

Article

Energy Transition Density of Driven Chaotic Systems: A Compound Trace Formula

Alfredo M. Ozorio de Almeida 

Centro Brasileiro de Pesquisas Físicas, Rua Xavier Sigaud 150, Rio de Janeiro 22290-180, RJ, Brazil; ozorio@cbpf.br

Abstract: Oscillations in the probability density of quantum transitions of the eigenstates of a chaotic Hamiltonian within classically narrow energy ranges have been shown to depend on closed compound orbits. These are formed by a pair of orbit segments, one in the energy shell of the original Hamiltonian and the other in the energy shell of the driven Hamiltonian, with endpoints that coincide. Viewed in the time domain, the same pair of trajectory segments arises in the semiclassical evaluation of the trace of a compound propagator: the product of the complex exponentials of the original Hamiltonian and of its driven image. It is shown here that the probability density is the double Fourier transform of this trace, and that the closed compound orbits emulate the role played by the periodic orbits in Gutzwiller's trace formula in its semiclassical evaluation. The phase of the oscillations with the energies or the evolution parameters agree with those previously obtained, whereas the amplitude of the contribution of each closed compound orbit is more compact and independent of any feature of the Weyl–Wigner representation in which the calculation was carried out.

Keywords: quantum energy transitions; semiclassical trace formulae; compound classical trajectories



Citation: Ozorio de Almeida, A.M. Energy Transition Density of Driven Chaotic Systems: A Compound Trace Formula. *Quantum Rep.* **2022**, *4*, 558–565. <https://doi.org/10.3390/quantum4040040>

Academic Editors: Andrei Klimov, Luis L. Sánchez-Soto and Hubert de Guise

Received: 8 October 2022

Accepted: 16 November 2022

Published: 30 November 2022

Publisher's Note: MDPI stays neutral with regard to jurisdictional claims in published maps and institutional affiliations.



Copyright: © 2022 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (<https://creativecommons.org/licenses/by/4.0/>).

1. Introduction

Initial quantum states which undergo manipulations in a laboratory are usually chosen to be simple, such as coherent states or the eigenstates of an integrable Hamiltonian. Nevertheless, there is, in principle, no impediment to the unitary evolution of the excited eigenstates of chaotic systems. It is true that they may be hard to single out in a dense energy spectrum with no selection rules, but this may be a further reason to focus on the transitions between energy windows, which contain many eigenstates, although they are classically narrow. Theoretically, this choice is motivated by the lack of an apt description for individual chaotic eigenstates, such as the semiclassical (SC) portrayal of the eigenstates of integrable systems through their Wigner functions [1,2].

Different features of the energy transition probability density, otherwise known as the transition density, were recently studied in two papers [3,4], labeled here as **I** and **II**. Whereas **I** concentrated on classical aspects and the occurrence of caustic singularities in the transition density, the nature of its SC oscillations away from caustics was the focus of **II**. Furthermore, this second paper generalized the special kind of transitions that were allowed in **I**. Thus, the initial eigenstates may evolve under the action of arbitrary Hamiltonians as long as this can be assumed to be a fast process in comparison with internal motions.

The transition density in **II** was calculated as a stationary phase approximation of an exact integral, which portrays the trace of a pair of operators, represented as a pair of spectral Wigner functions. Each of these is a superposition of the Wigner functions of the many eigenstates that may be found semiclassically within a classically narrow energy window. In **I**, the spectral Wigner function was even expressed as a path integral, but well-established SC approximations of the spectral Wigner were instead employed [5,6]. The full SC scenario combining the results of both papers is presented in **II**, and therefore the present contribution only deals with the improvement of the amplitudes previously obtained.

The energy transition density is basically an experimental property, and so it must be independent of the representation chosen to perform its calculation. It is thus pleasing that in the SC derivation of **II** for the transition density, the phase of the oscillations could erase any memory of the Weyl–Wigner representation, depending only on the action of closed compound orbits formed by a pair of orbit segments—one in an energy shell of the initial system and the other in an energy shell of the driven system. On the other hand, the amplitude of each compound orbit contribution resulted in a cumbersome product of the features of the pair of spectral Wigner functions that were selected by the stationary phase condition. Presumably, it is feasible to simplify this amplitude by clever manipulations, but an alternative path is presented here.

The object of the present paper is to provide a new derivation of the transition density, that starts from the trace of a pair of evolution operators and has a simple SC expression in terms of closed compound trajectories [7]. In this time domain, both the phase and the amplitude are free from the special features of the Wigner–Weyl representation. The main task is then to invert the dependence on the pair of times that characterize the trajectory segments forming the compound trajectory into a dependence on the pair of energies that emerge as the integral over time, performed again within the stationary phase approximation. (In most cases, the term trajectory will be employed in the time domain and the term orbit in the energy domain.) It so happens that the classical characterization of the compound orbits in the energy domain is more intuitively accessible than that in the time domain, and therefore delicate navigation between both pictures is needed. Thus, one obtains a more comprehensive view of the structure of closed compound orbits than in the original derivation in **II**, as well as the benefit of a simpler expression for the amplitude of their contribution.

The present derivation clarifies the parallelism of the structure of the energy transition density to that of the smoothed density of eigenenergies. The latter may also be expressed as a Fourier transform of the trace of the evolution operator and the semiclassical approximation of Gutzwiller [8,9] as well as of Balian and Bloch [10]; based on the classical periodic orbits in each energy shell. Currently, the periodic orbits are already present in the trace of the propagator itself, and it is only in the energy domain that smoothing is needed for convergence. In the present case of a compound trace combining two propagations, the semiclassical evaluation of the double Fourier transform relies instead on the compound orbits joining segments on both chosen energy shells. The classical bases of the static single energy density and the dynamical transition density are thus parallel and depend on closed structures with one dimension. However, compound orbits are of course much less familiar than periodic orbits, and their zoology then needs to be developed here.

The alternative exact formula for the transition density is presented in the following section in the form of a double Fourier transform of the trace of a compound evolution operator. Section 3 recalls the SC approximation of this trace, which was derived in [7] in terms of closed compound trajectories. Then, the Fourier integral is performed within the stationary phase approximation, hence producing the SC approximation to the energy transition density in terms of closed compound orbits. Section 4 constructs Poincaré sections, from which one establishes the existence of sequences of families of closed compound orbits parameterized by a pair of energies and hence sequences of closed compound trajectories parameterized by pairs of times, as assumed in Section 3. Finally, Section 5 compares the simpler SC expression for the energy transition density presented in Section 3 with its previous derivation in **II**.

2. Energy Transitions Driven by General Unitary Operators

Let us consider the probability density for the transition of a quantum system with a Hamiltonian $\hat{H}$ from an energy range centered on E and with a width ϵ , to an energy range centered on E' with the same width. It is driven by a one parameter family of unitary operators,

$$\hat{U}(\tau) = e^{-i\tau\hat{\Lambda}/\hbar}, \quad (1)$$

where $\hat{\Lambda}$ is the driving Hamiltonian and τ is the driving time. This was expressed in **II** as

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

Within the integral, each spectral Wigner function $W_E(\mathbf{x}, \epsilon)$ is directly defined as a superposition of the Wigner functions $W_k(\mathbf{x})$, for individual eigenstates $|k\rangle$ of $\hat{H}$, with energy E_k [5,6,11]:

$$W_E(\mathbf{x}, \epsilon) \equiv (2\pi\hbar)^N \sum_k \delta_\epsilon(E - E_k) W_k(\mathbf{x}). \quad (3)$$

They represent the spectral density operator

$$\hat{\rho}_E(\epsilon) \equiv \sum_k \delta_\epsilon(E - E_k) |k\rangle\langle k| \quad (4)$$

in the classically narrow energy range ϵ centered on an energy E , such that

$$\delta_\epsilon(E) \equiv \frac{1}{\pi} \frac{\epsilon}{\epsilon^2 + E^2} \quad (5)$$

integrates as a Dirac δ -function. In its turn, the unitary evolution of a pure state, that is, the driven pure state

$$|l\rangle\langle l|(\tau) \equiv \hat{U}(\tau)|l\rangle\langle l|\hat{U}(\tau)^\dagger \quad (6)$$

is represented by the driven Wigner functions $W_k(\mathbf{x}|\tau)$, which then result in the spectral Wigner function of the driven system below:

$$W_{E'}(\mathbf{x}, \epsilon|\tau) \equiv (2\pi\hbar)^N \sum_k \delta_\epsilon(E' - E_k) W_k(\mathbf{x}|\tau). \quad (7)$$

The alternative construction of the spectral Wigner function goes back to the Weyl propagator $V(\mathbf{x}, t)$, which represents the intrinsic unitary evolution operator

$$\hat{V}(t) = e^{-it\hat{H}/\hbar}, \quad (8)$$

that is,

$$W_E(\mathbf{x}, \epsilon) = \text{Re} \int_0^\infty \frac{dt}{\pi\hbar} \exp\left[\frac{it}{\hbar}(E + i\epsilon)\right] V(\mathbf{x}, t), \quad (9)$$

or more conveniently,

$$W_E(\mathbf{x}, \epsilon) = \int_{-\infty}^\infty \frac{dt}{2\pi\hbar} \exp\left[\frac{iEt}{\hbar} - \frac{\epsilon|t|}{\hbar}\right] V(\mathbf{x}, t). \quad (10)$$

On the other hand, the driven Hamiltonian generated by $\hat{U}(\tau)$,

$$\hat{H}(\tau) \equiv \hat{U}(\tau)\hat{H}\hat{U}(\tau)^\dagger, \quad (11)$$

generates the driven intrinsic evolution operator

$$\hat{V}(t|\tau) \equiv \hat{U}(\tau) e^{-it\hat{H}/\hbar} \hat{U}(\tau)^\dagger = \exp\left[-\frac{it}{\hbar}\hat{H}(\tau)\right], \quad (12)$$

which is represented by the corresponding Weyl propagator $V(\mathbf{x}, t|\tau)$. Thus, the driven spectral Wigner function is expressed as follows:

$$W_{E'}(\mathbf{x}, \epsilon|\tau) = \int_{-\infty}^\infty \frac{dt'}{2\pi\hbar} \exp\left[\frac{iE't'}{\hbar} - \frac{\epsilon|t'|}{\hbar}\right] V(\mathbf{x}, t'|\tau), \quad (13)$$

Introducing these expressions in (2) leads to the transition density in the following form:

$$P_{EE'}(\tau, \epsilon) = \frac{1}{(2\pi\hbar)^N} \int d^{2N}\mathbf{x} \left\{ \int_{-\infty}^{\infty} \frac{dt}{2\pi\hbar} \exp\left[\frac{iEt}{\hbar} - \frac{\epsilon|t|}{\hbar}\right] V(\mathbf{x}, t) \right\} \left\{ \int_{-\infty}^{\infty} \frac{dt'}{2\pi\hbar} \exp\left[\frac{iE't'}{\hbar} - \frac{\epsilon|t'|}{\hbar}\right] V(\mathbf{x}, t'|\tau) \right\}, \quad (14)$$

so that, switching the integrations, the following equation is obtained:

$$P_{EE'}(\tau, \epsilon) = \int_{-\infty}^{\infty} \frac{dt}{2\pi\hbar} \int_{-\infty}^{\infty} \frac{dt'}{2\pi\hbar} \exp\left[-\frac{\epsilon}{\hbar}(|t| + |t'|)\right] \exp\left[i\frac{(Et + E't')}{\hbar}\right] \int \frac{d^{2N}\mathbf{x}}{(2\pi\hbar)^N} V(\mathbf{x}, t) V(\mathbf{x}, t'|\tau). \quad (15)$$

At this stage, it is recalled that the property of the Wigner–Weyl representation (e.g., see [6]) that:

$$\int \frac{d^{2N}\mathbf{x}}{(2\pi\hbar)^N} V(\mathbf{x}, t) V(\mathbf{x}, t'|\tau) = \text{tr } \hat{V}(t) \hat{V}(t'|\tau), \quad (16)$$

that is, the trace of the product of operators, which may be interpreted as the single *compound evolution operator*

$$\hat{V}(t, t') \equiv \hat{V}(t) \hat{V}(t'|\tau), \quad (17)$$

as defined in [7]. Hence, the alternative exact expression for the energy transition density, which is the basis for the present SC approximations, is the double Fourier transform below:

$$P_{EE'}(\tau, \epsilon) = \int_{-\infty}^{\infty} \frac{dt dt'}{(2\pi\hbar)^2} \exp\left[\frac{i}{\hbar}(Et + E't')\right] \exp\left[-\frac{\epsilon}{\hbar}(|t| + |t'|)\right] \text{tr } \hat{V}(t, t'). \quad (18)$$

Since the integral runs over positive and negative times, all combinations of forward and backward evolutions for both families of operators are included in the integral. The simultaneous reversal of both times produces the complex conjugate, and hence the integral is real.

3. Semiclassical Approximations

The original discussion on compound evolution operators in the context of evolving quantum correlations considered products of an arbitrary number of evolutions in the Wigner–Weyl representation. It turns out that the SC trace of a compound operator derived in [7] depends on the action of *compound trajectories*: they join trajectory segments from each of the evolutions into piecewise smooth closed curves in phase space. Here, we shall be concerned with just a pair of curves, one evolved by the classical Hamiltonian $H(\mathbf{x})$ in positive or negative time t and the other evolved by the driven Hamiltonian $H(\mathbf{x}|\tau)$ in time t' . Thus, one defines $\mathbb{S}(t, t')$, the classical action of the compound trajectory, such that the SC contribution to the trace of the compound trajectory is expressed as follows:

$$\text{tr } \hat{V}(t, t') \approx \frac{2^N}{|\det[\mathbf{I}_d - \mathbf{M}(t, t')]|^{1/2}} \exp\left[\frac{i}{\hbar}(\mathbb{S}(t, t') + \hbar\sigma)\right]. \quad (19)$$

The linear approximation of the transformation generated by $H(\mathbf{x})$ near the t -trajectory being defined by the stability matrix, $\mathbf{M}(t)$ and the stability matrix for the linearized motion near the t' -trajectory being $\mathbf{M}'(t')$, then the full stability matrix for the compound trajectory is simply

$$\mathbf{M}(t, t') \equiv \mathbf{M}(t')\mathbf{M}(t), \quad (20)$$

whereas $\mathbf{I}_d$ is the identity matrix. One should note that the discontinuity of the derivative of the compound trajectory at the initial and final points of both trajectory segments implies that there is generally no zero eigenvalue in the full stability matrix, which is in contrast to smooth periodic trajectories. On the other hand, the determinant in the amplitude of (19) does not depend on the choice of the starting point between both trajectory endpoints.

There may be multiple branches of the action that meet along caustics in the (t, t') space, where the semiclassical amplitude diverges, that is, $[\det \mathbf{I}_d - \mathbf{M}(t, t')] = 0$. The phase σ is determined by the convergence of neighboring paths. (For convenience of notation, all such focal indices shall henceforth be denoted by the generic symbol σ , without specifying their generic values, which will be altered under the transformations to be carried out.) There are no caustics if both times t and t' are short [6], for which $\sigma = 0$; however, there is usually an increment to the phase at a caustic.

To evaluate integral (18) by stationary phase, one needs the time derivatives of the action of the compound trajectory. Within the Wigner–Weyl representation, this can be decomposed into a pair of center actions [6]:

$$\S(t, t') = S(\mathbf{x}, t) + S(\mathbf{x}, t'|\tau), \quad (21)$$

where $\mathbf{x}$ is the center of the vector joining the pair of endpoints of the pair of segments that form the compound trajectory. This is the action of a compound trajectory defined by a pair of times, which corresponds to the action of a compound orbit defined in Π by a pair of energies. Then,

$$\frac{\partial \S}{\partial t}(t, t') = \frac{\partial S}{\partial t}(\mathbf{x}, t) = -t E(t) \quad \text{and} \quad \frac{\partial \S}{\partial t'}(t, t') = \frac{\partial S}{\partial t'}(\mathbf{x}, t'|\tau) = -t' E(t'|\tau), \quad (22)$$

where $E(t)$ and $E(t'|\tau)$ are the respective energies of the t -trajectory and the t' -trajectories. (It should be noted that other choices for generating function, such as the ones depending on initial and final positions, result in the same partial derivatives of the action of the compound trajectory.) Therefore, the stationary phase conditions for the integrand of (19) are simply $E(t) = E$ and $E(t'|\tau) = E'$. Once both these conditions are satisfied, one can retrieve the energy action of the compound orbit in Π ,

$$\S(E, E') = \S(t(E, E'), t'(E, E')) + E t(E, E') + E' t'(E, E'), \quad (23)$$

which is just the symplectic area within the compound orbit, illustrated in Figure 1.

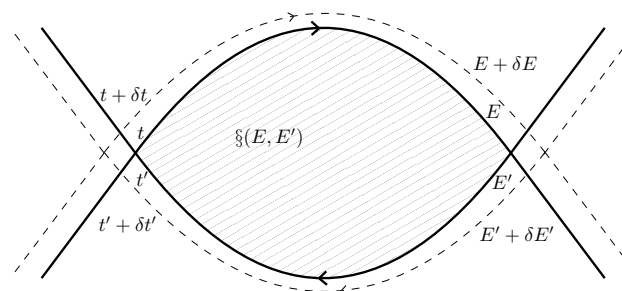


Figure 1. The action $\S(E, E')$ of the closed compound orbit is the symplectic area between both orbit segments, which coincide with the E -shell and the E' -shell if $N = 1$. It is a smooth function of both energies, as are the times $t(E, E')$ and $t'(E, E')$.

The assumption that one disposes of a two-parameter family of compound trajectories in time, which are a function of the pair of energy parameters, will be verified in the following section. Indeed, it will be ascertained that there is an infinite sequence of trajectory segments in both energy shells with increasing time, and hence in sequences of functions $t_j(E, E')$, $t'_j(E, E')$ and compound actions $\S_{j,j'}(E, E')$. Thus, by combining the

complex conjugate contributions of the compound orbits with their time reversal, the transition density takes the following form:

$$P_{EE'}(\tau, \epsilon) \approx \frac{2^N}{\pi \hbar} \sum_{j,j'} \exp\left(-\frac{\epsilon}{\hbar}(|t_j| + |t'_{j'}|)\right) \left| \det \frac{\partial(E, E')}{\partial(t_j, t'_{j'})} \det[\mathbf{I}_d - \mathbf{M}(t_j, t'_{j'})] \right|^{-1/2} \cos\left[\frac{1}{\hbar} \mathbb{S}_{j,j'}(E, E') + \sigma\right]. \quad (24)$$

4. Sections in Energy and Traversal Times

The derivatives in the amplitude of a compound orbit's SC contribution to the energy transition density imply that it belongs to a continuous family parameterized by t and t' . Even though the calculation is carried out in the time domain, this parametrization is most clearly justified in the energy domain. Let us start with the simple case where $N = 1$, so that the compound orbit is identified with segments of the energy shells $H(\mathbf{x}) = E$ and $H(\mathbf{x}|\tau) = E'$ joining their intersections, as shown in Figure 1. Evidently, each of these segments in the E -shell with j windings takes its time $t_j(E, E')$, just as the segments on the driven E' -shell have their duration $t'_{j'}(E, E')$. Then, locally, the inverse function theorem guarantees the existence of the functions $E_j(t, t')$ and $E_{j'}(t, t')$, so that the Jacobian determinant in (24) is simply

$$\det \frac{\partial(E_j, E_{j'})}{\partial(t, t')} = \left[\det \frac{\partial(t_j, t'_{j'})}{\partial(E, E')} \right]^{-1}. \quad (25)$$

The extension of this scenario for higher dimensions requires some care. As discussed in I and II, the pointwise intersection of the pair of energy shells is replaced by a $(2N - 2)$ -dimensional surface, the *evolved section*, which is a generalized Poincaré section of the E -shell by the driven E' -shell, or vice versa. Then the j th segment determines an orbit in the j th Poincaré map on the E -shell, whereas the j' th segment corresponds to an orbit on the j' th Poincaré map on the driven E' -shell. The compound orbit thus determines a fixed point for the product of the j -map with the j' -map.

The continuity of this construction for variations of E and E' indicates the existence of a two-parameter family of jj' -compound orbits, but this is best determined by constructing yet another surface of section. This can be an ordinary Poincaré section cutting, say the E -shell by a fixed $(2N - 1)$ -D plane. Then, a j -segment determines an initial point on the fixed section and maps it onto the evolved section. This point is then transported back to the evolved section by the continuing j' -segment in the E' -shell, from which a continuing j th segment takes it back to the fixed section. Obviously, a compound orbit once again determines a fixed point for this sequence of three mappings, but the advantage is that the energies E and E' are now mere parameters in the product Poincaré map. If the stability matrix $\mathbf{m}(E, E')$ for the this product map of the $2(N - 1)$ -D fixed section is nonsingular, i.e., $\det[\mathbf{I}_d - \mathbf{m}(E, E')] \neq 0$, then locally, there will be a two-parameter family of fixed points that corresponds to compound orbits with the full period $t_j(E, E') + t'_{j'}(E, E')$.

Thus, after all, the situation is just as depicted in Figure 1, but now, instead of the full E -shell and E' -shell in the simple case where $N = 1$, a single j -orbit segment in the E -shell and a j' -orbit segment in the E' -shell complete the compound circuit.

For parameters where there is no bifurcation of the closed compound orbits, one can use (25) for all dimensions so that the contributions of compound orbits to the transition density takes the following final form:

$$P_{EE'}(\tau, \epsilon) \approx \frac{2^N}{\pi \hbar} \sum_{j,j'} \cos\left[\frac{1}{\hbar} \mathbb{S}_{j,j'}(E, E') + \sigma\right] \exp\left(-\frac{\epsilon}{\hbar}(|t_j| + |t'_{j'}|)\right) \left| \det \frac{\partial(t_j, t'_{j'})}{\partial(E, E')} \right|^{1/2} \left| \det[\mathbf{I}_d - \mathbf{M}(t_j, t'_{j'})] \right|^{-1/2}. \quad (26)$$

The jj' -sum includes all combinations of forward and backward trajectory segments, always obtained as fixed points of the corresponding generalized Poincaré maps. However, it is certain that very long orbits will be exponentially dampened by the exponential factors, depending on the energy width ϵ . One must add to this the classical contributions of 'zero-length' orbits to the intersection of the pair of energy shells, that is, the evolved section, as discussed in **II**, in order to obtain the complete portrayal of the energy transition density.

5. Discussion

The SC approximation of the transition density obtained above can now be compared with that of the previous derivation in **II**. resulting from the direct stationary phase approximation of the integral in (2) over the SC approximation of the spectral Wigner functions,

$$W_E(\mathbf{x}, \epsilon) \approx \sqrt{\frac{2}{\pi\hbar}} \sum_j \frac{2^N}{[dE/d|t_j| |\det(\mathbf{I}_d + \mathbf{M}(\mathbf{x}, t_j))|]^{1/2}} e^{-\epsilon|t_j|/\hbar} \cos\left[\frac{S_j(\mathbf{x}, E)}{\hbar} + \sigma_j\right], \quad (27)$$

it can be expressed as follows:

$$P_{EE'}(\tau, \epsilon) \approx \frac{2^N}{\pi\hbar} \sum_{j,j'} \cos\left[\frac{1}{\hbar} S_{jj'}(E, E') + \sigma_j + \sigma_{j'} + \frac{\pi}{4} \sigma_{jj'}\right] \exp\left(\frac{\epsilon}{\hbar} (|t_j| + |t_{j'}|)\right) \left|\frac{dt_j}{dE} \frac{dt_{j'}}{dE'}\right|^{1/2} |\det(\mathbf{I}_d + \mathbf{M}(\mathbf{x}, t_j)) \det(\mathbf{I}_d + \mathbf{M}(\mathbf{x}, t_{j'}(\tau))) \det(2\mathbf{B}_j + 2\mathbf{B}_{j'} + \mathbf{B}_j \mathbf{J} \mathbf{B}_{j'} + \mathbf{B}_{j'} \mathbf{J} \mathbf{B}_j)|^{-1/2} \quad (28)$$

(with a correction for the constant factor in **II**).

The action of the closed compound orbit in each term is equal to that obtained in the present derivation, but the same cannot be said for the amplitude. This was carried over from the parent spectral Wigner functions, with the extra factor arising from the stationary phase integral, which depends on the Hessian matrices,

$$\mathbf{B}(\mathbf{x}, t) \equiv \frac{1}{2} \frac{\partial^2 S(\mathbf{x}, t)}{\partial \mathbf{x}^2}, \quad (29)$$

of the pair of actions combined in the action for the compound orbit. In all instances, $\mathbf{x} = \mathbf{x}_{jj'}$ is the stationary phase point at the center of the pair of endpoints of the pair of trajectory segments that comprise the jj' th compound orbit. Thus, the present incorporation into a single Jacobian of the separate stability matrices within a single determinant and the unification of the derivatives of the times with respect to the energies has somehow incorporated the intricate combination of Hessian determinants. The by-product is a considerable simplification of the amplitude.

One may recall that a special choice of coordinates allowed for the factoring into blocks of the stability matrix for a single orbit segment and hence the absorption of the energy derivative in the amplitude of the spectral Wigner functions in **II**. These amplitudes were used in the final amplitude of the transition density contributions in **II**, but in retrospect, this was not really an advantage. The problem is that the special coordinates for factoring the stability matrix depend on the trajectory segment. Hence, there are two different coordinate systems for the pair, one for each segment. There is no point in adopting such a procedure for the full compound orbit because there will be no way to include the full Jacobian determinant between the pair of times and the pair of energy derivatives with the full stability matrix.

Semiclassical approximations are generally robust if one keeps to the lowest orders that are strongly tied to the underlying classical infrastructure. An example is the equivalence of different quantum representations of the evolution operator under the stationary phase approximation of the integral transformations between them. In the present instance, one deals with the probability density of an energy transition, which is an experimental property independent of the representation employed in its calculation. The only difference

between both approaches is the order in which the trace and the Fourier transform are calculated. Considering that the amplitude of the SC oscillations with respect to changes in parameters (E, E', τ) is much simpler in its new form, there is no a priori reason not to adopt it. Their equivalence can then be presumed, even if it seems to be a hard task to show it directly. In any case, it is pleasing to know that the direct derivation in terms of spectral Wigner functions in **II** produces the same phases as those in the present double Fourier transform from times to energies.

The present paper closes a sequence which has undergone a somewhat nonlinear development, beyond adding technical refinement to semiclassical formulae for general transitions between coarsegrained energy levels. The initial paper I expanded an identity between pure Wigner functions, while bestowing it physical significance, though its main results did not go beyond purely classical energy transitions in a narrow context. This was followed in **II** by the addition of quantum terms to this classical background, which oscillate with the variation of the transition parameters, either the transition energies, or, for instance, the the duration of the external driving in an expanded context that included Hamiltonian evolution. The phase of the oscillations were identified with the action of closed compound orbits, composed of orbit segments in the in the initial and final energy shells, but their amplitude, derived by the stationary phase approximation of the original Wigner identity, was far from transparent.

It is only here, through the present rederivation of the transition density, that the amplitude of the semiclassical contribution of the compound orbits follows their phase in achieving full independence from the chosen Wigner–Weyl representation. In this way, the contributions of closed compound orbits to dynamical energy transitions, based on their classical actions and stability matrices, emulates the contributions of periodic orbits in a single energy shell to the static energy spectrum, in the manner disclosed by Gutzwiller’s ground-breaking work on the trace formula [9]. Once again, this work also deals with a trace, but it involves a product of operators, which leads to the replacement of simple periodic orbits by closed compound orbits.

The difficulty of working directly with these semiclassical formulae based on many trajectories has considerably delayed the significant numerical verification of formulae for the spectrum. Nevertheless, the fact that coarse-grained energy shells and hence cutoffs in the duration of the closed compound orbits are addressed here allows for the possibility that numerical simulations may be forthcoming.

Funding: This research received no external funding.

Data Availability Statement: Not applicable.

Acknowledgments: I would like to thank Gabriel Lando for his help in preparing the figures. Partial financial support from the National Institute for Science and Technology–Quantum Information and CNPq (Brazilian agencies) is gratefully acknowledged.

Conflicts of Interest: The authors declare no conflict of interest.

References

1. Wigner, E.P. On the quantum correction for thermodynamic equilibrium. *Phys. Rev.* **1932**, *40*, 749. [\[CrossRef\]](#)
2. Berry, M.V. Semi-classical mechanics in phase space: A study of Wigner’s function. *Phil. Trans. Roy. Soc A* **1977**, *287*, 237–271.
3. Ozorio de Almeida, A.M. Energy transitions driven by phase space reflection operators. *arXiv* **2021**, arXiv:2201.01812.
4. Ozorio de Almeida, A.M. Energy transition scars of driven chaotic systems. *arXiv* **2021**, arXiv:2203.10668.
5. Berry, M.V. Quantum scars of classical closed orbits in phase space. *Proc. R. Soc. Lond. A* **1989**, *423*, 219.
6. Ozorio de Almeida, A.M.; Koiller, J. A deceptively simple generalization. *J. Phys. A* **2016**, *49*, 491002. [\[CrossRef\]](#)
7. Ozorio de Almeida, A.M.; The Weyl representation in classical and quantum mechanics. *Phys. Rep.* **1998**, *295*, 265–342. [\[CrossRef\]](#)
8. Gutzwiller, M.C. Periodic orbits and classical quantization conditions. *J. Math. Phys.* **1971**, *12*, 343. [\[CrossRef\]](#)
9. Gutzwiller, M.C. *Chaos in Classical and Quantum Mechanics*; Springer: New York, NY, USA, 1990.
10. Balian R.; Bloch C. Solution of the Schrödinger equation in terms of classical paths. *Ann. Phys. N. Y.* **1974**, *85*, 514. [\[CrossRef\]](#)
11. Berry, M.V. Fringes decorating anticaustics in ergodic wavefunctions. *Proc. R. Soc. Lond. A* **1989**, *424*, 279.