

## Semiclassical Propagation of Gaussian Wave Packets

Raphael N. P. Maia, Fernando Nicacio, and Raúl O. Vallejos

*Centro Brasileiro de Pesquisas Físicas (CBPF), Rua Dr. Xavier Sigaud 150, 22290-180 Rio de Janeiro, Brazil*

Fabrizio Toscano

*Fundação Centro de Ciências e Educação Superior a Distância do Estado do Rio de Janeiro, 20943-001 Rio de Janeiro, Brazil*  
*Instituto de Física, Universidade Federal do Rio de Janeiro, Cx. P. 68528, 21941-972 Rio de Janeiro, Brazil*

(Received 16 July 2007; published 6 May 2008)

We analyze the semiclassical evolution of Gaussian wave packets in chaotic systems. We show that after some short time a Gaussian wave packet becomes a primitive WKB state. From then on, the state can be propagated using the standard time-dependent WKB scheme. Complex trajectories are not necessary to account for the long-time propagation. The Wigner function of the evolving state develops the structure of a classical filament plus quantum oscillations, with phase and amplitude being determined by geometric properties of a classical manifold.

DOI: [10.1103/PhysRevLett.100.184102](https://doi.org/10.1103/PhysRevLett.100.184102)

PACS numbers: 05.45.Mt, 03.65.Sq

*Introduction.*—The standard approach to semiclassical evolution is time-dependent WKB theory (TDWKB) [1–4]. This theory provides a clear geometric description of the dynamics: a time-dependent quantum state is associated with an evolving Lagrangian manifold in classical phase space. [A phase-space manifold  $(p(q), q)$  is Lagrangian if  $p = \nabla S(q)$ , for some generating function  $S$  [5].] For TDWKB to be applicable the initial state must itself be related to a Lagrangian manifold. This is the case, e.g., of eigenstates of position or momentum operators (related to planes) [5], or highly excited eigenstates of bounded integrable Hamiltonians (related to tori) [3].

Somewhat surprisingly TDWKB has never been used to propagate Gaussian wave packets. It is probably the static point of view what blocked the use of standard TDWKB: If a Gaussian state is thought of as the ground state of some harmonic oscillator, then it certainly does not qualify as an initial WKB state. However, by taking the dynamics into consideration, a new perspective arises. In chaotic systems, when one observes the evolution of an initially Gaussian wave packet through a phase-space representation (like Husimi or Wigner) [6], it becomes manifest that, after some time, the wave packet acquires the form of a thin filament, very similar to the classical evolution of the initial density [7–10] (in the case of the Wigner function the filament is decorated by interference fringes). The smaller  $\hbar$  (as compared with the relevant action scales), the stronger the localization of the wave packet along some classical manifold. With this picture in mind it is natural to conjecture that the wave packet evolves into a WKB state, its support being a real phase-space manifold [8,11,12]. The purpose of this Letter is to provide concrete evidence in support of this statement.

We show that, after some (short) time, a Gaussian wave packet becomes a primitive WKB state. From then on, the state can be propagated using the standard TDWKB scheme. Complex trajectories [13–15] are not necessary

to describe the long-time propagation of wave packets, but they may be used to describe the evolution during the initial stage. The present approach not only offers an intuitive geometric description of the evolving state, but can be very accurate, as we demonstrate with a numerical example.

We focus on the Wigner function for its ability to reflect subjacent phase-space structures [16], and because it is the standard representation when dealing with decoherence (arising from coupling to the environment [9]) in semiclassical regimes.

*TDWKB approach.*—In order to eliminate some unnecessary complications we consider a 1 degree of freedom Hamiltonian  $H(p, q, t)$ , the dependence on  $t$  being periodic with period  $\tau$ . Let us assume that the one-period map,  $M_\tau(p(t), q(t)) = (p(t + \tau), q(t + \tau))$ , has a hyperbolic fixed point at the origin, and, without loss of generality, choose the  $q$  axis to coincide with the unstable subspace. At  $t = 0$  we launch a Gaussian wave packet at the origin:

$$\psi_0(q) = (2\pi\sigma^2)^{-1/4} \exp(-q^2/4\sigma^2). \quad (1)$$

Note that we have preserved the essential ingredient of chaotic dynamics, i.e., the exponential stretching and folding of phase-space manifolds.

If the  $q$  uncertainty ( $\sigma$ ) of the initial wave packet (1) is large enough [e.g., a classical length,  $\sigma \sim \hbar^0$ ], then (1) is already a primitive WKB state,

$$\psi_0(q) = A_0(q) \exp[iS_0(q)/\hbar], \quad (2)$$

given that both the amplitude  $A_0(q)$  and phase  $S_0(q) = 0$  vary slowly on the quantum scale [2]. The associated Lagrangian manifold is  $p = 0 = dS_0/dq$ . Accordingly, this state can be successfully evolved using the TDWKB scheme, as we showed in Ref. [17].

Let us now analyze what happens when a small circular wave packet is launched at an unstable fixed point. Numerical simulations show that the positive part of the

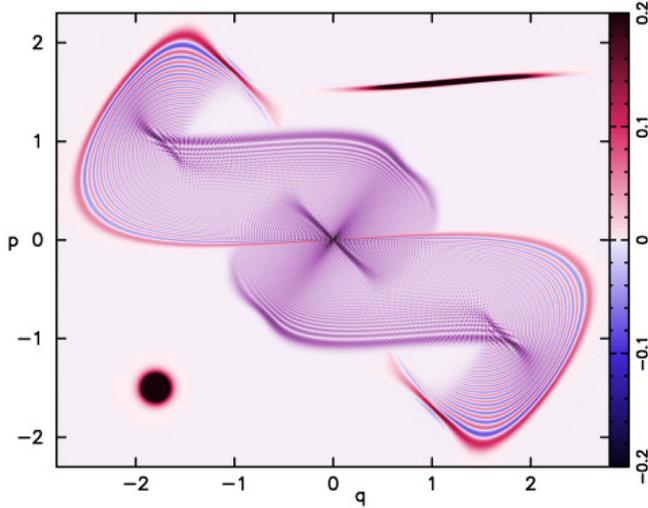


FIG. 1 (color online). Linear density plot of the exact Wigner function  $[\pi\hbar W(p, q)]$  after six periods of evolution with the kicked harmonic oscillator (see the text for a description of the system). We also show displaced versions of (i) the initial state (a circular Gaussian at the origin, left-bottom), (ii) the Wigner function after two steps (top, right).

Wigner function gets stretched along the unstable manifold. As this positive part bends, interference fringes appear. The picture is that of a positive (classical) thin filament decorated by an oscillatory pattern (see Fig. 1).

The fact that the structures in Fig. 1 are very similar to those found in the Wigner functions related to WKB eigenstates [18], leads us to enquire: does the Wigner function of Fig. 1 correspond to a WKB state, i.e., can we write

$$\psi_t(q) \approx \sum_{\nu} A_t^{(\nu)}(q) \exp[iS_t^{(\nu)}(q)/\hbar]? \quad (3)$$

Here  $\nu$  labels the different branches of the hypothetical Lagrangian manifold supporting the WKB state ( $p^{(\nu)} = dS^{(\nu)}/dq$ ) [5]. It is understood that the expression above must be valid during some time interval, during which amplitudes and phases evolve according to TDWKB theory [2–5]; i.e., amplitudes are convected by the classical flow in  $q$  space,  $A_t(q') = A_0(q) |\partial q'/\partial q|^{-1/2}$ , and the generating function, which solves the Hamilton-Jacobi equation, can be written as an integral over the classically evolved manifold [3]:  $S_t(q') = S_t(q_0) + \int_{q_0}^{q'} pdq$ .

In the case of only one branch, i.e., before the classical manifold folds, a numerical simulation is sufficient to answer the question posed above, as we show in the following. For this purpose we introduce the concrete model system that will serve as our test bench. This is the kicked harmonic oscillator [10,19]:  $H(p, q, t) = p^2/2m + m\omega^2 q^2/2 + K \cos(kq) \sum_{n=0}^{\infty} \delta(t - n\tau)$ . The parameters  $m = \omega = k = 1$ ,  $K = 2$  (in appropriate units [10]), and  $\tau = \pi/(3\omega)$  guarantee a large chaotic region

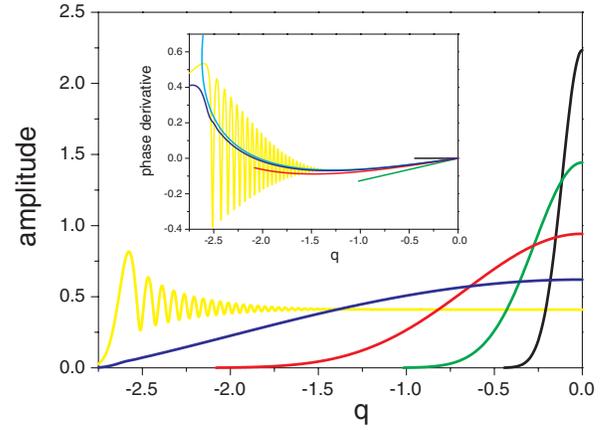


FIG. 2 (color online). Wave function amplitude  $|\psi_t(q)|$  and phase derivative  $d\phi_t/dq$  (inset) at  $t/\tau = 0, 1, 2, 3, 4$  (black, green, red, blue, yellow, respectively). Also shown is the unstable manifold (inset, cyan). Because of parity symmetry we only plot the region  $q \leq 0$ .

around the hyperbolic fixed point located at the origin [10]. The unstable direction is close to the  $q$  axis. We considered an initial circular state ( $t = 0^-$ ) given by Eq. (1) with  $\sigma = 0.08$  (corresponding to  $\hbar = 0.0128$ ). Some snapshots of its evolution (Wigner functions) are shown in Fig. 1.

In Fig. 2 we show amplitude  $\rho_t(q)$  and phase derivative  $d\phi_t/dq$  of the evolved state for short times [ $\psi \equiv \rho \exp(i\phi/\hbar)$ ]. Both quantities must be smooth on the quantum scale for the state to qualify as a primitive WKB state. We see that as time grows the amplitude gets smoother: at  $t = 0$  it was localized in a region of size  $\mathcal{O}(\hbar^{1/2})$ , at  $t = 3$  it has acquired the maximal (classical) width. The derivative of the phase, which is the candidate to Lagrangian support of the WKB state, stays smooth, and close to the unstable manifold, until  $t \approx 3$ . For larger times,  $t \geq 4$ , the turning point is reached and a fold is born, giving rise to quantum oscillations in both  $\rho(q)$  and  $\phi(q)$ . For smaller  $\hbar$  a similar behavior is observed, the only difference being that it takes longer to reach the turning point (this time goes like  $\log \hbar$ ). Our claim is that, for small enough  $\hbar$ , there is a time window ( $t_{\min}, t_{\max}$ ) where  $\psi_t$  is to good accuracy (see below) a primitive WKB state, meaning that it can be propagated further on according to TDWKB. In our numerical example, we checked that the optimal time for starting the TDWKB scheme is  $t = 2$ . At  $t = 3$  the interference effects of the turning point are already significant (even if not apparent in Fig. 2). At  $t = 1$  the wave packet is still not wide enough.

The next step is thus to evolve  $\psi_{t=2}$  using TDWKB and compare with the exact propagation. In order to unfold subjacent phase-space structures, the comparison will be made at the level of Wigner functions.

*Semiclassical Wigner function.*—The Wigner function of a general WKB state [Eq. (3)] can be calculated analytically, using the stationary phase method, in a way analo-

gous to that followed by Berry and Balazs for the special case of semiclassical eigenstates of integrable Hamiltonians [3]. We start with the usual definition of Wigner function, specialized to our case,

$$W(\bar{p}, \bar{q}, t) = \frac{1}{\pi\hbar} \int d\xi A_t(\bar{q} + \xi) A_t(\bar{q} - \xi) e^{i\phi(\xi)/\hbar}, \quad (4)$$

where the phase is given by  $\phi(\xi) = S_t(\bar{q} + \xi) - S_t(\bar{q} - \xi) - 2\bar{p}\xi$ . We assume that  $\bar{p}, \bar{q}$  is not far away from the manifold. In this case only one branch of  $S_t$  is relevant [3]. The stationary phase condition reads  $p_t(\bar{q} + \xi) + p_t(\bar{q} - \xi) = 2\bar{p}$ , where  $p_t(q) = dS_t/dq$ . If the point  $\bar{x} = (\bar{p}, \bar{q})$  is on the concave side of the evolved manifold but not too far away, there are in general two solutions  $\pm\xi^*$ , defining two points on the manifold,  $x_+$  and  $x_-$ . These are the tips of a chord having  $\bar{x}$  as midpoint (Fig. 3). When the stationary points are not coalescing they give individual complex conjugate contributions to the integral. The corresponding Wigner function reads

$$W(\bar{p}, \bar{q}, t) = \frac{2\sqrt{2}}{\sqrt{\pi\hbar}} A_0(q_+) A_0(q_-) \frac{\cos(\mathcal{A}/\hbar - \pi/4)}{\sqrt{|v_+ \wedge v_-|}}. \quad (5)$$

The phase structure was extracted literally from Ref. [3]; i.e.,  $\mathcal{A}$  is the (symplectic) area between the manifold and the chord. The amplitude is different from Berry and Balazs', as they considered a different initial density. Here  $A_0(q_{\pm})$  is the initial amplitude at the preimages of  $x_{\pm}$  and  $v_{\pm} = dx_{\pm}/dq_0$  denote tangent vectors at  $x_{\pm}$ , their moduli representing local rates of expansion ( $dq_0$  is the  $q$

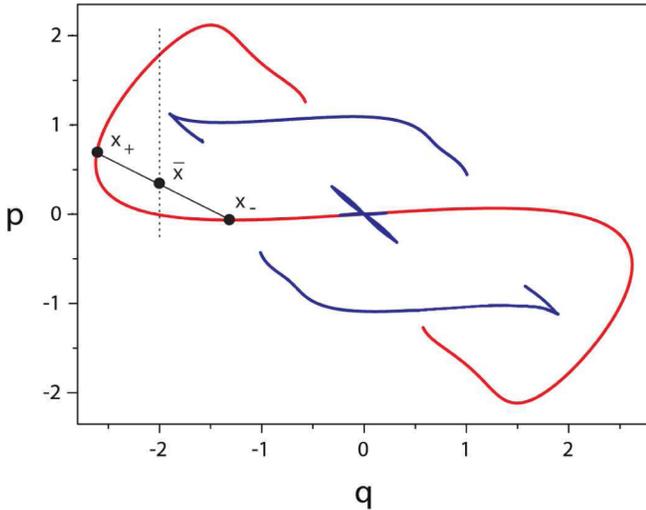


FIG. 3 (color online). Classical manifold corresponding to the state depicted in Fig. 1 (red). This manifold is itself a caustic of the Wigner function. The “ghost” lines (blue) also belong to the caustic. The point  $\bar{x}$  is the center of the chord with tips at  $x_-$  and  $x_+$ . A point  $\bar{x}$  belongs to the caustic if the vectors tangent to the manifold at  $x_-$  and  $x_+$  are parallel. The dashed vertical line at  $q = -2.0$  indicates a special section for testing the semiclassical approximations (see Fig. 4).

component of a displacement along the initial manifold, at the preimage of  $x_{\pm}$ ).

Equation (5) is a good semiclassical approximation, except in the vicinity caustic points, where  $|v_+ \wedge v_-| = 0$ , i.e., when tangent vectors at the tips of the chords are parallel (see Fig. 3). At caustics stationary phase points coalesce and one must use transitional (or uniform) approximations [18]. If  $(\bar{p}, \bar{q})$  is close enough to the classical manifold, we can obtain a crude transitional approximation to Eq. (4) as follows: (i) Approximate the manifold by the quadratic curve  $\bar{p} \approx p_* + p'_*(q - q_*) + p''_*(q - q_*)^2/2$ . This leads to a cubic phase  $\phi(\xi)$ . (ii) Neglect variations of the amplitude, i.e.,  $A_t(q) \approx A_t(q_*)$ . If we traverse the caustic along the line  $\bar{q} = q_*$ , and assuming  $p''_* > 0$ , then [12,20]:

$$W(\bar{p}, q_*, t) \approx \frac{2A_t^2(q_*)}{(\hbar^2 p''_*)^{1/3}} \text{Ai} \left[ -\frac{2(\bar{p} - p_*)}{(\hbar^2 p''_*)^{1/3}} \right], \quad (6)$$

Ai standing for the Airy function.

We are now in position for the final step in our program: the comparison of exact and semiclassical evolutions. Figure 1 displays the exact Wigner function after six steps of evolution. It is evident that its skeleton is the caustic of the manifold of Fig. 3, which was obtained by evolving during four steps the manifold (phase derivative) associated to the exact  $\psi_{t=2}(q)$ .

For a quantitative examination, in Fig. 4 we plotted the section  $q = -2$  of the exact Wigner function together with the semiclassical prediction, Eqs. (5) and (6). Inside their respective domains of validity both approximations are excellent. This completes our argumentation.

*Concluding remarks.*—We reported for the first time the use of standard TDWKB for semiclassical propagation of wave packets in chaotic systems.

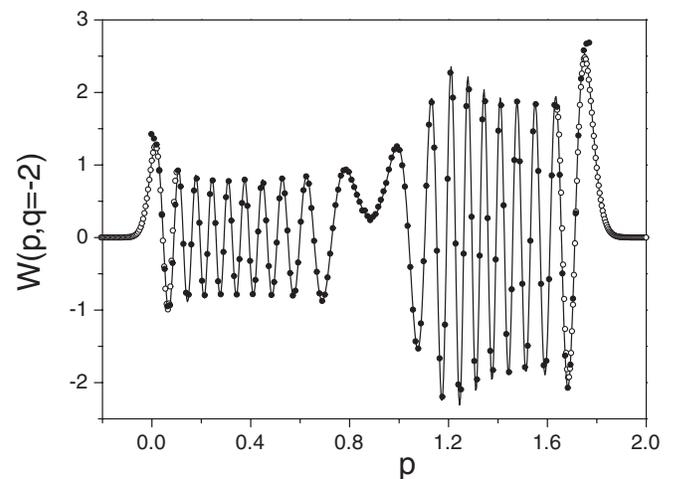


FIG. 4. A section of the exact Wigner function  $W(p, q = -2)$  of Fig. 1 (line) vs WKB approximation. Full circles correspond to the standard stationary phase result [Eq. (5)] and open circles to the transitional approximation [Eq. (6)].

The key point is that chaotic dynamics provides the initial expansion that defines the appropriate Lagrangian manifold for starting the TDWKB scheme. In particular we showed that localized states typically evolve into WKB states, and explained how to calculate amplitudes and phases explicitly. The applicability of the method in its present form requires stretching of the wave packet before folding starts. This condition may not be met in every example considered, but is otherwise guaranteed in deep-enough semiclassical regimes.

Our results provide a novel perspective for reexamining important previous work on long-time wave packet propagation. Consider, for instance, the remarkable calculations of Tomsovic and Heller's, who used a multiple linearization scheme to obtain accurate autocorrelation functions for large times [7]. In the light of our findings, their scheme can now be understood as arising from the linearization of the WKB wave function  $\psi_t(q)$  (which is globally valid) in the vicinity of a periodic point. The family of "homoclinic" intersections in Ref. [7], essential for organizing the summation of recurrences, corresponds, in the TWKB context, to the set of intersections between the Lagrangian manifold of the evolved state and the stable manifold of the fixed point. In this way, we expect the present Letter will contribute to the ongoing debate about the time scale for the breakdown of semiclassical propagation. Whether the break time diverges like  $\log\hbar$  [11,12] or, more plausibly, like some power of  $\hbar$  [7,21] is a question still awaiting a definitive answer.

One important feature of TDWKB is that it can be easily supplemented to accommodate decoherence effects. Let us briefly analyze the example of the Lindblad master equation corresponding to a chaotic Hamiltonian system coupled to a high temperature reservoir [10,22] (or, similarly, the nonselective weak continuous measurement of  $\hat{q}$  and/or  $\hat{p}$  [22,23]). In the formalism of quantum trajectories [22], the quantum jumps associated to such an environment (or weak measurement scheme), amount to random rigid translations in phase space [24]. The alternation of random translations with Hamiltonian evolution leads to a final density matrix represented by a weighted ensemble of pure WKB states, each one related to a particular history of random translations. The corresponding Wigner function is thus suggestively expressed as an average over filamentary Wigner functions like the one depicted in Fig. 1.

We thank A.M. Ozorio de Almeida, L.A. Pachón, M. Sieber, E. Vergini, T. Dittrich, J. Vanicek, L. Kaplan,

G. Alber, and E. J. Heller for interesting comments. Partial financial support from CNPq, CAPES, PROSUL, The Millennium Institute for Quantum Information (Brazilian agencies), and UNESCO/IBSP Project 3-BR-06 is gratefully acknowledged.

- 
- [1] J.H. Van Vleck, Proc. Natl. Acad. Sci. U.S.A. **14**, 178 (1928).
  - [2] P. A. M. Dirac, *Principles of Quantum Mechanics* (Oxford University Press, Oxford, 1947).
  - [3] M.V. Berry and N.L. Balazs, J. Phys. A **12**, 625 (1979).
  - [4] V.P. Maslov and M.V. Fedoriuk, *Semiclassical Approximations in Quantum Mechanics* (Reidel, Dordrecht, 1981).
  - [5] R.G. Littlejohn, J. Stat. Phys. **68**, 7 (1992).
  - [6] W.P. Schleich, *Quantum Optics in Phase Space* (Wiley-VCH, Berlin, 2001).
  - [7] S. Tomsovic and E.J. Heller, Phys. Rev. Lett. **67**, 664 (1991); Phys. Rev. E **47**, 282 (1993).
  - [8] P.G. Silvestrov, J. Tworzydło, and C.W.J. Beenakker, Phys. Rev. E **67**, 025204(R) (2003).
  - [9] W.H. Zurek, Rev. Mod. Phys. **75**, 715 (2003).
  - [10] F. Toscano, R.L. de Matos Filho, and L. Davidovich, Phys. Rev. A **71**, 010101(R) (2005).
  - [11] R. Schubert, Commun. Math. Phys. **256**, 239 (2005).
  - [12] P.G. Silvestrov and C.W.J. Beenakker, Phys. Rev. E **65**, 035208(R) (2002).
  - [13] V.P. Maslov, *The Complex WKB Method for Nonlinear Equations I* (Birkhäuser, Basel, 1994).
  - [14] D. Huber, E. J. Heller, and R. G. Littlejohn, J. Chem. Phys. **89**, 2003 (1988).
  - [15] M. A. M. de Aguiar, M. Baranger, L. Jaubert, F. Parisio, and A. D. Ribeiro, J. Phys. A **38**, 4645 (2005).
  - [16] A. M. Ozorio de Almeida, Phys. Rep. **295**, 265 (1998).
  - [17] R. N. P. Maia, F. Nicacio, R. O. Vallejos, and F. Toscano, arXiv:0707.2423v1.
  - [18] M. V. Berry, Phil. Trans. R. Soc. A **287**, 237 (1977).
  - [19] G.P. Berman, V. Yu. Rubaev, and G.M. Zaslavsky, Nonlinearity **4**, 543 (1991).
  - [20] M. A. Alonso and G.W. Forbes, J. Opt. Soc. Am. A **17**, 2288 (2000).
  - [21] R. Schubert, arXiv:0705.0134v1.
  - [22] H.-P. Breuer and F. Petruccione, *The Theory of Quantum Open Systems* (Oxford University Press, Oxford, 2002).
  - [23] K. Jacobs and D.A. Steck, Contemp. Phys. **47**, 279 (2006).
  - [24] M. J. W. Hall, Phys. Rev. A **50**, 3295 (1994).