\partial H/\partial X$ averaged over the shell is zero. Although the Gaussian assumption is not quite at a par with the uniformity principle, the arguments presented above make it plausible. Nothing is yet known of the relation between higher moments $\overline{Q^m}$ and $\overline{Q^2}$, so as to obtain a more rigorous result. Numerical simulations for the particular case where the external parameter is a magnetic flux line [8] provide further support to (23).

The average in Eq. (22) can be evaluated using (23):

$$\langle e^{iQX/\hbar} \rangle = \exp \left[ -\frac{X^2}{2\hbar^2 \overline{Q^2}(E, \mathbf{X}, t)} \right].$$

(26)

As we commented previously, the energy average was already utilized in obtaining the periodic orbits with fixed period. Strictly, we should now average (26) over $\mathbf{X}$, but both $\overline{Q^2}$ and the Gaussian (23) are smooth functions of $\mathbf{X}$, so we may just evaluate the latter at the center of the averaging range. As for the time dependence of the mean square parametric velocity, we refer to previous treatments [9,20], leading to the result
\( \overline{Q^2} = \alpha |t| \), \quad \text{with} \quad \alpha(E, X) = 2 \int_0^\infty dt \left\langle \frac{\partial H}{\partial p}(p(t), q(t)) \frac{\partial H}{\partial p}(p(0), q(0)) \right\rangle_{\text{e.s.}}. \)

(27)

Here, the average over the periodic orbits has been substituted by an average over the entire energy shell, in accordance with the uniformity principle. It is important to note that the decay of the classical correlation function in (27) need only be integrable, since many available chaotic systems do not exhibit full exponential decay of the correlations. Strictly, the linear dependence of \( \overline{Q^2} \) on \( t \) should only hold for times longer than that of the decay of the correlation function, but numerical investigations [8,21] have found this feature to be quite robust. (Notice that there is a factor 2 missing in the definition of \( \alpha \) in Ref. [8]. Modifying \( \alpha \) accordingly the semiclassical prediction for \( X_c \) changes by a factor \( \sqrt{2} \). As a result, the agreement between the numerics and the semiclassical theory becomes excellent.)

Substituting (27) and (26) into Eq. (22) and evaluating the integral in the limit \( \tau \to 0 \), we finally arrive at the main result of this section

\[
K_D^{\text{sc}}(\Omega, X) = -\frac{1}{\beta \pi^2} \frac{\Omega^2 - (\alpha X^2/2\hbar + 2\eta)^2}{\Omega^2 + (\alpha X^2/2\hbar + 2\eta)^2},
\]

(28)

where \( \beta = 2/g \). The nongeneric long-wave oscillations in the correlation, characteristic of each individual system, appear as we choose \( \tau \) equal or greater to the period of the shortest periodic orbit. The above expression corresponds to the leading non-oscillatory term of the asymptotic expansion of the correlation function exactly calculated within RMT [Eqs. (13) and (14)], and hence presumed to hold for generic chaotic systems.

On the other hand, this formalism gives a recipe for calculating \( \alpha \), which is a system-specific quantity and fixes the value of the parametric rescaling factor \( X_c \). From this point-of-view, the semiclassical method and the RMT are complementary for a full understanding of \( K(\Omega, X) \). An important immediate application concerns possible transitions from GOE families to GUE families of Hamiltonians. If this occurs for a small variation of a second parameter as in [20], the classical parameter \( \alpha \) should remain unchanged, whereas \( X_c \) must grow because of increased level repulsion. By comparing the invariant form of Eq. (28) with (13) and (14), we can predict that \( X_c \) will increase by a factor \( \sqrt{2} \).

IV. REQUANTIZATION AND ITS IMPLICATIONS FOR THE DENSITY CORRELATION FUNCTION

In a recent paper, Bogomolny and Keating [10] proposed a new semiclassical procedure to obtain the density correlation function \( K(\Omega, 0) \) and its parametric extension, \( K(\Omega, X) \). Their result for \( K(\Omega, 0) \) coincides with the exact GUE expression for systems with broken time-reversal invariance and gives the leading GOE oscillatory and non-oscillatory terms in powers of \( \omega^{-2} \) for time-reversal symmetric systems. We will here rederive their results within the wider context of parametric variations.

The starting point of the derivation in Ref. [10] is standard and considers the sum over periodic orbits in the Gutzwiller trace formula (14) up to some value of \( T^* \). As a consequence, the information about energy scales smaller than \( \hbar/T^* \) is washed out, and strictly speaking,
the connection to RMT results cannot be made in such an energy range. However, one can still introduce information related to the discrete nature of the spectrum through the following “requantization” condition \[22\]

\[
N_{T^*}(E_\nu(T^*)) = \nu + \frac{1}{2},
\]

by which, for a given value of \(T^*\), one has a well-defined procedure to obtain a set of eigenvalues \(\{E_\nu(T^*)\}\). It has to be stressed that such a procedure does not imply any control on accuracy. This is equivalent to say that, by increasing the value of \(T^*\), it is not guaranteed that \(\{E_\nu(T^*)\}\) will converge to the exact spectrum. Actually, this quantization rule is not applicable for \(T^* > t_H\) since for such periods the cumulative semiclassical level density can become a non-monotonic function.

The requantized level density, defined as

\[
D_{T^*}(E, X) = \sum_\nu \delta(E - E_\nu(T^*, X)),
\]

can be rewritten in the form

\[
D_{T^*}(E, X) = \rho_{T^*}(E, X) \sum_\nu \delta(N_{T^*}(E, X) - \nu - 1/2)
= \rho_{T^*}(E, X) \sum_{k=\infty}^{+\infty} (-1)^k \exp[2\pi i k N_{T^*}(E, X)],
\]

with \(\rho_{T^*}(E, X)\) standing for the parametric level density given by the truncated trace formula. It is immediate to see that averaging Eq. (31) yields

\[
\langle D_{T^*}(E, X) \rangle_{E, X} = \langle \rho_{T^*}(E, X) \rangle_{E, X} \equiv \rho_{\text{Weyl}}(E, X),
\]

equivalent to the usual level density, easily obtained from the Weyl formula.

The advantages of this procedure become evident once we analyze the spectral fluctuations. Let us study the 2-point spectral correlation function for \(D_{T^*}(E)\) in order to compare with the results of the preceding sections. It is useful to write the density correlation function in the form

\[
K(\Omega, X) = \langle D_{T^*} \left( E + \frac{\Omega}{2}, X + \frac{X}{2} \right) D_{T^*} \left( E - \frac{\Omega}{2}, X - \frac{X}{2} \right) \rangle_{E, X} - \left( \rho_{\text{Weyl}} \right)^2.
\]

The averages are defined as in Section III. Thus,

\[
K(\Omega, X) = \left\langle \rho_{T^*} \left( E + \frac{\Omega}{2}, X + \frac{X}{2} \right) \rho_{T^*} \left( E - \frac{\Omega}{2}, X - \frac{X}{2} \right) \right\rangle_{E, X}
= \sum_{k_1, k_2} (-1)^{k_1 - k_2} \exp \left( 2\pi i \left[ k_1 N_{T^*} \left( E + \frac{\Omega}{2}, X + \frac{X}{2} \right) - k_2 N_{T^*} \left( E - \frac{\Omega}{2}, X - \frac{X}{2} \right) \right] \right)_{E, X} - \left( \rho_{\text{Weyl}} \right)^2.
\]

One can recover the standard semiclassical result discussed in the previous section by considering the simplest term in the double sum, namely, \(k = k_1 = k_2 = 0\):
This is the same calculation as presented in the previous section, except that now the exponential cutoff is substituted by a sharp truncation at $T^*$. This causes a spurious oscillatory term which only becomes negligible in the asymptotic regime where $\alpha X^2/2\hbar \gg \Delta$. In other words, the semiclassical result only becomes independent of the cutoff at the asymptotic limit, where it coincides with RMT. In Ref. [10], this term with $k_1 = k_2 = 0$ was called “diagonal approximation”. This should not be confused with the standard diagonal approximation discussed in the previous section.

We are left to discuss the terms with $k_1 \neq 0$ and $k_2 \neq 0$. It is easy to see that the ones with $k_1 \neq k_2$ give a negligible contribution to the correlation function. Indeed, dividing the spectrum for the unfolded system (34) into a smooth and a fluctuating part ($N_{T^*} = N^{\text{Weyl}} + N_{T^*}^{\text{fl}}$) we have $N^{\text{Weyl}}(E, X) = E/(2\pi\hbar)^d$. For this part, the average (34) furnishes

\[
\langle \exp \left\{ 2\pi i \left[ k_1 N^{\text{Weyl}} \left( E + \frac{\Omega}{2}, X + \frac{X}{2} \right) - k_2 N^{\text{Weyl}} \left( E - \frac{\Omega}{2}, X - \frac{X}{2} \right) \right] \right\} \rangle_{E, X} = \left( \frac{(2\pi\hbar)^d}{(k_1 - k_2)\delta E} \right) \sin \left[ \frac{(k_1 - k_2)\delta E}{(2\pi\hbar)^d} \right] = \frac{\sin[(k_1 - k_2)\delta N]}{(k_1 - k_2)\delta N},
\]

which is negligible if the averaging region $\delta E$ extends over many states, unless $k_1 = k_2$. Thus,

\[
K^{k\neq0}(\Omega, X) = \frac{1}{4\pi^2} \frac{\partial^2}{\partial \Omega_1 \partial \Omega_2} \sum_{k \neq 0} \frac{1}{k^2} \exp \left[ 2\pi i k (\Omega_1 - \Omega_2) \right] \Phi_k(\Omega_1, \Omega_2, X_1, X_2)
\]

(evaluated at $\Omega_1 = -\Omega_2 = \Omega$ and $X_1 = -X_2 = X$), where $k \equiv k_1 = k_2$ and

\[
\Phi_k(\Omega_1, \Omega_2, X_1, X_2) = \langle \exp \left\{ 2\pi i k \left[ N_{T^*}^{\text{fl}}(E + \Omega_1, \overline{X} + X_1) - N_{T^*}^{\text{fl}}(E + \Omega_2, \overline{X} + X_2) \right] \right\} \rangle_{E, X}.
\]

One is now left with the formidable task of averaging (38), for which there is no clear controllable strategy. Bogomolny and Keating [11] proposed a kind of Gaussian ansatz, which in practice simplifies the average by making $\langle \exp[iG(E)] \rangle = \exp[-\langle G^2(E) \rangle/2]$. Although appealing, this ansatz is harder to justify classically than a similar passage in the previous section. Moreover, it is not clear how to implement the averaging in a consistent way. In Appendix C, we justify the validity of the Gaussian assumption (for large energy differences as compared to $\Delta$) using solely the diagonal approximation. Based on that, we have

\[
\Phi_k(\Omega_1, \Omega_2, X_1, X_2) = \exp \left\{ -2\pi^2 k^2 \left\langle \left[ N_{T^*}(E + \Omega_1, \overline{X} + X_1) - N_{T^*}(E + \Omega_2, \overline{X} + X_2) \right] \right\}^2 \right\}_{E, X}.
\]

There are at least two straightforward ways to evaluate the average in (39), both giving the same final result. The first one is by direct subtraction of the cumulative densities, followed
by the use of the diagonal approximation. The second one has the nice property of putting in evidence some of the delicate points of the semiclassical averaging procedure, and will be discussed now. An important point to have in mind, however, is that the average in the exponent of Eq. (39) is just the usual number variance $\Sigma^2(\Omega)$ when $X_1 = X_2$. If we were interested in $X = 0$ correlations at $\Omega \ll \Delta$ and simply substituted into Eq. (39) the exact RMT expression for $\Sigma^2(\Omega)$, we would obtain an incorrect result for the level density correlation function. We interpret this fact as a clear indication that the Gaussian ansatz of Ref.[10], which neglects correlation between orbits, is problematic for $\Omega/\Delta \ll 1$. This limitation will appear more explicitly below.

Let us start writing (39) as

$$\Phi_k(\Omega_1, \Omega_2, X_1, X_2) = \left[ \frac{\Lambda(\Omega_1, \Omega_2, X_1, X_2)}{\Lambda_0} \right]^{k^2}$$

(40)

with

$$\ln \Lambda(\Omega_1, \Omega_2, X_1, X_2) = 4\pi^2 \left\langle N_{T^*}^f(E + \Omega_1, X + X_1) N_{T^*}^f(E + \Omega_2, X + X_2) \right\rangle_{E, X}$$

(41)

and $\Lambda_0 = \Lambda(0, 0, 0, 0)$. Then, we evaluate $\Lambda_0$ using the diagonal approximation (see for instance [23]),

$$\left\langle \left[ N_{T^*}^f(E, X) \right]^2 \right\rangle_{E, X} = \frac{g}{2\pi^2} \int_{T^*} T^* \frac{dt}{t} = \frac{g}{2\pi^2} \ln \left( \frac{T^*}{\tau} \right).$$

(42)

The lower bound of integration is of the order of the shortest periodic orbit, beyond which we cannot even extrapolate the uniformity principle. Recalling that in our case the energy of the shell is identified with its volume, we obtain, from purely geometrical considerations, that

$$\tau = \frac{\partial S}{\partial E} \propto E^{-(1-1/d)}.$$  

(43)

If we now choose $T^* = \kappa t_H$ ($t_H$ is the Heisenberg time), Eq. (42) becomes

$$\left\langle \left[ N_{\kappa t_H}^f(E, X) \right]^2 \right\rangle = \frac{2}{g\pi^2} \left( 1 - \frac{1}{d} \right) \ln \left( \frac{E}{\Delta} \right) + \text{constant}.$$  

(44)

It is interesting that we recover the RMT result only in the limit where the phase space dimension $d \to \infty$. (Incidentally, the above formula accounts for the spectral rigidity of the integrable limit of $d = 1$.)

Applying now the diagonal approximation to the numerator of (39), we write

$$\ln \Lambda(\Omega_1, \Omega_2, X_1, X_2) = 2g \text{Re} \int_{\tau}^{T^*} dt \frac{1}{t} \exp \left[ \frac{i}{\hbar} (\Omega_1 - \Omega_2) t - \frac{\alpha (X_1 - X_2)^2 t}{2\hbar^2} \right],$$  

(45)

which can be expressed in a compact form as

$$\ln \Lambda(\Omega_1, \Omega_2, X_1, X_2) = 2g \text{Re} \left[ E_1(\xi \tau) - E_1(\xi T^*) \right],$$  

(46)
with $\xi = -i(\Omega_1 - \Omega_2)/h + \alpha(X_1 - X_2)^2/2\hbar^2$ and $E_1$ denoting the exponential integral \[14\].

Recalling that $T^*$ is of the order of $\hbar/\Delta$ and $\tau$ is a much shorter time scale, we have $|\xi T^*| \gg 1$ and $|\xi \tau| \ll 1$. As a consequence, $E_1(\xi T^*)$ is exponentially small and $E_1(\xi \tau)$ can be expanded up to first order \[14\]. The result is

$$\ln \Lambda(\Omega_1, \Omega_2, X_1, X_2) \approx 2g \Re \left[ -\gamma - \ln(\xi \tau) \right]$$

$$\approx 2g \Re \left[ -\gamma + \ln \left( \frac{T^*}{\tau} \right) - \ln(\xi T^*) \right], \quad (47)$$

where $\gamma$ is the Euler constant. Collecting the above results into \[39\], we see that the first two terms in the r.h.s. of \[17\] are cancelled by $\ln \Lambda_0$, and

$$\Phi_k(\Omega_1, \Omega_2, X_1, X_2) = \left[ -\frac{i}{\hbar}(\Omega_1 - \Omega_2) + \frac{\alpha(X_1 - X_2)^2}{2\hbar^2} \right] e^{\gamma T^*} \xi T^* \eta T^*/h \exp \left( -\frac{\alpha X^2 T^*}{2\hbar^2} \right) \exp \left( -\frac{\alpha X^2 T^*}{2\hbar^2} \right) \tau/h \right), \quad (48)$$

Hence, the sum over $k$ in \[37\] is an asymptotic series in inverse powers of $\xi T^*$. To obtain the parametric generalization of Bogomolny and Keating result \[10\], we cutoff this series in the first term and choose $T^* e^{-\gamma} = t_H/2$, obtaining

$$K_{|k|=1}(\Omega, X) = \frac{\cos(2\pi\Omega/\Delta)}{2\Delta^2} \left| \frac{\Delta}{-i\pi \Omega + \alpha \pi^2 X^2/\hbar} \right|^{1/\beta}, \quad (49)$$

which, after proper rescaling, is exactly \[13\] or \[14\], depending on the symmetry class labelled by $\beta = 2/g$.

It thus appears that requantization has reproduced precisely the asymptotic form of the correlation function calculated exactly within RMT if we postulate the same factor of $\sqrt{2}$ for the change in $X_0$ from GOE to GUE. However, in taking a sharp cutoff for the periodic orbit sum, we add the spurious oscillatory term

$$\frac{g T^* \cos \left( \frac{\Omega T^*}{\hbar} - \phi \right) \exp \left( -\frac{\alpha X^2 T^*}{2\hbar^2} \right)}{2\pi^2 \hbar \left( \Omega^2 + \left( \frac{\alpha X^2}{\hbar} \right)^2 \right)}, \quad (50)$$

to \[28\] with $\eta = 0$ [above, $\phi = \tan^{-1}(2\hbar \Omega/\alpha X^2)$]. This will certainly be negligible if $\alpha X^2 T^*/2\hbar^2 \gg 1$, but we cannot push $\alpha X^2/\hbar$ down to the averaged level spacing. Indeed, our deduction of \[49\] does not hold at this level either, since there one should not neglect the upper limit of \[15\].

These conclusions are maintained if we substitute $N_T$ by the integral of the smoothed density of section \[11\] in the requantization of Bogomolny and Keating. The steps in the calculation of the correlation function remain the same, so that now $K_{|k|=0}(\Omega, X)$ is exactly \[28\] with a finite $\eta$. The expression for

$$\ln \Lambda(\Omega_1, \Omega_2, X_1, X_2) = 2g \Re \int_0^\infty dt \frac{1}{t} \exp \left\{ i(\Omega_1 - \Omega_2)t/h - \left[ \alpha(X_1 - X_2)^2/2\hbar^2 + 2\eta/h \right] t \right\}$$

$$= 2g \Re E_1 \left[ -i(\Omega_1 - \Omega_2)/h + \alpha(X_1 - X_2)^2/2\hbar^2 + 2\eta\tau/h \right], \quad (51)$$

now holds, in principle, for any value of $\Omega_j$ or $X_j$, including zero. We can now use the same approximation for the exponential integral function as in \[17\] to obtain
\[ \Phi_k(\Omega_1, \Omega_2, X_1, X_2) = \left| -\frac{i}{\hbar} (\Omega_1 - \Omega_2) + \frac{\alpha (X_1 - X_2)^2}{2\hbar^2} + 2\eta/\hbar \right|^{2\eta k^2} \]

which leads to (13) when we choose \( \eta = \Delta/2\pi \) and assume \( \Omega \) and \( \alpha X^2/2\hbar \) to be much greater than the mean level spacing. In this sense, the energy smoothing with \( \eta \) corresponds to the cutoff time \( T^* (\eta T^* \sim \hbar) \).

V. FINAL DISCUSSION AND CONCLUSIONS

The Gutzwiller series does not converge in the limit of small smoothing. Indeed, it can be argued that the exponential smoothing used in Section [11] is insufficient, but Gaussian smoothing does work and leads to equivalent results. The application of the periodic orbit theory for nongeneric long-range oscillations of the energy level correlation functions was pushed in the last decade to a range where contact could be made with the universal regime of Random Matrix Theory. This involves the uniformity principle for long periodic orbits, as well as the diagonal approximation. In our study we have used the semiclassical trace formula to show the universality of the level density parametric correlation function for classically chaotic systems. This universality manifests itself after a proper rescaling of the correlation function variables. Within the range of validity of the semiclassical formulation and in the diagonal approximation, we have obtained the same functional dependence on energy and external parameter found by the method of RMT.

From a purely utilitary point of view, it may appear unnecessary to rederive RMT results within a semiclassical theory. Yet, it is only in this way that we can calculate the arbitrary parameters in RMT, as well as derive the nongeneric long-range oscillations characteristic of the individual systems that we wish to measure. In the present case, we obtain the result that the unfolded mean square parametric velocity diminishes by a factor of \( \sqrt{2} \) when the time-reversal symmetry is broken.

The semiclassical description of parametric correlations relies on the ansatz proposed in (23), which is based on the central limit theorem and leads to (27). To demonstrate rigorously the validity of (24) for a generic classical chaotic system, a systematic study of higher moments of \( Q_\gamma \) is required, which is a quite difficult task. Notwithstanding, there is solid numerical evidence [8, 21] to support the proposed Gaussian ansatz. As a consequence of (27), \( \alpha X^2/2\hbar \) will always appear in the same footing as \( \Omega \) in the semiclassical approach.

In general, this is not the case in the RMT, as one can see in Section [1]. Only after linearizing the “effective action” (what we do to generate the asymptotic expansion), we see the semiclassical structure emerging.

It seemed that one would have to proceed beyond the diagonal approximation to recover the oscillatory behavior which RMT predicts at short scales. However, the remarkable requantization scheme advanced by Bogomolny and Keating shows that it is only necessary to feed in the discreteness of the quantum spectrum to obtain an expression for the correlation functions that extrapolate to the correct oscillatory RMT result in the asymptotic limit of large \( \Omega^2 + \alpha^2 X^4/4\hbar^2 \). It is also important to stress that only diagonal information about periodic orbits enters into this result. In other words, nothing is said about correlations among orbit actions, so that these may only affect higher terms in the asymptotic expansion.
In fact, to obtain higher-order corrections matching the exact series, one would certainly need to introduce information about inter-level correlations as well, which is apparently beyond the capability of any present semiclassical approach, specially in the case of arbitrary parameter variations.

The intrinsic limitation of the semiclassical method to cover small energies at the quantum scale is remarkably manifest in the parametric correlations. The lack of accuracy in energy ranges $\Omega \lesssim \Delta$ imposes a limitation in the accuracy of parametric correlation function for $X \lesssim X_c$, as one can see from Eq. (28). In the standard derivation of Sec. III, this is a direct consequence of the necessity of smoothing the level density. Even in the requantization scheme, although not explicitly, the same problem occurs, since both sharp and smooth cutoffs in the Gutzwiller series do not assure convergence to the actual eigenvalues.

Finally, remark that in this work we did not attempt to investigate deviations from the universal, RMT behavior due to large scale structures in the spectrum which can be ultimately related to short periodic orbits of the system (see, for instance, the supersymmetric treatment used in Ref. [24] for finite conductance disordered systems). Again, the requantization scheme seems to be a good starting point for such systematic studies from a purely semiclassical point-of-view. Unfortunately, at present we only know how to proceed safely by restricting ourselves to the energy range where the diagonal approximation is accurate. There is a possibility that the resummation technique could, in principle, extract additional information from the $\Lambda$ function, but this work has still to be done for generic systems. This is one of the major challenges of the semiclassical theory.

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APPENDIX A: RMT ASYMPTOTIC EXPANSIONS

Here we carry out the asymptotic expansion of $k(\omega, x)$ to lowest order in $x^{-2}$ and $\omega^{-2}$ starting from the exact RMT expressions (8), (9), (11), and (12). Although, for the GUE, one could start from (10), we decided to use the integral expression to illustrate the method. Essentially, we have to separate the contributions coming from the two maximum-amplitude points. For the GUE case, we begin by expanding $F_{GUE}$ around $\lambda = \lambda_1 = 1$:

$$k^{GUE}_{1,1}(\omega, x) \approx \frac{1}{2} \text{Re} \int_0^\infty ds \int_0^\infty ds_1 \exp[-(\pi^2 x^2 - i\pi \omega^+)(s + s_1)]$$

$$\approx \frac{1}{2} \text{Re} \frac{1}{(\pi^2 x^2 - i\pi \omega^+)^2}, \quad (A1)$$

where $s \equiv 1 - \lambda$ and $s_1 \equiv \lambda_1 - 1$. Notice that the integrand in (A1) is only appreciable for $s, s_1 \sim O(x^{-2})$ and, since we only need the lowest order in $x^{-2}$, we can neglect quadratic terms in $s$. Equation (A1), however, is still correct even if $x = 0$, provided that keep $\omega \gg 1$.

Next, we expand $F_{GUE}$ around $\lambda = -\lambda_1 = -1$:
\[ k_{-1,1}^{GUE}(\omega, x) \approx \frac{1}{2} \text{Re} e^{2i\pi \omega^+} \int_0^\infty dr \int_0^\infty ds_1 \exp[-\pi^2 x^2 (r + s_1) - i\pi \omega^+(r - s_1)] \]
\[ \approx \frac{1}{2} \text{Re} \left( \frac{e^{2i\pi \omega^+}}{\pi^2 x^2 - i\pi \omega^+} \right), \quad (A2) \]

where \( r \equiv \lambda + 1 \). This result is also valid for \( x = 0 \) and \( \omega \gg 1 \). Notice moreover that, contrary to the previous contribution, this one is oscillating in \( \omega \) on a scale \( O(1) \) and therefore contains information about the discreteness of the spectrum. We can add (A1) to (A2) to obtain Eq. (13).

The GOE case is similar, but slightly more complicated due to the additional structure in the integrand. Beginning with \( \lambda = \lambda_1 = \lambda_2 = 1 \), we can expand \( F^{GOE} \) and the rest of the integrand around this point to get
\[ k_{1,1,1}^{GOE}(\omega, x) \approx \text{Re} \left[ \frac{1}{(\pi^2 x^2/2 - i\pi \omega^+)^2} \right] \]
\[ \times \int_0^{\pi/2} d\phi \int_0^{\pi/2} d\theta \frac{\sin 2\theta}{[1 + \sin 2\theta (\cos \phi + \sin \phi) + (\cos 2\theta + 1) \sin \phi \cos \phi]^2} \]
\[ \approx \text{Re} \left[ \frac{1}{(\pi^2 x^2/2 - i\pi \omega^+)^2} \right]. \quad (A3) \]

(Here we have resorted to a numerical method to solve the double integral.) Finally, we can expand around the other maximal point, which is \( \lambda = -\lambda_1 = -\lambda_2 = -1 \), and obtain
\[ k_{-1,1,1}^{GOE}(\omega, x) \approx \text{Re} \left\{ e^{2i\pi \omega^+} \int_0^\infty dr \int_0^\infty ds_1 \int_0^\infty ds_2 \frac{(2r)(-2)}{(-4)^2} \right. \]
\[ \times \exp\left[-(\pi^2 x^2/2)(r + s_1 + s_2) - i\pi \omega^+(r - s_1 - s_2)\right] \}
\[ \approx \frac{1}{2} \text{Re} \left( \frac{e^{2i\pi \omega^+}}{\pi^2 x^2/2 - i\pi \omega^+} \right). \quad (A5) \]

Since this contribution is of higher order than (A3), we should only keep the oscillating part and neglect the rest. With this in mind, we arrive at Eq. (14).

**APPENDIX B: PARAMETRIC VARIATION OF PERIODIC ORBIT**

It may be surprising that we can integrate the parametric velocity \( Q_\gamma \) in (24), obtained from classical perturbation theory to yield the exact result:
\[ S(E, X_2) - S(E, X_1) = \int_{X_1}^{X_2} dX \int_0^{T(E,X)} dt \frac{\partial H}{\partial X}(\xi(t), X) \]  

where \( \xi = (p, q) \) are vectors in the classical phase space. Thus there is no limit on the period of the orbit if we keep the right order of integration. We can obtain the expression above by embedding the one parameter family of Hamiltonians \( H(\xi, X) \) into a single Hamiltonian \( \mathcal{H} \) in a phase space that is expanded by two more coordinates. Hence, we add the parameter \( X \) itself and a conjugate variable \( Y \), defining the Hamiltonian so that

\[ \mathcal{H}(\xi, X, Y) \equiv H(\xi, X) \]

at each point. Then, Hamilton’s equations determine that \( X \) is a constant of the motion, whereas the equations for \( \xi \) are unaltered, so that the energy of the original systems is still constant, equal to \( E \). However, the periodic orbits of the original systems now correspond to helicoidal orbits such that

\[ \Delta Y = Q_\gamma(E, X) = \int_0^{T_\gamma} dt \dot{Y}(\xi(t), X) = \int_0^{T_\gamma} dt \frac{\partial H}{\partial X}(\xi(t), X). \]

Conservation of \( E \) and \( X \) implies that each of these helicoidal orbits lies within a two-parameter family in the extended phase space. Fixing the energy \( E \), we thus obtain a two-dimensional surface, along which

\[ \oint dq \cdot p + \oint dX \ Y - \oint dt \ H = 0 \]

for any reducible circuit (as a consequence of the Poincaré-Cartan theorem \[25\]). The last integral cancels, because the full energy has been chosen identical to the energies of the original system, a constant along the surface. Picking the circuit so as to connect two helicoids (corresponding to periodic orbits) with different parameters, we obtain

\[ \oint_{X_2} dq \cdot p - \oint_{X_1} dq \cdot p = \int_{X_1}^{X_2} dX \ Y , \]

recovering (B1).

It is important to note that the action difference refers to a continuous family of periodic orbits. In the case where there is a set of multiply symmetry-connected orbits, (B1) can also be used if the change of parameter does not break the symmetry.

We also point out that (B1) refers strictly to an action difference at constant energy. Of course, it is possible to choose different one-parameter families of periodic orbits within the two-parameter family in our problem. Goldberg et al. \[9\] choose constant volume for the shell instead. This coincides with constant energy for unfolded dynamical systems.

**APPENDIX C: JUSTIFICATION FOR THE GAUSSIAN ANSATZ**

In this appendix we motivate the Gaussian ansatz used in Ref. \[10\] using arguments based solely on the diagonal approximation. Let us start by Taylor expanding the exponential term
of $\Phi_k$ of Eq. (38), thus recasting the original exponential averaging problem into an averaging of increasing powers of $(\delta N_{T'}^H)^n$, with $\delta N_{T'}^H \equiv N_{T'}^H(E, X) - N_{T'}^H(E', X')$.

The lowest-order term of the Taylor expansion ($n = 1$), taken within the validity range of classical perturbation theory, can be written as

$$\langle N_{T'}^H(E + \Omega_1, X + X_1) - N_{T'}^H(E + \Omega_2, X + X_2) \rangle_{E, X} =$$

$$\frac{1}{\pi^2} \left\langle \sum_{r, T, \gamma} A_{rT, \gamma} \exp \frac{irS_\gamma(E + \Omega_1, X + X_1)}{\hbar} - \exp \frac{irS_\gamma(E + \Omega_2, X + X_2)}{\hbar} \right\rangle_{E, \bar{X}}, \quad (C1)$$

which clearly vanishes, since

$$\langle e^{i r S_\gamma(E, \bar{X})/\hbar} \left[ e^{i r T_\gamma(E, \bar{X}) \Omega_1/\hbar + i r Q_\gamma(E, \bar{X}) X_1/\hbar} - e^{i r T_\gamma(E, \bar{X}) \Omega_2/\hbar + i r Q_\gamma(E, \bar{X}) X_2/\hbar} \right] \rangle_{E, \bar{X}} = 0 \quad (C2)$$

due to the very rapid oscillations of the term in $S_\gamma/\hbar$ in the averaging interval $\delta E$.

Generally, in order to energy average the $n$-th power of $\delta N_{T'}^H$, we have to calculate terms like

$$I_{\{r, \gamma\}}^{(n)} = \left\langle \exp \left[ \frac{1}{\hbar} (r_1 S_{\gamma_1} + r_2 S_{\gamma_2} + \cdots + r_n S_{\gamma_n}) \right] \right\rangle_E. \quad (C3)$$

In fact, neglecting repetitions (see comment below), we conclude that $I^{(n)} \approx 0$, whenever $n$ is odd, as in (C1). Moreover, for even values of $n$, we can always find a set of actions that cancel each other, yielding $I^{(n)}_{\{r, \gamma\}} \neq 0$. Due to phase-space restrictions, the largest contribution will come from sets where the actions are grouped pairwise. This allows $\langle (\delta N_{T'}^H)^n \rangle$ to be factorized into powers of $\langle (\delta N_{T'}^H)^2 \rangle$, leading to the Gaussian formula used in Ref. [10]. Note, however, that our argument relies on

$$\frac{1}{\hbar} (r_1 S_{\gamma_1} + r_2 S_{\gamma_2} + \cdots + r_n S_{\gamma_n}) \gg 1, \quad (C4)$$

for any distinct combination of trajectories. This condition is not necessarily satisfied when $n \gg 1$.

Finally, in a first inspection, the inclusion of repetitions would seem to spoil our arguments in favour of the Gaussian ansatz. However, using again phase-space considerations, it is simple to see that the number of terms obtained by cancelling actions using repetitions is much smaller than the number of simple pairwise cancellations of primitive orbits. Thus the effect of the repetitions is not expected to be important.
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