Semiclassical propagator of the Wigner function

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Propagation of the Wigner function is studied on two levels of semiclassical propagator, one based on the van-Vleck propagator, the other on phase-space path integration. Leading quantum corrections to the classical Liouville propagator take the form of a time-dependent quantum spot. Its oscillatory structure depends on whether the underlying classical flow is elliptic or hyperbolic. It can be interpreted as the result of interference of a pair of classical trajectories, indicating how quantum coherences are to be propagated semiclassically in phase space. The phase-space path-integral approach allows for a finer resolution of the quantum spot in terms of Airy functions.

Quantum propagation in phase space has always been in the shadow of propagation in conventional (position, momentum) representations. Yet it is superior in various respects, particularly in the semiclassical realm: It avoids all problems owing to projection, such as singularities at caustics. Canonical invariance of all classical quantities involved is manifest. Boundary conditions are imposed consistently at a single (initial or final) time, thus removing the so-called root-search problem and allowing for initial-value representations. Semiclassical approximations to the quantum-mechanical propagator have predominantly been seeked in the form of coherent-state propagations [4] and its numerous modifications. By now, a broad choice of phase-space propagation schemes is available which score very well if compared to other semiclassical techniques.

Almost all of these developments refer to the propagation of wavefunctions in some Hilbert space. Less attention has been paid to the propagation of Wigner and Husimi functions. They live in projective Hilbert space, i.e., represent the density operator and are bilinear in the wavefunction. Besides their popularity, they have a crucial virtue in common: An extension to non-unitary time evolution is immediate. This opens access to a host of applications that combine complex quantum dynamics, where a phase-space representation facilitates the comparison to the corresponding classical motion, with decoherence or dissipation: quantum optics and quantum chemistry, nanosystems in biophysics and electronics, quantum measurement and computation.

By the scales involved, many of them call for semiclassical approximations. However, only few such studies exist, for specific systems predominantly in quantum chaos [5], including dissipative systems [6]. By contrast, Ref. [7] discusses a new method, Wigner-function propagation analogous to the solution of classical Fokker-Planck equations.

As a major challenge, any attempt to directly propagate Wigner functions requires an appropriate treatment of quantum coherences. As early as 1976, Heller [8] argued that the “dangerous cross terms”, i.e., the off-diagonal elements of the density matrix in the relevant representation, can give rise to a complete failure of semiclassical propagation of the Wigner function. Quantum coherences are reflected in the Wigner function as “sub-Planckian” oscillations. They plague semiclassical approximations by their small scale and by propagating along paths that can deviate by any degree from classical trajectories.

In this Letter, we point out how Heller’s objections are resolved by considering pairs of trajectories as basis of semiclassical approximations, and present corresponding expressions for the propagator of the Wigner function. The concept of trajectory pairs has been introduced in the present context by Rios and Ozorio de Almeida [11, 12], albeit working in a strongly restricted space of semiclassical Wigner functions. We here give a general derivation of the propagator, independently of any initial or final states.

Moreover, we go beyond the level of approximations based on stationary phase. Employing a phase-space path-integral technique, we construct an improved semiclassical Wigner propagator in terms of Airy functions. It resolves all singularities and contains the semiclassical approximations based on trajectory pairs as a limiting case. The interference patterns we obtain depend, up to scaling, only on the nature of the underlying classical phase-space flow—elliptic vs. hyperbolic—and in this sense are universal. While living in projective Hilbert space, this result is superior to Gaussian wave-packet propagation in that it allows Gaussians to evolve into non-Gaussians.

In order to fix units and notations, define the Wigner function corresponding to a density operator \( \hat{\rho} \) as

\[
W(r) = \int dq' e^{i \frac{q'}{\hbar} \cdot r - \frac{i}{2} \left[ (q + q')^2/\hbar^2 \right] \hat{\rho} \left[ q - q'/2 \right]}
\]

where \( r = (p, q) \) is a vector in \( 2T \)-dimensional phase space. Its time evolution is generated by a Hamiltonian \( H(p, q) \) through the equation of motion \( (\partial / \partial t) W(q, r, t) = \{ H(q, r), W(q, r, t) \}_M \) converges to the Poisson bracket for \( \hbar \to 0 \). As this equation of motion is linear, the evolution of the Wigner function over a finite time can be expressed as an inte-
gral kernel, \( W(r'', t'') = \int d^{2} r' G(r'', t''; r', t') W(r', t') \), defining the Wigner propagator \( G(r'', t''; r', t') \). For autonomous Hamiltonians, it induces a one-dimensional dynamical group parameterized by \( t = t'' - t' \) (in what follows, we restrict ourselves to this case and use \( t \) as the only time argument). This implies, in particular, the initial condition \( G(r'', r'; 0) = \delta (r'' - r') \) and the composition (Chapman-Kolmogorov) equation \( G(r'', r'; t) = \int d^{2} r G(r'', r, t-t') G(r, r', t') \).

The Wigner propagator can be expressed in terms of the Weyl transform of the unitary time-evolution operator \( U(r, t) = \int d^{2} q e^{-i \text{p} \cdot \text{q}/\hbar} \left[ q + i q'/2 \right] U(t) \mid q - i q'/2 \rangle \), called Weyl propagator, as a convolution,

\[
G(r'', r', t) = \int d^{2} r e^{i \pi (r'' - r') R} U^{*}(\tilde{r}_{+}, t) U(\tilde{r}_{+}, t),
\]

with \( \tilde{r}_{+} \equiv (r' + r'' \pm R)/2 \). It serves as a suitable starting point for a semiclassical approximation, invoking an expression for the Weyl propagator semiclassically equivalent to the van-Vleck approximation [13, 14].

\[
U(r, t) = 2^{f} \sum_{j} \frac{\exp(\delta S_{j}(r, t)/\hbar - \mu_{j} \pi/2)}{\sqrt{\det(M_{j}(r, t) + 1)}}.
\]

The sum includes all classical trajectories \( j \) connecting phase-space points \( r_{j}', r_{j}'' \) in time \( t \) such that \( r = r_{j} \equiv (r_{j}' + r_{j}'')/2 \). \( M_{j} \) is the corresponding stability matrix, \( \mu_{j} \) its Maslov index. The action \( S_{j}(r_{j}, t) = A_{j}(r_{j}, t) - H(r_{j}, t) \), with \( A_{j} \), the symplectic area enclosed between the trajectory and the straight line (chord) connecting \( r_{j}' \) and \( r_{j}'' \) (hashed areas \( A_{j,\pm} \) in Fig. 1).

Substituting Eq. (2) in Eq. (1) leads to a sum over pairs \( j_{+}, j_{-} \) of trajectories whose respective chord centers \( r_{j_{\pm}} \) are separated by the integration variable \( R \). Otherwise, the two trajectories are unrelated. A coupling between them, as expected on classical grounds, comes about only upon evaluating the \( R \)-integral by stationary phase. Stationary points are given by \( r'' - r' = (r_{j_{+}}' - r_{j_{-}}') + (r_{j_{+}}'' - r_{j_{-}}'')/2 \). Together with the conditions for the two chords, \( r_{j_{+}}' + r_{j_{-}}'' \pm R \equiv r_{j_{+}}' + r_{j_{-}}'' \), this implies

\[
r = r' \equiv (r_{j_{+}}' + r_{j_{-}}')/2, \quad r'' \equiv (r_{j_{+}}'' + r_{j_{-}}'')/2.
\]

Stationary points are thus given by pairs of classical trajectories such that the initial (final) stage of the propagator is in the middle between their respective initial (final) points (Fig. 2b). This does not require these trajectories to be identical! They do coincide as long as \( r' \) and \( r'' \) are on the same classical trajectory, but bifurcate as \( r'' \) moves off the classical trajectory \( r_{cl}(r', t) \) starting at \( r' \), if the dynamics is not harmonic.

The resulting semiclassical approximation for the Wigner propagator is (dot indicating time derivative)

\[
G(r'', r', t) = \frac{4^{f}}{h^{f}} \sum_{j} \frac{2 \cos(S_{j}(r'', r', t)/\hbar - f \pi/2)}{\sqrt{\det(M_{j} + M_{j'})}}
\]

\[
S_{j}(r'', r', t) = (\tilde{r}_{j_{+}} - \tilde{r}_{j_{-}}) \cdot (r'' - r') + S_{j_{+}} - S_{j_{-}}
\]

\[
= \int_{0}^{t} ds [\tilde{r}_{j}(s) \cdot \tilde{r}_{j}(s) - H_{j_{+}}(r_{j_{+}}) + H_{j_{-}}(r_{j_{-}})].
\]

FIG. 1: The reduced action (shaded) of the Wigner propagator in van-Vleck approximation, Eq. (4), is the symplectic area enclosed between the two classical trajectories \( r_{j_{\pm}}(t) \) and the two transverse vectors \( r_{j_{+}}' - r_{j_{-}}' \) and \( r_{j_{+}}'' - r_{j_{-}}'' \) (schematic drawing). The full central line is the classical trajectory \( r_{cl}(r', t) \), the broken line is the propagation path \( \tilde{r}_{j}(r', t) \).

with \( \tilde{r}_{j}(t) \equiv (r_{j_{+}}(t) + r_{j_{-}}(t))/2, R_{j}(t) \equiv r_{j_{+}}(t) - r_{j_{-}}(t), \) and \( S_{j_{+}} \equiv A_{j_{+}}(r_{j_{+}}') - H_{j_{+}}(r_{j_{+}}'), t \). The reduced action \( A_{j} = \int_{0}^{t} ds [\tilde{r}_{j}(s) \cdot \tilde{r}_{j}(s)] \) is the symplectic area enclosed between the two trajectory sections and the vectors \( r_{j_{+}}'' - r_{j_{-}}'' \) and \( r_{j_{+}}' - r_{j_{-}}' \) (Figs. 12b). In general, Eq. (4), as a function of \( r'' \), describes a distribution that extends from the classical trajectory into the surrounding phase space, forming a “quantum spot” (Fig. 3b) with a characteristic oscillatory pattern that results from the interference of the contributing classical trajectories. In general, it fills only a sector with opening angle \( < 2\pi \) (Fig. 2b), where the sum contains two trajectory pairs (four stationary points). Outside this “illuminated area”, stationarity cannot be fulfilled, that is, the “shadow region” is not accessible even for mean paths \( r_{j}(t) \). The border is formed by phase-space caustics along which there is exactly one solution (two stationary points). As \( r'' \) approaches the classical trajectory \( r_{cl}(r', t) \) starting in phase-space (from the illuminated sector, the two solutions \( j_{+}, j_{-} \) coalesce to \( M_{j_{+}} = M_{j_{+}} \), and Eq. (4) becomes singular. If the potential is purely harmonic, all mean paths coincide with \( r_{cl}(r', t) \), and the classical Liouville propagator, \( G(r'', r', t) = \delta (r'' - r_{cl}(r', t)), \) is retained. In all other cases, Eq. (4), though based on the van-Vleck propagator, reflects the structure of stationary points of the action including third-order terms, with one pair of extrema and one pair of saddle points. It is formulated in terms of canonically invariant quantities related to classical trajectories and thus generalizes immediately to an arbitrary number of degrees of freedom. The propagation of Wigner functions defined semiclassically in terms of Lagrangian manifolds [11] is contained in Eq. (4) as a special case.

We are now able to resolve Heller’s objections [9]: If the two trajectories \( j_{+}, j_{-} \) are sufficiently separated and the potential is sufficiently nonlinear, then (i), the propagation path \( \tilde{r}(r', t) \) can differ arbitrarily from \( r_{cl}(r', t) \), and (ii), the phase factor in [11] exhibits sub-Planckian oscillations. They would couple resonantly to corresponding features in the initial Wigner function, generating a similar pattern in the final Wigner function around the end-
pically, keeping track of the symplectic area $A$ of the Feynman path integral, their middle. (ii) Propagate trajectory pairs around the initial argument (Fig. 2): (i) Define a local grid (e.g., in polar coordinates) at $r^t$ that deforms the region accessed by two midpoints $r^t$ of the propagator, identifying pairs of classical trajectories that straddle the propagation path as stationary solutions.

We will now include cubic terms in the action, with respect to variations of the path variables. To keep technicalities at a minimum, we restrict ourselves from now on to a single degree of freedom and to Hamiltonians of the standard form $H(p,q) = T(p) + V(q)$, where $T(p) = p^2/2m$ while the potential $V(q)$ may contain non-linearities of arbitrary order. With this form, $H_W(r)$ coincides with the Hamiltonian function “quantized” by merely replacing operators with classical variables. As the path integral readily allows to treat time-dependent potentials, chaotic classical motion remains within reach.

Expanding the action around $r(t) = r_{cl}(t,t)$ and $R(t) = (P(t),Q(t)) = 0$, there remain only linear terms in $P$ and linear and cubic terms in $Q$. Evaluating the $R$-sector of the path integral thus results in an Airy spreading of the propagator, with a rate $\sim V'''(q_{cl}(t))$, in the $p$-direction. It is superposed to the classical phase-space flow around the trajectory, i.e., rotation (shear) if it is elliptic (hyperbolic). As a consequence, a spot of the full phase-space dimension develops. Scaling $\rho = (\eta,\xi) = (\mu^{1/4}, \mu^{-1/4}q)$, with $\mu = T''(p_{cl})/V'''(q_{cl})$, we express the linearized classical motion as a dimensionless map,

$$M(\phi(t)) = \begin{bmatrix} \cos \phi(t) & -\sin \phi(t) \\ \sin \phi(t) & \cos \phi(t) \end{bmatrix}. \quad (8)$$

These maps form a group parameterized by the angle $\phi(t) = \int_0^t ds \sqrt{T''(p(s))V'''(q(s))}$. It is real (imaginary) if the linearized dynamics is elliptic (hyperbolic).

This allows to evaluate also the $r$-sector of the path integral. Transforming the Wigner function to Fourier phase space, $\tilde{W}(\gamma) = (FW)(\gamma) = (2\pi)^{-1} \int d^2 r e^{i(\gamma \cdot r)} W(r)$, and the propagator accordingly, $\tilde{G} = FGF^{-1}$, we obtain

$$\tilde{G}(\gamma'', \gamma', t) = \delta(\gamma'' - M(\phi(t))\gamma') \exp \left( -i \frac{a_{\text{cl}}}{3} \alpha^3 + a_{21} \alpha^2 \beta' + a_{12} \alpha \beta'^2 + \frac{a_{33}}{3} \beta'^3 \right). \quad (9)$$

The coefficients $a_{kl} = \int_0^t ds \sigma(s)(\sin\phi(s))^{l}(\cos\phi(s))^{k}$ depend on where along the classical trajectory how much quantum spreading $\sim \sigma(t) = (\mu(t))^{3/4} h^2 V'''(q_{cl}(t))/8$ is picked up and thus on the specific system and initial conditions. The Fourier transform from Eq. (9) back to the

Two paths, $r(t)$ and $R(t)$, have to be integrated over. The former is subject to boundary conditions $r(0) = r'$ and $r(t) = r''$, the latter is free. The path action is

$$S(\{r\}, \{R\}) = \int_0^t ds [\dot{r}(s) \wedge R(s) + H_W(r(s) + R(s)/2) - H_W(r(s) - R(s)/2)]. \quad (7)$$

Equation (4) is recovered upon evaluating the path-integral representation in stationary-phase approximation: Defining $r_{\pm}(t) \equiv r(t) \pm R(t)/2$, with boundary conditions analogous to Eq. (3) and requiring stationarity leads to the Hamilton equation of motion for $r_{\pm}(t)$: We again find pairs of classical trajectories that straddle the propagation path as stationary solutions.

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original Wigner propagator can be done analytically, after transforming the third-order polynomial in the phase to a normal form

The internal structure and the time evolution of the quantum spot described by Eq. (3) are qualitatively different for elliptic and hyperbolic classical trajectories (real and imaginary \( \phi \), resp.). In the elliptic case, the spot is a periodic function of \( \phi \). In particular, it collapses approximately to a point whenever \( \phi = 2\pi l \), \( l \) integer. Close to these nodes, it shrinks and grows again along a straight line in the \( p \)-direction, reflecting the fact that for short time, the quantum Airy spreading \( \sim t^{1/3} \) outweighs the classical rotation \( \sim t \). Only sufficiently far from the nodes, while rotating around the trajectory by \( \phi(t)/2 \), the one-d. distribution fans out into a two-d. interference pattern formed as the overlap of the bright (oscillatory) sides of two Airy functions, with a sharp maximum on the classical trajectory (Fig. 3b). In comparison with the corresponding exact quantum-mechanical result (Fig. 3a) for the quantum spot, obtained by expanding the propagator in energy eigenstates \( \{ \psi \} \), the path-integral solution resolves the caustics far better than Eq. (4) (Fig. 3c). The hyperbolic case is obtained replacing trigonometric by the corresponding hyperbolic functions. As a result, along unstable trajectories there are no periodic recurrences as in the elliptic case; the spot continues expanding in the unstable and contracting in the stable direction (Fig. 3d). Isolated unstable periodic orbits embedded in a chaotic region of phase space exhibit a degeneracy of the Weyl propagator \( \text{Weyl} \). It allows to account for scarring in terms of the Wigner propagator \( \text{Wigner} \).

We have obtained a consistent picture of incipient quantum effects in the Wigner propagator, both in the van-Vleck approach and in the path-integral formalism: (i) for anharmonic potentials, the delta function on the classical trajectory is replaced by a quantum spot extending into phase space, (ii) its structure shows a marked time dependence, qualitatively different for elliptic and hyperbolic dynamics, (iii) it exhibits interference fringes arising as a product of Airy functions, (iv) it can be expressed in terms of canonically invariant quantities associated to pairs of underlying classical trajectories, (v) within each level of semiclassical approximation used, the propagator retains its dynamical-group structure. Open issues include: extension to higher dimensions and to higher-order terms in the action, performance in the presence of tunneling, application to unstable periodic orbits and implications for scars, trace formulae, and spectral statistics, regularization of the ballistic nonlinear \( \sigma \)-model, semiclassical propagation of entanglement, and generalization to non-unitary time evolution.

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