

## Semiclassical Propagator of the Wigner Function

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Propagation of the Wigner function is studied on two levels of semiclassical propagation: 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.

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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 root-search problem and allowing for initial-value representations. Semiclassical approximations to the quantum-mechanical propagator have predominantly been sought in the form of coherent-state path integrals [1–3]. Closely related are Heller’s Gaussian wave-packet dynamics [4] and its 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 wave functions 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 wave function. Besides their popularity, they have a crucial virtue in common: An extension to nonunitary 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, nano-systems 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 [6,7]. By contrast, Ref. [8] 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 [9] argued

that the “dangerous cross terms,” i.e., the off-diagonal elements of the density matrix, 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 [10]. 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 the 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 [11,12], 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  $W(\mathbf{r}) = \int d^f q' \exp(-i\mathbf{p} \cdot \mathbf{q}'/\hbar) \langle \mathbf{q} + \mathbf{q}'/2 | \hat{\rho} | \mathbf{q} - \mathbf{q}'/2 \rangle$ , where  $\mathbf{r} = (\mathbf{p}, \mathbf{q})$  is a vector in  $2f$ -dimensional phase space. Its time evolution is generated by a Hamiltonian  $\hat{H}(\hat{\mathbf{p}}, \hat{\mathbf{q}})$  through the equation of motion  $(\partial/\partial t)W(\mathbf{r}, t) = \{H(\mathbf{r}), W(\mathbf{r}, t)\}_{\text{Moyal}}$ , involving the Weyl symbol  $H(\mathbf{r})$  of the Hamiltonian  $\hat{H}$ . The Moyal brackets  $\{.,.\}_{\text{Moyal}}$  [13] converge to the Poisson brackets for  $\hbar \rightarrow 0$ . As this equation of motion is linear, the evolution of the Wigner function over

a finite time can be expressed as an integral kernel  $W(\mathbf{r}'', t'') = \int d^2f r' G(\mathbf{r}'', t''; \mathbf{r}', t') W(\mathbf{r}', t')$ , defining the Wigner propagator  $G(\mathbf{r}'', t''; \mathbf{r}', t')$ . For autonomous Hamiltonians, it induces a one-dimensional dynamical group parametrized 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  $G(\mathbf{r}'', \mathbf{r}'; 0) = \delta(\mathbf{r}'' - \mathbf{r}')$  and the composition rule  $G(\mathbf{r}'', \mathbf{r}', t) = \int d^2f r G(\mathbf{r}'', \mathbf{r}, t - t') G(\mathbf{r}, \mathbf{r}', t')$ .

The Wigner propagator can be expressed in terms of the Weyl transform of the unitary time-evolution operator  $U(\mathbf{r}, t) = \int d^f q' \exp(-i\mathbf{p} \cdot \mathbf{q}'/\hbar) \langle \mathbf{q} + \mathbf{q}'/2 | \hat{U}(t) | \mathbf{q} - \mathbf{q}'/2 \rangle$ , called the Weyl propagator, as a convolution

$$G(\mathbf{r}'', \mathbf{r}', t) = \int d^2f R e^{-i/\hbar(\mathbf{r}'' - \mathbf{r}') \wedge \mathbf{R}} U^*(\tilde{\mathbf{r}}_-, t) U(\tilde{\mathbf{r}}_+, t), \quad (1)$$

with  $\tilde{\mathbf{r}}_{\pm} \equiv (\mathbf{r}' + \mathbf{r}'' \pm \mathbf{R})/2$ . 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 [14,15],

$$U(\mathbf{r}, t) = 2^f \sum_j \frac{\exp(iS_j(\mathbf{r}, t)/\hbar - i\mu_j\pi/2)}{\sqrt{|\det(M_j(\mathbf{r}, t) + I)|}}. \quad (2)$$

The sum includes all trajectories  $j$  connecting points  $\mathbf{r}'_j, \mathbf{r}''_j$  in time  $t$  such that  $\mathbf{r} = \tilde{\mathbf{r}}_j \equiv (\mathbf{r}'_j + \mathbf{r}''_j)/2$ .  $M_j$  is the corresponding stability matrix;  $\mu_j$  is its Maslov index. The action  $S_j(\mathbf{r}_j, t) = A_j(\mathbf{r}_j, t) - H(\mathbf{r}_j, t)t$ , with  $A_j$  the symplectic area enclosed between the trajectory and the straight line (chord) from  $\mathbf{r}'_j$  and  $\mathbf{r}''_j$  [14] (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  $\tilde{\mathbf{r}}_{j\pm}$  are separated by the integration variable  $\mathbf{R}$ . Otherwise, the two trajectories are unrelated. A coupling between them, as expected on classical grounds, comes about only upon evaluating the  $\mathbf{R}$  integral by stationary phase. Stationary points are given by  $\mathbf{r}'' - \mathbf{r}' = (\mathbf{r}''_{j-} - \mathbf{r}'_{j-} + \mathbf{r}''_{j+} - \mathbf{r}'_{j+})/2$ . Together with the conditions for the two chords,  $\mathbf{r}' + \mathbf{r}'' \pm$

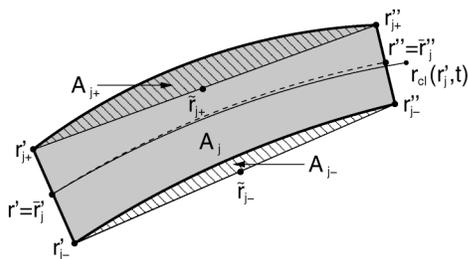


FIG. 1. The reduced action (shaded) of the Wigner propagator in the Van Vleck approximation, Eq. (5), is the symplectic area enclosed between the two classical trajectories  $\mathbf{r}_{j\pm}(t)$  and the two transverse vectors  $\mathbf{r}'_{j+} - \mathbf{r}'_{j-}$  and  $\mathbf{r}''_{j+} - \mathbf{r}''_{j-}$  (schematic drawing). The solid central line is the classical trajectory  $\mathbf{r}_{cl}(\mathbf{r}', t)$ ; the broken line is the propagation path  $\tilde{\mathbf{r}}_j(\mathbf{r}', t)$ .

$\mathbf{R} = \mathbf{r}'_{j\pm} + \mathbf{r}''_{j\pm}$ , this implies

$$\mathbf{r}' = \tilde{\mathbf{r}}' \equiv \frac{1}{2}(\mathbf{r}'_{j-} + \mathbf{r}'_{j+}), \quad \mathbf{r}'' = \tilde{\mathbf{r}}'' \equiv \frac{1}{2}(\mathbf{r}''_{j-} + \mathbf{r}''_{j+}). \quad (3)$$

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

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

$$G(\mathbf{r}'', \mathbf{r}', t) = \frac{4^f}{h^f} \sum_j \frac{2 \cos(S_j(\mathbf{r}'', \mathbf{r}', t)/\hbar - f\pi/2)}{\sqrt{|\det(M_{j+} - M_{j-})|}}, \quad (4)$$

$$\begin{aligned} S_j(\mathbf{r}'', \mathbf{r}', t) &= (\tilde{\mathbf{r}}_{j+} - \tilde{\mathbf{r}}_{j-}) \wedge (\mathbf{r}'' - \mathbf{r}') + S_{j+} - S_{j-} \\ &= \int_0^t ds [\dot{\tilde{\mathbf{r}}}_j(s) \wedge \mathbf{R}_j(s) - H_{j+}(\mathbf{r}_{j+}) + H_{j-}(\mathbf{r}_{j-})], \end{aligned} \quad (5)$$

with  $\tilde{\mathbf{r}}_j(t) \equiv (\mathbf{r}_{j-}(t) + \mathbf{r}_{j+}(t))/2$ ,  $\mathbf{R}_j(t) \equiv \mathbf{r}_{j+}(t) - \mathbf{r}_{j-}(t)$ , and  $S_{j\pm} \equiv A_{j\pm}(\tilde{\mathbf{r}}_{j\pm}, t) - H_{j\pm}(\tilde{\mathbf{r}}_{j\pm}, t)t$ . The reduced action  $A_j = \int_0^t ds \dot{\tilde{\mathbf{r}}}_j(s) \wedge \mathbf{R}_j(s)$  is the symplectic area enclosed between the two trajectory sections and the vectors  $\mathbf{r}'_{j+} - \mathbf{r}'_{j-}$  and  $\mathbf{r}''_{j+} - \mathbf{r}''_{j-}$  [Figs. 1 and 2(b)]. In general, Eq. (4), as a function of  $\mathbf{r}''$ , describes a distribution that extends from the classical trajectory into the surrounding phase space, forming a ‘‘quantum spot’’ [Fig. 3(b)] with a characteristic

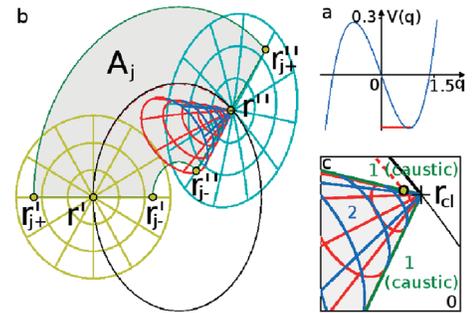


FIG. 2 (color). (a) Classical building blocks entering the Wigner propagator according to Eqs. (4) and (5), for a stable trajectory starting at  $\mathbf{r}' = (0.636, 0)$  near the minimum of the cubic potential  $V(q) = 0.329q^3 - 0.69q$ . (b) Classical trajectory  $\mathbf{r}_{cl}(\mathbf{r}', t)$  (black line), a pair of auxiliary trajectories  $\mathbf{r}_{j\pm}(t)$  (green lines), and the corresponding propagation path  $\tilde{\mathbf{r}}_j(\mathbf{r}', t)$  (red dashed line). The grid of auxiliary initial points  $\mathbf{r}'_{j\pm}$  around  $\mathbf{r}'$  (yellow) is parametrized by polar coordinates. Propagated classically over time  $t$ , it deforms into the turquoise pattern around  $\mathbf{r}''$ . The red/blue cone is formed by midpoints  $\tilde{\mathbf{r}}''_{j\pm}$  that correspond to extrema/saddles of the action. Its boundaries form caustics separating the region accessed by two midpoints  $\tilde{\mathbf{r}}''$  from the inaccessible rest. (c) Enlargement of the area around  $\mathbf{r}''$ , indicating the number of trajectory pairs that access each region.

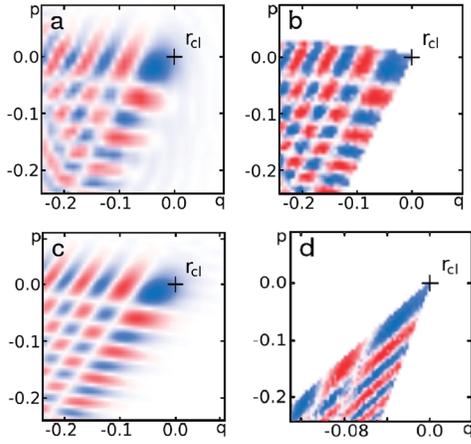


FIG. 3 (color). Quantum spot replacing the classical delta function on a stable (elliptic) trajectory near the minimum of a cubic potential as shown in Fig. 2(a), at  $t = 1.8$  ( $\phi \approx 2\pi/3$ ). (a) shows the exact quantum result for the Wigner propagator; (b) and (c) are semiclassical approximations based on Eqs. (4) and (9), respectively, all for  $\hbar = 0.01$ . Frames coincide with that in Fig. 2(c). (d) Quantum spot, according to Eq. (4), for an unstable classical trajectory near the maximum of the same potential, at  $t = 1.0$ . Crosses mark the classical trajectory. Color code ranges from red (negative) to blue (positive).

oscillatory pattern that results from the interference of the contributing classical trajectories. In general, it fills only a sector with an opening angle  $< 2\pi$  [Fig. 2(c)], 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  $\bar{\mathbf{r}}_j(t)$ . The border is formed by phase-space caustics along which there is exactly one solution (two stationary points). As  $\mathbf{r}''$  approaches the classical trajectory  $\mathbf{r}_{cl}(\mathbf{r}', t)$ , from the illuminated sector, the two solutions  $j - , j +$  coalesce so that  $M_{j-} \rightarrow M_{j+}$ , and Eq. (4) becomes singular. If the potential is harmonic, all mean paths coincide with  $\mathbf{r}_{cl}(\mathbf{r}', t)$ , and the classical Liouville propagator  $G(\mathbf{r}'', \mathbf{r}', t) = \delta(\mathbf{r}'' - \mathbf{r}'_{cl}(\mathbf{r}', t))$  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  $\bar{\mathbf{r}}(\mathbf{r}', t)$  can differ arbitrarily from  $\mathbf{r}_{cl}(\mathbf{r}', t)$ , and (ii) the phase factor in (4) 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 point of the

nonclassical propagation path. In this way, quantum coherences are faithfully propagated within a semiclassical approach.

Equations (4) and (5) translate into a straightforward algorithm for the numerical calculation of the propagator (Fig. 2): (i) Define a local grid (e.g., in polar coordinates) around the initial argument  $\mathbf{r}'$  of the propagator, identifying pairs of auxiliary initial points  $\mathbf{r}'_{j-}, \mathbf{r}'_{j+}$  with  $\mathbf{r}'$  in their middle. (ii) Propagate trajectory pairs  $\mathbf{r}_{j\pm}(t)$  classically, keeping track of the symplectic area  $\mathbf{A}_j$  between them. (iii) Find the amplitude and phase contributed by each trajectory pair and associate them to the final midpoints  $\bar{\mathbf{r}}''_j$ . They constitute a deformed cone, projected onto phase space [Fig. 2(c)]. Its “lower” (“upper”) surface [red (blue) in Fig. 2(c)] corresponds to pairs of extrema (saddles) of the action, respectively. (iv) Superpose the contributions of the two surfaces, after smoothing amplitude and phase over midpoints  $\bar{\mathbf{r}}''_j$  within each of them.

The caustics in Eq. (4) result from applying stationary-phase integration in a situation where pairs of stationary points can come arbitrarily close to one another. Since the underlying Van Vleck propagator admits only up to quadratic terms in the phase, we seek a superior approach, corresponding to a uniform approximation. It is available in the form of a path-integral representation of the Wigner propagator [16], in close analogy to the Feynman path integral,

$$G(\mathbf{r}'', \mathbf{r}', t) = \frac{1}{h^f} \int D\mathbf{r} \int D\mathbf{R} e^{-iS(\{\mathbf{r}\}, \{\mathbf{R}\})/\hbar}. \quad (6)$$

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

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

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

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

Expanding the action (7) around  $\mathbf{r}(t) = \mathbf{r}_{cl}(\mathbf{r}', t)$  and  $\mathbf{R}(t) \equiv (P(t), Q(t)) = \mathbf{0}$ , there remain only linear terms

in  $P$  and linear and cubic terms in  $Q$ . Evaluating the  $\mathbf{R}$  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  $\rho = (\eta, \xi) = (\mu^{1/4}p, \mu^{-1/4}q)$ , 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 parametrized by the angle  $\phi(t) = \int_0^t ds \sqrt{T''(p_{cl}(s))V''(q_{cl}(s))}$ . It is real (imaginary) if the linearized dynamics is elliptic (hyperbolic).

To evaluate the  $\mathbf{r}$  sector of the path integral, we Fourier transform the Wigner function  $\tilde{W}(\gamma) \equiv (FW) \times (\gamma) = (2\pi)^{-1} \int d^2r \exp(-i\gamma \wedge \mathbf{r})W(\mathbf{r})$  and the propagator accordingly,  $\tilde{G} = FGF^{-1}$ . We get  $[\gamma' \equiv (\alpha', \beta')]$

$$\tilde{G}(\gamma'', \gamma', t) = \delta(\gamma'' - M(\phi'')\gamma') \exp\left(-i\left(\frac{a_{30}}{3}\alpha'^3 + a_{21}\alpha'^2\beta' + a_{12}\alpha'\beta'^2 + \frac{a_{03}}{3}\beta'^3\right)\right). \quad (9)$$

The coefficients  $a_{jk} = \int_0^t ds \sigma(s)(\sin\phi(s))^j(\cos\phi(s))^k$  depend on where along the classical trajectory how much quantum spreading  $\sim \sigma(t) = (\mu(t))^{3/4}\hbar^2 V'''(q_{cl}(t))/8$  is picked up and thus on the specific system and initial conditions. The Fourier transform from Eq. (9) back to the original Wigner propagator can be done analytically, after transforming the third-order polynomial in the phase to a normal form [17].

The internal structure and the time evolution of the quantum spot described by Eq. (9) are qualitatively different for elliptic and hyperbolic classical trajectories (real and imaginary  $\phi$ , respectively). In the elliptic case, the spot is a periodic function of  $\phi$ . In particular, it collapses approximately to a point whenever  $\phi = 2l\pi$ ,  $l$  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-dimensional distribution fans out into a two-dimensional interference pattern formed as the overlap of the bright (oscillatory) sides of two Airy functions, with a sharp maximum on the classical trajectory [Fig. 3(b)]. In comparison with the corresponding exact quantum-mechanical result [Fig. 3(a)] for the quantum spot, obtained by expanding the propagator in energy eigenstates [18], the path-integral solution [Fig. 3(c)] resolves the caustics far better than Eq. (4). 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 direction and contracting in the stable direction [Fig. 3(d)]. Isolated unstable periodic orbits embedded in a chaotic region of phase space exhibit a degeneracy of the Weyl propagator [14]. It allows one to account for scarring in terms of the Wigner propagator [17].

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) 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 formulas, and spectral statistics, regularization of the ballistic nonlinear  $\sigma$  model, semiclassical propagation of entanglement, and generalization to nonunitary time evolution.

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