Energy transition scars of driven chaotic systems

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Abstract.

Trajectory segments in the energy $E$-shell, which combine to form a closed curve with segments in another canonically driven energy $E'$-shell, add oscillatory semiclassical structure to the smooth classical background of the energy transition probability density. In this, they resemble the contributions of scars to the spectral Wigner function in the neighbourhood of periodic orbits in a single static energy shell. The exact representation of the transition density as an integral over spectral Wigner functions, that was previously derived for the special case where the system undergoes a reflection in phase space, is here generalized to arbitrary unitary transformations. If these are generated continuously by a driving Hamiltonian, there will be a finite lapse in the driving time for the transition to start, until the initially nested shells touch each other and then start to overlap.

The stationary phase evaluation of the multidimensional integral for the transition density selects the pair of matching trajectory segments on each shell, which close to form a piecewise smooth compound orbit supporting a transition scar. Each compound orbit shows up as a fixed point of a product of mappings that can be interpreted as generalized Poincaré maps on the intersection of the shells. Thus, the closed compound orbits are isolated if the original Hamiltonian is chaotic. The actions of the compound orbits are functions of the driving time. Repetitions have no place in the sum over transition scars, but phase reinforcement can occur if the endpoints of a contributing segment lie close to the stable and unstable manifolds of an ordinary Bohr-quantized periodic orbit.
1. Introduction

The discovery of the scars of periodic orbits in the quantum eigenfunctions of classically chaotic systems by Heller in 1984 [1] jostled the view that these should only reflect uniform ergodic coverage of the corresponding energy shell, as, for instance, in the conjecture of Voros and Berry [2, 3]. Periodic orbits in the energy shell of a chaotic system are isolated. The phase reinforcement of their contribution to a mixed state in a narrow energy window was derived semiclassically (SC) by Bogomolny [4]. Then Berry [5] transported these results into phase space, where scars became a feature of the spectral Wigner function of classically chaotic systems. Later it was shown [6] that caustics in the interior of the energy shell touch it along each periodic orbit, so there is a profusion of caustics separating the multiple contributions of open trajectory segments to the ordinary (complex exponential) SC spectral Wigner function.

The action of an external quantum Hamiltonian drives the eigenstates through a continuous group of unitary transformations and the spectral Wigner function along with them, while the corresponding classical Hamiltonian drives canonically the energy shells and trajectory segments, which are the ingredients of the SC approximation of the driven spectral Wigner function. The eigenenergies are not altered in the driven Hamiltonian and likewise the driven energy shell keeps the same energy constant for the driven classical Hamiltonian, but the original Hamiltonian is not usually constant along a driven trajectory segment, nor is the driven Hamiltonian constant along a trajectory segment of the original Hamiltonian. Since all the points in an original $E$-shell are transported to the driven $E'$-shell, the only contribution to the (original) $E \mapsto E'$ classical transition is due to those points that are driven onto the intersection of the $E$-shell with the driven $E'$-shell.

The special role played in the Weyl-Wigner representation by the continuous set of unitary operators that correspond to classical reflections about any point in phase space, i.e. dislocated parity operators [7, 8], was instrumental for an initial investigation of the probability of $E \mapsto E'$ energy transitions of quantum systems that are driven by these transformations. No distinction between regular, mixed or hard chaotic motion arose in the classical approximation in [9] (henceforth referred to as I), constructed solely on the geometry of the classical $E$-shell, the classical reflection of the $E'$-shell and their intersection. Semiclassically, this may be considered as the contribution of very short trajectory segments, to which are here added the fully oscillatory SC contributions of long segments on both shells with endpoints lying on their intersection.

This paper presents transition scars constructed on closed piecewise smooth compound orbits [10], formed by a trajectory segment in the original $E$-shell and joined at both tips to a segment in a driven $E'$-shell. Just like the scars of true periodic orbits in a single energy shell, these compound orbits will generically be isolated if the return maps to the intersection of the shells are chaotic. The transition scars add oscillations to the smooth classical background presented in I as a parameter of the driving unitary transformation of the system is varied.
This enriched picture results from the stationary evaluation of the exact integral for the energy transition probability density (or transition density for short) between a pair of coarsegrained energies. It was derived in I from an exact integral identity for pure state Wigner functions, but here it is generalized to any unitary transformation with a classically evolving Weyl propagator. Beyond the previous reflections, this includes phase space translations (the Heisenberg group) and the metaplectic group, corresponding to symplectic (linear canonical) phase space transformations. Even for general unitary transformations, it is still valid semiclassically to evolve the Hamiltonian classically and then reconstruct the trajectories on the evolved $E'$-shell and thence the evolved Wigner function. The integral in which it enters for the transition density is then evaluated within the stationary phase, which is again semiclassical. Thus, one can estimate energy transitions for continuous groups of unitary transformations starting from the identity, such as generated by any external driving Hamiltonian. There will be a finite interval before the driven $E'$-shell touches the stationary $E$-shell, provoking a caustic peak in the time dependence of the transition density.

The exact expression for the energy transition density driven by general unitary transformations is derived in the following section. It integrates over the spectral Wigner function for the energy $E$ and the evolved spectral Wigner function for the energy $E'$. As it happens, the focus on ordinary scars limited previous derivations [5, 6] to the neighbourhood of periodic orbits, whereas here open trajectory segments are required. Thus, section 3 extends the SC approximation of spectral Wigner functions and their evolution. The multidimensional stationary phase approximation is then obtained in section 4, which completes the picture of general transition densities in section 5, including the classical term derived in I.

Over fifty years of collaboration with Michael Berry and the wonderful group that grew around him in Bristol has taught me a lot more than Wigner functions. I hope to continue this interaction way beyond the landmark of his eightieth birthday!

**2. Energy transitions driven by general unitary operators**

Consider the evolution of pure eigenstates $|k\rangle$ of a Hamiltonian $\hat{H}$ with energy $E_k$, under the action of a one parameter family of unitary operators

$$\hat{U}(\tau) = e^{-i\tau\hat{\Lambda}/\hbar},$$

(2.1)

where $\hat{\Lambda}$ is the driving Hamiltonian. The probability of a transition to a state $|l\rangle$ in the driving time $\tau$ is

$$P_{kl}(\tau) = |\langle k|\hat{U}(\tau)|l\rangle|^2 = \langle k|\hat{U}(\tau)|l\rangle\langle l|\hat{U}^\dagger(\tau)|k\rangle$$

$$= \text{tr} \hat{U}(\tau)|l\rangle\langle l|\hat{U}(\tau)^\dagger|k\rangle = \text{tr} |l\rangle\langle l|\hat{U}(\tau)|k\rangle\langle k|,$$

(2.2)

where one defines the driven pure state

$$|l\rangle\langle l|\langle l|\equiv \hat{U}(\tau)|l\rangle\langle l|\hat{U}(\tau)^\dagger.$$
Introducing the Wigner-Weyl representation, within the corresponding classical phase space $\mathbb{R}^{2N}$ with its points $\{x = (p, q)\}$, the transition probability is expressed in terms of the Wigner functions $W_k(x)$ and $W_l(x|\tau)$ for the pair of eigenstates as

$$P_{kl}(\tau) = (2\pi\hbar)^N \int d^{2N}x \ W_k(x) \ W_l(x|\tau).$$

(2.4)

If one replaces $\hat{U}(\tau)$ by the phase space reflection operator $\hat{R}_x$ in the preceding formulae, it is recognized that (2.4) is a generalization of of the Wigner function identity on which I was constructed. Of course, an essential element in the original identity is the property that the Wigner function evolves classically under reflections. This classical propagation of the Wigner function is also generated by the Heisenberg operators,

$$\hat{T}_{\xi} = \exp \left[ \frac{2i}{\hbar} \xi \wedge \hat{x} \right] = \int dNq \ |q + \xi_q\rangle\langle q - \xi_q| \exp \left[ \frac{2i}{\hbar} \xi_p \wedge q \right],$$

(2.5)

where $\xi$ is the halfchord for the corresponding phase space translation $x \mapsto x + 2\xi$, as well as the metaplectic operators, which correspond to symplectic, i.e. linear canonical transformations in phase space. §

In general, the SC approximation of a driven eigenstate $W_l(x|\tau)$ does not equal its simple classical evolution, which is known as the truncated Wigner approximation (TWA), but it will be justified in the following section that it is identified with the Wigner function of the $l$'th eigenstate of the driven Hamiltonian:

$$\hat{H}(\tau) \equiv \hat{U}(\tau) \hat{H} \hat{U}(\tau)^\dagger,$$

(2.6)

with the same energy $E_l$.

Now one coarsegrains the transition probability as in I by invoking of the spectral Wigner function [5, 12, 6]

$$W_E(x, \epsilon) \equiv (2\pi\hbar)^N \sum_k \delta_\epsilon(E - E_k) \ W_k(x),$$

(2.7)

which represents the spectral density operator

$$\hat{\rho}_E(\epsilon) \equiv \sum_k \delta_\epsilon(E - E_k) \ |k\rangle\langle k|$$

(2.8)

for a classically narrow energy range $\epsilon$ centred on the energy $E$, such that $\delta_\epsilon(E)$ integrates as a Dirac $\delta$-function and likewise

$$W_E(x, \epsilon|\tau) \equiv (2\pi\hbar)^N \sum_k \delta_\epsilon(E - E_k) \ W_k(x|\tau)$$

(2.9)

is the spectral Wigner function for the driven system. Then the probability density for the transition $E \mapsto E'$

$$P_{EE'}(\tau, \epsilon) \equiv \text{tr} \ \hat{\rho}_E(\epsilon) \ \hat{\rho}_{E'}(\epsilon|\tau)$$

(2.10)

§ In fact, the translation operators are the basis for the chord representation, equivalent to the Wigner-Weyl representation, so one could construct the whole SC theory for energy transitions on the chord function instead of the Wigner function, but there is no immediate advantage, being that the latter are much more familiar. Here, we adopt the notation in [13] in which the halfchord $\xi$ lables half the translation, instead of the full translation as in all my previous papers.
results from the summation over both indices in (2.4) as

$$P_{EE'}(\tau, \epsilon) = (2\pi\hbar)^N \sum_{k,l} \delta_\epsilon(E - E_k) \delta_\epsilon(E' - E_l) \int d^{2N}x \ W_k(x) W_l(x|\tau)$$

(2.11)

$$= \frac{1}{(2\pi\hbar)^N} \int d^{2N}x \ W_E(x, \epsilon) W_{E'}(x, \epsilon|\tau).$$

Even though the limitation to the continuous group of unitary transformations generated by a particular external Hamiltonian is in no way essential, it should be noted that the reflection operator $\hat{R}_x$ is never close to the identity $\hat{I}$. Indeed, the reflections do not form a group and it is only in combination with the Heisenberg group of translation operators $\hat{T}_\xi$ that the quantum version of the affine group is formed [14, 6]. Thus, the translation operators will be the main example, for which the transition densities for general translations $2\xi$ take the specific form

$$P_{EE'}(\xi, \epsilon) = \frac{1}{(2\pi\hbar)^N} \int d^{2N}x \ W_E(x, \epsilon) W_{E'}(x + 2\xi, \epsilon).$$

(2.12)

bearing in mind that the simplest driving Hamiltonian $\Lambda(x) = \alpha \wedge x/2$ generates the subgroup of translations with the half chord $\xi(\tau) = \tau \alpha$.

A further advantage of focusing on the translations is that a reflection through a general point $x$ combines a reflection through the origin with a translation by $2\xi = 2x$. If $H(x)$ is symmetric with respect to the origin, there is no difference between the reflected energy shell and the shell merely translated by $2x$. We can then keep in mind the structures of centre sections explored in I, but in general the reflection centre $x$ does not need to be close to the $E$-shell, where lies the caustic of the SC spectral Wigner function that was there analyzed. On the other hand, a subgroup of translations by $2\tau\alpha$ of a nearby energy shell will take a short time interval until the smaller section touches the larger one from its inside. With further translations the section quickly grows into a large manifold, though it may still have the topology of a sphere, just as common Poincaré sections. One can expect most if not all periodic orbits to traverse the section, so that their successive intersections with the section become periodic points of the generalized Poincaré map.

The transition density $P_{EE'}(\tau, \epsilon)$ is expressed in (2.11) as an integral over a spectral Wigner function and a driven spectral Wigner function. A first appraisal of the transition density is provided by the intersection of the pair of energy shells involved in the transition. It was shown in I that near a caustic one can get away with an integral just over their intersection. For large sections one needs to add a full SC description of the spectral Wigner functions in terms of trajectory segments, each with a phase determined by its classical action.

3. Spectral Wigner functions revisited

The SC approximation for $W_E(x, \epsilon)$ is based on trajectory segments in the $E$-shell with their tips $x_\pm$ centred on $x$ [5, 12, 6]. Let us return to its construction from the Weyl
The action, $S(x, t)$, is just the symplectic area between the trajectory from $x^-$ to $x^+$ and its chord $2\xi$, from which one subtracts $Et$, where $E$ is the energy of the trajectory.

The propagator $V(x, t)$, which represents the intrinsic unitary evolution operator

$$\hat{V}(t) = e^{-it\hat{H}/\hbar},$$

that is,

$$W_E(x, \epsilon) = \text{Re} \int_0^\infty \frac{dt}{\pi \hbar} \exp \left( i\frac{t}{\hbar}(E + i\epsilon) \right) V(x, t).$$

In the simplest case, the Weyl propagator has the SC approximation

$$V(x, t) \approx 2^N \left| \det(I + M(t)) \right|^{1/2} \exp \left[ i\frac{1}{\hbar}(S(x, t)) + \hbar \pi \sigma \right],$$

if there is just a single classical trajectory centred on the point $x$; otherwise there will be a superposition of similar terms. The geometric part of the centre or Weyl action $S(x, t)$ is just the symplectic area between the trajectory $\dot{x}(t, x_-)$ and the chord $2\xi = x_+ - x_-$, as shown in Fig.1. From this, one subtracts $-Et$, where $E$ is the energy of the trajectory.

The centre action specifies the classical canonical transformation, $x_\pm \mapsto x_\pm$, corresponding to $\hat{V}(t)$ indirectly through

$$2\xi = -J \frac{\partial S}{\partial x}, \quad x_\pm = x \pm \xi,$$

where the standard symplectic matrix is

$$J = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$$

in terms of $(p, q)$ blocks. The linear approximation of this transformation near the $x$-centred trajectory is defined by the stability matrix $M$. There may be multiple solutions to the variational problem that identifies trajectories with a given centre $x$, so the actions may have many branches and these branches meet along caustics where the semiclassical amplitude diverges. For short times there are no caustics and $\sigma = 0$. 

**Figure 1.** The action, $S(x, t)$, is just the symplectic area between the trajectory from $x^-$ to $x^+$ and its chord $2\xi$, from which one subtracts $Et$, where $E$ is the energy of the trajectory.
The stationary phase evaluation of \[ (3.2) \] singles out the trajectory segments on the \( E \)-shell with their tips \( x_{\pm} \) centred on \( x \). Their times \( t_j \) may be positive or negative, i.e. one also includes \( \tilde{x}(-t) \), exchanging the endpoints \( x_{\pm} \) centred on \( x \), because of taking the real part, with the result

\[
W_E(x, \epsilon) \approx \sqrt{\frac{2}{\pi \hbar}} \sum_{j} \frac{2^N}{|dE/dt_j| \left| \det(\mathbf{I} + \mathbf{M}(t_j)) \right|^{1/2}} e^{-|t_j|/\hbar} \cos \left[ \frac{S_j(x, E)}{\hbar} + \lambda_j \right]. \tag{3.6}
\]

The only change in the energy action branches \( S_j(x, E) \) with respect to the time action \( S(x, t) \), for the same trajectory segment that is centred on \( x \), is the absence of the term \(-Et\). Thus the relation \[ (3.4) \] between the centre \( x \) and the endpoints still holds for the branches of the energy action, even though it is only the time action that plays the role of a generating function for the respective canonical transformation.

Previous treatments of the spectral Wigner function have been mostly concerned with their scars in the neighbourhood of periodic orbits, so that the endpoints nearly coincide. Then it is possible to adopt time-energy variables locally, which limits the stability matrix to the remaining transverse variables. Even though distant endpoints cannot be so simply treated, a variant of the velocity plane introduced in I is of help. Indeed, the 2-D plane spanned by the endpoint velocities \( \dot{x}_{\pm} \) may be chosen for the \((p,q)\) coordinates of the \( N \)'th conjugate plane in a symplectic coordinate system for the \( 2N \)-D phase space. Each of these velocities has a \((2N-1)\)-D skew-orthogonal plane, \( \parallel \), identified with the pair of tangent planes to the energy shell at \( x_{\pm} \). Then any vector \( y \) in the \( 2(N-1)\)-D intersection of these planes is skew orthogonal to the velocity plane and one may choose an arbitrary symplectic coordinate system on \( y \) together with \((p,q)\) to complete the \( 2N \) symplectic coordinates for the phase space \[ 16 \].

Following I and originally \[ 15 \] one introduces the pair of displaced Hamiltonians

\[
H_+ = H(x + \xi) \quad \text{and} \quad H_- = H(x - \xi), \tag{3.7}
\]

which can be considered as either functions of the centre \( x \), for a fixed halfchord \( \xi \), or vice versa. Then Hamilton's equations for the pair of basis vectors \( \dot{x}_{\pm} \) can be expressed as

\[
\dot{p}_{\pm} = -\frac{\partial H_{\pm}}{\partial q} \quad \text{and} \quad \dot{q}_{\pm} = \frac{\partial H_{\pm}}{\partial p}, \tag{3.8}
\]

whereas

\[
\dot{y}_{\pm} = J \frac{\partial H_{\pm}}{\partial y} = J \frac{\partial H}{\partial y}(x_{\pm}) = 0. \tag{3.9}
\]

Furthermore, the Jacobian matrix for adopting the displaced Hamiltonians themselves as (nonsymplectic) coordinates on the velocity plane, instead of \((p,q)\), is just

\[
\frac{\partial (H_+, H_-)}{\partial (p, q)} = \frac{\partial H_+}{\partial p} \frac{\partial H_-}{\partial q} - \frac{\partial H_+}{\partial q} \frac{\partial H_-}{\partial p} = \dot{x}_+ \wedge \dot{x}_- = \{H_+, H_-\}, \tag{3.10}
\]

which is identified as the full Poisson bracket of the pair of displaced Hamiltonians.

\[ || \] that is, the plane orthogonal to \( J \dot{x}_{\pm} \).
Let us now consider the stability matrix for the linearized motion surrounding the chosen trajectory segment centred on \( x \) in the time \( t_j \): \( \delta x_+ = M(t_j) \delta x_- \). This symplectic transformation takes a tangent plane to the \( E \)-shell at \( x_- \) to its tangent plane at \( x_+ \), so that by energy conservation any displacement of the form \( \delta x_- \) is transported to \( (\delta y_+ = M_y(t_j) \delta y_-) \). Conversely if \( \delta y_- = 0 \), then the only component of \( \delta x_- \) in the initial tangent plane lies along \( \dot{x}_- \), whereas the component of \( \delta x_+ \) in the tangent plane at \( x_+ \) follows \( \dot{x}_+ \), so that we also have \( \delta y_+ = 0 \). In short, the stability matrix separates into a tangent block \( M_y \) and a 2-D block \( m \) in the velocity plane, identified with the full matrix \( M \) itself in the case of a single degree of freedom. Then we have 

\[
\det(I + M(t_j)) = \det(I + m(t_j)) \det(I + M_y(t_j)) \quad \text{in the denominator of (3.6), noting that}
\]

\[
(I + m)^{-1} = [\det(I + m)]^{-1} (I + m^{-1}). \tag{3.11}
\]

The energy derivative in the SC spectral Wigner function presupposes trajectories with a fixed centre \( x \), but it is more natural to fix the initial point \( x_- \), so that for \( x(t, x_-) \) we impose

\[
\delta x = \frac{\partial x}{\partial x_-} \delta x_- + \frac{\partial x}{\partial t} \delta t = \frac{1}{2} (I + m(t_j)) \delta x_- + \frac{1}{2} \dot{x}_+(x_-, t) \delta t = 0, \tag{3.12}
\]

that is,

\[
\frac{\partial x_-}{\partial t}(x, t) = -(I + m)^{-1} \dot{x}_+(x_-, t) \tag{3.13}
\]

and hence, for fixed \( x \),

\[
\frac{dE}{dt} = \frac{\partial H}{\partial x_-} \cdot \frac{\partial x_-}{\partial t}(x, t) = -(J \dot{x}_-) \cdot (I + m)^{-1} \dot{x}_+
\]

\[
= [\det(I + m)]^{-1} \dot{x}_- \wedge (\dot{x}_+ + \dot{x}_-)
\]

\[
= [\det(I + m)]^{-1} \{H_-, H_+\}, \tag{3.14}
\]

using (3.11).

In conclusion, the SC approximation for the spectral Wigner function becomes

\[
W_E(x, \epsilon) \approx \sqrt{\frac{2}{\pi \hbar}} \sum_j \frac{2^N}{\sqrt{\{|\{H_-, H_+\}_j | (I + M_y(t_j))\}|^{1/2}}} e^{-\epsilon|t_j|/\hbar} \cos \left[ \frac{S_j(x, E)}{\hbar} + \lambda_j \right]. \tag{3.15}
\]

In the case of a single freedom, there are no transverse \( y \)-coordinates and hence no determinant remains in the denominator, which becomes singular at the caustic as \( x \) touches the energy shell. The remaining Poisson bracket of the displaced Hamiltonians is proportional to the Poisson bracket of the pair of action variables in the SC expression for a pure state Wigner function in [15].

In general, averaging over oscillations in \(|W_E(x, \epsilon)|^2 \) one obtains a classical envelope in terms of the full denominators \( \{H_+, H_+\}_j \) in the sum over all trajectory segments-\( j \). This is here a discrete sum, instead of the integral in \( I \) (effectively over a continuum of \( t = 0 \) trajectories), being that here the transverse factor \( |\det(I + M_y(t_j))| \) in the denominator brings in the stability of each finite trajectory segment. Defining the centre
section 6 (also reviewed in I), each contributing segment determines a fixed point of some iteration of a generalized Poincaré map.

So far the focus has been on the original spectral Wigner function, but we also need its evolved form (2.9). This is determined by a purely classical evolution of its argument in the simple cases of reflections and translations, which may be combined with symplectic transformations, but not general canonical evolutions generated by a driving Hamiltonian \( \Lambda(x) \) with higher than second order terms. Nonetheless, the SC approximation of the Weyl representation of the driven quantum Hamiltonian (2.6) is merely

\[
H(x|\tau) = H(\tilde{x}(-\tau, x)),
\]

that is, the driven classical Hamiltonian. On the other hand, the intrinsic evolution operator (3.1) generated by the driven Hamiltonian is simply

\[
\hat{V}(t|\tau) \equiv \hat{U}(\tau) e^{-it\hat{H}/\hbar} \hat{U}(\tau)^\dagger = \exp \left[-\frac{it\hat{H}}{\hbar} \right].
\]

(3.16)

It follows that the corresponding SC approximation for the evolved Weyl propagator \( V(x, t|\tau) \) is just (3.3) based on the classical trajectories of the driven classical Hamiltonian and consequently (3.2) supplies the SC evolved spectral Wigner function in the form of (3.6).

Explicitly then the SC approximation for the evolved spectral Wigner function for the coarse-grained energy shell \( H(x|\tau) = E' \) is

\[
W_{E'}(x, \epsilon|\tau) \approx \sqrt{\frac{2}{\pi\hbar}} \sum_j 2^N \left[ \frac{\{H_-, H_+\}_j(\tau)}{\det(I + M_y(t_j|\tau))} \right]^{1/2} \exp \left[-\frac{\epsilon|t_j|}{\hbar} \right] \cos \left[ \frac{S_j(x, E'|\tau)}{\hbar} + \lambda_j \right].
\]

(3.17)

Here the driven pair of displaced classical Hamiltonians \( H_\pm(x|\tau) = H(x_\pm(t_j|\tau)) \) has the Poisson bracket \( \{H_+, H_+\}_j(\tau) \), though the dependence on the centre \( x \), as that of the stability matrix, is not shown explicitly. Indeed, one should keep in mind that even the time \( t_j \) of each trajectory segment is \( x \)-dependent and that the index-\( j \) runs over positive and negative times. The derivative of the driven action \( S_j(x, E'|\tau) \) with respect to \( x \) supplies the driven chord \( \xi_{j'}(x|\tau) \) and hence the endpoints, which lie on the driven energy shell according to (3.3).

4. Stationary phase evaluation of the scars in the transition density

Inserting the SC approximations (3.15) and (3.17) of the original and the evolved spectral Wigner functions in the exact expression (2.11) for the transition density results in a sum of integrals over complex exponentials labeled by all the windings of the trajectory segments lying on either energy shell, such that their centre is the integration variable \( x \):

\[
P_{EE'}(\tau, \epsilon) \approx \text{Re} \left( \frac{2}{\pi\hbar} \right)^{N+1} \sum_{j, j'} \sum_{j, j'}
\]

(4.1)

\[\updownarrow\text{In this way, the usual procedure of constructing SC approximations based on evolving Lagrangian manifolds is extended to structures of different dimensionality in phase space.}\]
The stationary phase condition for the integral in each term then singles out the stationary points \( \mathbf{x} = \mathbf{x}_{jj'} \), for which

\[
\frac{d}{d\mathbf{x}} [S_j(\mathbf{x}, E) + S_j'(\mathbf{x}, E'|\tau)] = 0. \tag{4.3}
\]

According to \((3.4)\) this implies that the halfchords \( \xi_j(\mathbf{x}_{jj'}) + \xi_{jj'}(\mathbf{x}_{jj'}|\tau) = 0 \) (allowing for the notation \( \xi(\mathbf{x}_{jj'}) = \xi_j(\mathbf{x}_{jj'}) = -\xi_{jj'}(\mathbf{x}_{jj'}|\tau) \)), so that the pairs of segments centred on the stationary points join continuously at both their endpoints.

\[
\mathbf{x}_+(\mathbf{x}_{jj'}, t_j) = \mathbf{x}_-(\mathbf{x}_{jj'}, t_j') \quad \text{and} \quad \mathbf{x}_+(\mathbf{x}_{jj'}, t_j') = \mathbf{x}_-(\mathbf{x}_{jj'}, t_j). \tag{4.4}
\]

In other words, each stationary phase contribution to the transition density is ascribed to a single continuous piecewise smooth trajectory joining both energy shells. This is an example of a (closed) compound orbit and its total action is

\[
S_{jj'} = S_j(\mathbf{x}_{jj'}, E) + S_j'(\mathbf{x}_{jj'}, E'|\tau). \tag{4.5}
\]

The full evaluation of \((4.2)\) by stationary phase requires the variation of the sum of the chord areas of both segments as their common centre \( \mathbf{x} \) moves out from \( \mathbf{x}_{jj'} \). Then they no longer fit together and the tips of their chords \( 2\xi_j(\mathbf{x}) \) and \( 2\xi_{jj'}(\mathbf{x}|\tau) \), both centred on \( \mathbf{x} = \mathbf{x}_{jj'} + \delta\mathbf{x} \), can be joined in an elongated polygonal figure of eight. Illustrated in Fig. 2, it has zero symplectic area because of the central symmetry. This continuous displacement of the centre from zero to \( \delta\mathbf{x} \) brings with it a continuous family of trajectory segments on the \( E \)-shell. The displacement of the endpoints \( \delta\mathbf{x}_\pm(E) \) (shown in red in the figure) connect opposite corners of the figure of eight at \( \mathbf{x}_\pm(\mathbf{x}_{jj'} + \delta\mathbf{x}) \) to the endpoints \( \mathbf{x}_\pm(\mathbf{x}_{jj'}) \) of the stationary chord. By the Poincaré-Cartan theorem [16], the elongated circuit formed by this family of trajectory segments also has zero symplectic area. The analogous construction for the elongated circuit on the border of trajectory segments on the driven \( E' \)-shell is closed by another pair of (red) displacements \( \delta\mathbf{x}_\pm(E') \), also with tips at \( \mathbf{x}_\pm(\mathbf{x}_{jj'}) \). Adding and subtracting these three circuits with zero symplectic area to the original pair of actions, it is verified that all that is left in the overall variation of the sum of the actions is the pair of small triangles, here illustrated in red.

In terms of the Hessian matrices

\[
B_j = \frac{1}{2} \frac{\partial^2 S_j}{\partial \mathbf{x}^2}(\mathbf{x}_{jj'}, E) \quad \text{and} \quad B_{jj'} = \frac{1}{2} \frac{\partial^2 S_{jj'}}{\partial \mathbf{x}^2}(\mathbf{x}_{jj'}, E'|\tau) \tag{4.6}
\]

the variation of the endpoints is

\[
\delta\mathbf{x}_\pm(E) = (\mathbf{I} \pm B_j)\delta\mathbf{x} \quad \text{and} \quad \delta\mathbf{x}_\pm(E') = (\mathbf{I} \pm B_{jj'})\delta\mathbf{x}. \tag{4.7}
\]

It should be noted that the coincidence of the pair of endpoints does not carry over to the velocities \( \dot{\mathbf{x}}_\pm(\mathbf{x}_{jj'}, t_j) \) and \( \dot{\mathbf{x}}_\pm(\mathbf{x}_{jj'}, t_j') \), leading to different Poisson brackets in the denominator of the integrand, which is just their skew product, according to \((3.10)\). Thus, one should also distinguish the variables \( \mathbf{y}(t_j) \) and \( \mathbf{y}(t_j') \) that are transverse to the respective velocity planes.

* Originally constructed from trajectory segments in SC Weyl propagators in [10].
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\begin{align}
\frac{d^2}{dx^2} [S_j(x, E) + S_j'(x, E'|\tau)] &= 2B_j + 2B_{j'} + B_j BB_{j'} + B_{j'} JB_j. \\
\end{align}

Thus, defining the signature \(\sigma_{jj'}\) of this matrix, the SC approximation for the contribution of the transition scars to the transition density becomes

\begin{align}
P_{EE'}(\tau, \epsilon) &\approx \text{Re} \left( \frac{2}{\pi\hbar} \right)^{N+1} \sum_{j,j'} \exp \left[ \frac{i}{\hbar} S_{jj'} + i(\lambda_j + \lambda_{j'} + \pi \sigma_{jj'}) - \frac{\epsilon}{\hbar} (|t_j| + |t_{j'}|) \right] \\
&\cdot \left\{ \langle [H_-, H_+], [H_-, H_+] \rangle^{1/2} \text{det}(I + M_y(t_j)) \text{det}(I + M_y(t_{j'}|\tau)) \right. \\
&\left. \text{det}(2B_j + 2B_{j'} + B_j BB_{j'} + B_{j'} JB_j) \right\}^{-1/2}. \\
\end{align}

It should be noted that the most important ingredient in the above scar contributions preserves no imprint of the Wigner-Weyl representation within which it was derived. Indeed, the action \(S_{jj'}\) of each closed compound orbit need not be decomposed into two centre actions and one would obtain the same result in another representation. For instance, an inverse Weyl-Wigner transformation of the spectral Wigner function furnishes the spectral density operator \(\hat{\rho}_E(\epsilon)\) as \(\langle q_-|\hat{\rho}_E(\epsilon)|q_+\rangle\), its position representation. Again the SC approximation is based on trajectory segments, but constrained by their fixed end positions \(q_\pm\), while the derivative of the actions supplies the end momenta \(p_\pm = p(q_\pm, E)\). Then the trace of the product operator in (2.10) becomes an integral over \(q_-\) and \(q_+\) instead of \(x\) and the stationary condition is just

\begin{align}
p(q_+, E) = p(q_-, E'|\tau) \quad \text{and} \quad p(q_+, E'|\tau) = p(q_-, E). \\
\end{align}

Hence, one obtains again the transition scars based on closed compound orbits with the same action as before. The amplitude of the scars will not be immediately translatable.
into that in (4.12) and it may be worthwhile to try to rework these alternatives into a simpler more compact form in the future.

5. Semiclassical scenario for energy transitions

The stationary phase evaluation of the transition scars should now be completed with a broader picture of the transition density. This relies on further generalizations of Poincaré sections to those presented in I, following [6]. Let us recall that the centre section of the $E$-shell is the intersection with its reflection or that of another $E'$-shell through a given point, here chosen as $x_{jj'}$. The $j$-segment, contributing to the spectral Wigner function and hence to the above SC approximation, participates in the mapping of the section onto itself. Originally in I, the reflected shell was identified with the driven shell, but this no longer holds here, so that one can also define the evolved centre section in complete analogy, that is, the intersection of the driven $E'$-shell with its reflection through the same stationary point $x_{jj'}$. Then it is the $j'$-segment, contributing to the driven spectral Wigner function, that participates in the $j'$-mapping of the evolved centre section onto itself, in which the label $j'$ indicates the number of times the segment crosses the section. These centre sections are defined for any centre $x$, but it is only at the stationary points $x_{jj'}$ that both segments meet to form the closed $jj'$-compound orbit.

The pairs of centre sections and their mappings may be considered as scaffolding, superseded by the alternative evolved section resulting from the intersection of the $E$-shell with the driven the $E'$-shell. Clearly, the pair of stationary trajectory segments also have their tips on this section for all $j$ and $j'$ windings, so that one may consider the smooth extension to neighbouring trajectories, thus defining the $j$-mapping and the $j'$-mapping of the evolved section onto itself. It follows that all stationary contributions to the transition probability density are constructed on the fixed points of the product of a $j$-mapping with a $j'$-mapping of the driven section onto itself. The common centre $x_{jj'}$ of each of the related closed compound orbits depends on $j$ and $j'$. Both the $j$-segment on the $E$-shell and the $j'$-segment on the driven $E'$-shell are smooth solutions of their respective Hamilton equations, joined together by their endpoints, which lie on the evolved section.

The evolved section coincides with the centre section if the evolution is a reflection. Likewise the classical approximation constructed in I for that case can be immediately extended to general evolutions. Indeed, the extra contribution of very short trajectories, is not obtained by stationary phase, but it will be identified as the 00-term in the full SC expression for the transition density. This approximation holds where both spectral Wigner functions are adequately described by Dirac $\delta$-functions on their respective energy shells. Within this approximation, the integral (2.11) for the transition density is constrained to the evolved section and

$$P_{EE'}(\tau, \epsilon)_{00} \approx \int dx \delta(H_-(x) - E) \delta(H_+(x|\tau) - E'). \quad (5.1)$$
Thus, following $I$, one obtains the generalized classical contribution as

$$P_{EE}(\tau,\epsilon)_{00} \approx \oint_{x_0} d\mathbf{x} \left|\{H_-(\mathbf{x}), H_+(\mathbf{x}|\tau)\}\right|^{-1}, \quad (5.2)$$

where the single Poisson bracket here matches the Hamiltonian with its evolved image, hence the change in notation. As discussed in $I$, the integrand only becomes singular over the evolved section at caustics, but the result is finite if $N > 1$.

The families of evolved sections along with their $jj'$-mappings are identified by a single continuous parameter the time $\tau$, or $2N$ parameters such as either a translation $\xi$ or a reflection centre $\mathbf{x}$. Thus, a smooth family of evolved sections leads to smooth families of $j$-mappings and $j'$-mappings, which give rise to smooth families of $jj'$-fixed points, each on a compound orbit of the respective $jj'$-mapping. It is then possible to follow the $jj'$-families of compound orbits numerically like ordinary periodic orbit families $[18]$, converging by Newton’s method for each small parameter increment, even through eventual bifurcations.

The finite width of the coarsegrained energy shells dampens exponentially the compound orbits for which $|t_j| + |t_{j'}| > \hbar/\epsilon$, effectively cutting off their contribution to the SC sum for the transition density. It should be noted that no repetition of the compound orbit is included, unlike usual periodic orbit theory, since a single $j$-segment on the $E$-shell is followed by a single $j'$-segment on the $E'$-shell, no matter how many individual windings are indicated by $j$ and $j'$. This pair of segments is responsible for the particular $jj'$-mapping of the evolved section onto itself: the product of the $j$-mapping on this section of the $E$-shell and the $j'$-mapping on the same section of the driven $E'$-shell. Both these mappings will be chaotic, if so is the original Hamiltonian $H(\mathbf{x})$, implying that the compound orbits will be just as isolated as the periodic orbits in the original $E$-shell. Hence, the transition scars will be isolated for chaotic systems.

There is no reinforcement through phase coherence of contributions for Bohr-quantized compound orbits, since they are unique for each $j$ and $j'$. The only similar eventuality that comes to mind is for the endpoints of a $j$-segment (or a $j'$-segment) to lie near a pair of stable and unstable manifolds of a true periodic orbit that is Bohr-quantized. Then there will be a sequence of $j$-segments contributing to a sequence of $jj'$-compound orbits converging to a common phase and hence a possible peak in the transition density. This eventual phase reinforcement depends basically on the energy $E$, or alternatively on the energy $E'$ of the evolved shell, since the action of the approximated periodic orbit is canonically invariant. Then changes of $\tau$ only affect smoothly the endpoints of the pair of segments forming the compound orbit, which can wander away from the stable and unstable manifolds and hence the segment may wind further away from the Bohr-quantized orbit.

The subgroup of translations $\xi(\tau) = \tau\alpha$ generated by the driving Hamiltonian $\Lambda(\mathbf{x}) = \alpha \wedge \mathbf{x}$ provides the simplest example of time evolutions, being that, as for Wigner functions, the quantum evolution of chord functions is purely classical. The
chord function for a pure state $|\psi\rangle$ is
\[
\chi(\xi) = \frac{1}{(2\pi\hbar)^N} \langle \psi | \hat{T}_{2\xi} | \psi \rangle
\] (5.3)
and, if the original Hamiltonian $H(x)$ has a centre of symmetry, then chord functions for its eigenstates and their mixtures are real and equal to the respective Wigner functions. Then both representations of a an eigenstate have their maximum at the origin. This peak is shared by the spectral Wigner functions and the diagonal term of the transition density (for no energy transition) is merely $|W_E(x, \epsilon)|^2$. Semiclassically it becomes a supercaustic: Instead of being merely tangent at a single point, the yet to be evolved image of the energy shell coincides with the shell. Then, early in the evolution, it cuts the shell along a maximal section, such that any trajectory segment of the unperturbed shell reaching the section is the initial point of a returning segment along the evolved shell that nearly reaches its initial point, that is, all points on the evolved section are nearly fixed points! There is then a minimal interval before the global participation of all the points on the evolved section condenses onto the orthodox SC contribution of selected trajectory segments. This is a very short transit, because the pair of segments are long and all that is needed is for the action between them to be of order $\hbar$. Far from caustics, the diagonal transition density has SC contributions by the same compound orbits as the Wigner function and the chord function, but with their full action, instead of its half. The essential difference if $E \neq E'$ is that $P_{EE'}(\tau = 0, \epsilon) = 0$: It takes a finite $\tau$ for the driven $E'$-shell to touch the static $E$-shell, generically at a tangent point in a true caustic of the transition density, and it is only then that the previously evanescent transition density starts to oscillate semiclassically.

Unlike the external caustics discussed in I, which limit the parameters for which the evolved $E'$-shell lies entirely outside the $E$-shell, this internal caustic marks the parameter for which they are no longer nested inside each other. Beyond this caustic parameter, the pair of segments forming the compound orbit quickly elongate to reach a growing section, which becomes nearly maximal as in the diagonal case. From then on, both cases are similar and the evolved section slowly shrinks again, until the external caustic is reached. Even with the cutoff in time supplied by the finite energy widths, there will be many closed compound orbits that generate transition scars in the various $jj'$-mappings of a large evolved section. However, as the section diminishes on the approach of an external caustic, fewer contributions of sufficiently small period cross the section, so that in the neighbourhood of the caustic there will only be a SC scar if the section is traversed by a short periodic orbit of either energy shell. Then the closed compound orbit is a mere perturbation of the periodic orbit, which will lead to phase reinforcement of this scar in case of Bohr quantization.

The SC approximation for the transition density in terms of exponential oscillations becomes singular as either caustic is approached and it needs to be replaced by a uniform approximation, already discussed in I in the case of phase space reflections. The reflection symmetry between the $E$-shell and its evolution simplifies the uniform approximation, which is expressed in terms of the Airy function [19], but for the
nondiagonal expression and generally for the chord function of nonsymmetric energy shells, one needs the complete fold-catastrophe expression including the derivative of the Airy function, as described by Berry [20] and implemented for chord functions in [21]. In any case, the approximation [6]

$$S_j(x_{jj'}) \approx \frac{2^{5/2}}{3} \frac{(E - H(x_{jj'}))^3/2}{(x_{jj'} H_{jj'} x_{jj'})^{1/2}}$$

(5.4)

for the action of a contribution of a short trajectory segment to the spectral Wigner function if \( x \) lies close to the \( E \)-shell, with

$$H_{jj'} = \frac{\partial^2}{\partial x^2} H(x_{jj'}) ,$$

(5.5)

leads to the dominant contribution to the Hessian matrix (4.6) as

$$B_j \approx \sqrt{\frac{2}{(E - H(x_{jj'}))(x_{jj'} H_{jj'} x_{jj'})}} \frac{\partial H}{\partial x} \otimes \frac{\partial H}{\partial x} .$$

(5.6)

This is a large positive matrix near a caustic and \( B_{jj'} \) will follow suit. Hence, the scar contributions vanish on the caustic just as the main classical contribution, as was shown in I. Since these matrices are positive, the signature in (4.11) follows that of \(-B_j^2\), that is, \(\sigma_{jj'} = -2N\). So it will remain, as the driving parameter changes continuously, until there is a zero eigenvalue in (4.10) entailing a singularity in the SC approximation for the transition scar.

The fact that the spectral Wigner functions represent a mixed state for a classically narrow \( \epsilon \)-window of energies, effectively a coarsegrained microcanonical ensemble, may seem a disadvantage. Taking \( \epsilon \to 0 \) to obtain a sharp transition rather than a density is problematic, as are resummation procedures to obtain a finite sum [22, 6]. On the other hand, it should be borne in mind that an eventual future preparation in a real laboratory of an initial highly excited eigenstate may be quite difficult for a typical quantum system. If it corresponds to prevalent classical motion, the complete absence of the very selection rules, which allow one to pick out an individual state within a dense spectrum, may be a serious obstacle, though this is current practice, for instance, for integrable highly excited Rydberg atoms.

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