An Initial Value Representation with Complex Trajectories

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Abstract

We present an Initial Value Representation for the semiclassical coherent state propagator based on complex trajectories. We map the complex phase space into a real phase space with twice as many dimensions and use a simple procedure to automatically eliminate non-contributing trajectories. The resulting semiclassical formulas do not show divergences due to caustics and provide accurate results.

Key words: semiclassical methods; coherent states; initial value representations; complex trajectories

1 Introduction

The investigation of wavepackets dynamics by semiclassical methods has practical importance for calculations of several processes involving atoms and molecules. It is also a fundamental topic in the study of the classical-quantum connection, especially for chaotic systems and for open systems, coupled to environments.

The history of semiclassical methods goes back to the origins of quantum mechanics itself. One fundamental result is the so called Van Vleck approximation to the

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coordinate propagator, derived in 1928 [1], that can be written as

\[
\langle x_f | e^{-i\hat{H}\tau/\hbar} | x_i \rangle \approx \frac{1}{\sqrt{2\pi m_{qp}}} e^{iS(x_i,x_f,T)/\hbar - i\pi/4 - i\pi k/2}.
\] (1)

In this expression \(S(x_i,x_f,T)\) is the classical action of a trajectory connecting coordinates \(x_i\) to \(x_f\) in the time \(T\), \(m_{qp}\) is an element of the tangent matrix, that controls the motion in the vicinity of this trajectory, and \(k\) is the number of focal points (where \(m_{qp}\) goes to zero) along the trajectory. If more than one trajectory satisfying these boundary conditions exists, one has to sum their contributions. From this basic propagator one can compute the time evolution of arbitrary wavefunctions.

A more direct approach to calculate the time evolution of wavepackets in given by the propagator in the coherent state representation. The coherent states of the harmonic oscillator are minimum uncertainty wavepackets and define a representation involving both the coordinates and the momenta that can be readily visualized in the phase space. The coherent state propagator \(\langle z_f | e^{-\frac{i}{\hbar}\hat{H}T} | z_0 \rangle\) represents the amplitude probability that the initial wavepacket \(|z_0\rangle\) centered on \(q_0,p_0\) is found at the state \(|z_f\rangle\), centered on \(q_f,p_f\), after a time \(T\). However, the direct evaluation of the semiclassical limit of this propagator results in an expression bearing the same difficulties of the Van Vleck formula [2,3,4,5], namely: (a) the classical trajectories needed are defined by mixed initial-final boundary conditions, rendering the calculation hard, specially in multidimensional or chaotic systems and; (b) the formula diverges at phase space focal points. Moreover, the trajectories are complex and some of them, even satisfying the appropriate boundary conditions, lead to unphysical contributions and must be discarded [6,7,8,9,10,11,13,14].

Several methods have been developed to overcome these difficulties, most of them based on the idea of initial value representations (IVR) [15,16,17,18,19,20,21,22,23,24]. Among these, the Herman-Kluk propagator [18] and the method of linearized cellular dynamics developed by Heller and Tomsovic [25,26] stands out as very accurate. More recent derivations and corrections to the basic Herman-Kluk formula have also provided new insight into this class of approximation [27,28,29,30].

In spite of the many difficulties involved in the calculation of the coherent state propagator with complex trajectories, this approximation turns out to be very accurate...
Recent work on Bohmian mechanics have also employed complex trajectories, providing a new formulation leading to accurate results [31,32]. In this paper we propose the construction of an initial value representation for this approximation that removes most of its problems: the mixed conditions defining the trajectories are replaced by initial conditions; the complex trajectories are mapped into real trajectories of an associated Hamiltonian; the divergences due to focal points are eliminated and; a simple and automatic filtering is used to eliminate the non-contributing trajectories.

This paper is organized as follow. The next section reviews the semiclassical coherent state propagator and its semiclassical approximation in terms of complex trajectories. In section 3 we develop the initial value representation for complex trajectories (CIVR). It presents what we call the sudden CIVR, where only trajectories satisfying the original mixed conditions are considered, and the smooth CIVR where the neighborhood of the relevant trajectories are considered as well. We also discuss how the complex trajectories calculations are performed in terms of real trajectories. This section ends with a discussion of the criteria used for filtering out the non-contributing trajectories. In section 4 the smooth CIVR is applied to an anharmonic quartic oscillator and some final comments are made. In two appendices useful relations of the tangent matrix are derived for both real and complex trajectories.

2 The semiclassical coherent state propagator

The coherent state $|z\rangle$ of a harmonic oscillator of mass $m$ and frequency $\omega$ is defined by

$$|z\rangle = e^{-\frac{1}{2}|z|^2} e^{z \hat{a}^\dagger} |0\rangle$$  \hspace{1cm} (2)

with $|0\rangle$ the harmonic oscillator ground state and

$$\hat{a}^\dagger = \frac{1}{\sqrt{2}} \left( \frac{\hat{q}}{b} - i \frac{\hat{p}}{c} \right), \hspace{1cm} z = \frac{1}{\sqrt{2}} \left( \frac{q}{b} + i \frac{p}{c} \right).$$  \hspace{1cm} (3)

In these equations $\hat{q}$, $\hat{p}$, and $\hat{a}^\dagger$ are operators; $q$ and $p$ are real numbers and $z$ is complex. The parameters $b = (\hbar/m\omega)^{\frac{1}{2}}$ and $c = (\hbar m\omega)^{\frac{i}{2}}$ define the length and
momentum scales, respectively, and their product is $\hbar$.

For a time-independent Hamiltonian operator $\hat{H}$, the propagator in the coherent states representation is the matrix element of the evolution operator between states $|z_0\rangle$ and $|z_f\rangle$ [33]:

$$K(z^*_f, z_0, T) = \langle z_f | e^{-i \hat{H} T} | z_0 \rangle.$$  \hspace{1cm} (4)

The semiclassical evaluation of $K(z^*_f, z_0, T)$ was presented in detail in [3,4]. The result is given by

$$K_{sc}(z^*_f, z_0, T) = \sum_{\nu} \sqrt{\frac{i}{\hbar} \frac{\partial^2 S}{\partial z_0 \partial z^*_f}} \exp \left\{ \frac{i}{\hbar} (S + I) - \frac{1}{2} (|z_f|^2 + |z_0|^2) \right\},$$  \hspace{1cm} (5)

where

$$S = S(z^*_f, z_0, t) = \int_0^t dt' \left[ \frac{i \hbar}{2} (\dot{u}v - \dot{v}u) - H(u, v, t') \right] - \frac{i \hbar}{2} (u(T) z^*_f + z_0 v(0))$$  \hspace{1cm} (6)

is the action and the classical Hamiltonian function is calculated from the Hamiltonian operator as $H(u, v) = \langle v | \hat{H} | u \rangle$. The term

$$I = \frac{1}{2} \int_0^T \frac{\partial^2 H}{\partial u \partial v} dt$$  \hspace{1cm} (7)

is a correction to the action. The sum over $\nu$ represents the sum over all contributing (complex) classical trajectories satisfying Hamilton’s equations with boundary conditions

$$\frac{1}{\sqrt{2}} \left( \frac{q(0)}{b} + i \frac{p(0)}{c} \right) = z_0, \quad \frac{1}{\sqrt{2}} \left( \frac{q(T)}{b} - i \frac{p(T)}{c} \right) = z^*_f.$$  \hspace{1cm} (8)

In all these expressions the variables $u$ and $v$ are defined by

$$u = \frac{1}{\sqrt{2}} \left( \frac{q}{b} + i \frac{p}{c} \right), \quad v = \frac{1}{\sqrt{2}} \left( \frac{q}{b} - i \frac{p}{c} \right).$$  \hspace{1cm} (9)

They are manifestly independent ($u \neq v^*$ since $q$ and $p$ are complex), and replace $z$ and $z^*$ to avoid confusion. In these variables the boundary conditions become

$$u(0) = z_0, \quad v(T) = z^*_f.$$  \hspace{1cm} (10)
3 A complex initial value representation

3.1 Basic idea

The first of the boundary conditions (10) specifying the complex trajectory can be written explicitly as

$$\frac{q(0)}{b} + ib\frac{p(0)}{\hbar} = \frac{q_0}{b} + ib\frac{p_0}{\hbar},$$

(11)

where \(q_0\) and \(p_0\) define the initial coherent state \(|z_0\rangle\). This condition is not sufficient to determine the trajectory, since \(q(0)\) and \(p(0)\) are complex. The missing condition is given by the second equation in (10) and refers to the final propagation time \(T\).

In order to avoid dealing with mixed initial-final conditions, let us first suppose we have had a second equation of the form

$$\frac{q(0)}{b} - ib\frac{p(0)}{\hbar} = \frac{q_1}{b} - ib\frac{p_1}{\hbar}.$$  

(12)

By solving for \(q(0)\) and \(p(0)\) one finds

$$q(0) = \frac{1}{2} \left[ (q_0 + q_1) + i\frac{b^2}{\hbar}(p_0 - p_1) \right]$$

$$p(0) = \frac{1}{2} \left[ (p_0 + p_1) + i\frac{b}{\hbar}(q_1 - q_0) \right].$$

(13)

For \(q_0\) and \(p_0\) fixed, each \(q_1\) and \(p_1\) defines a trajectory with end points \(q(T)\) and \(p(T)\).

Let \(\tilde{q}_1\) and \(\tilde{p}_1\) be the values of \(q_1\) and \(p_1\) such that the second of equations (10) is satisfied, i.e., for which the initial conditions (13) leads to

$$\frac{q(T)}{b} - ib\frac{p(T)}{\hbar} = \frac{q_f}{b} - ib\frac{p_f}{\hbar},$$

(14)

where \(q_f\) and \(p_f\) define the final coherent state \(|z_f\rangle\). Then, we can rewrite the semiclassical propagator of Eq. (5) as

$$K_{sc}(z_f^*, z_0, T) = \int dq_1dp_1\delta_a(q_1 - \tilde{q}_1)\delta_a(p_1 - \tilde{p}_1)$$
\[ \psi(z^*_f, T) = \frac{1}{2\pi\hbar} \int K_{sc}(z^*_f, z_0, T)\psi(z^*_0, 0)\delta_a(q_1 - \tilde{q}_1)\delta_a(p_1 - \tilde{p}_1)\, dq_0 dp_0 dq_1 dp_1. \]  

We note that the second derivative of the action with respect to its arguments, as appearing in the pre-factor of the semiclassical propagator, can be written in terms of the tangent matrix, that controls the classical motion in the vicinity of a given trajectory. In appendix A we derive several useful relations between the tangent matrix in \( u, v \) and \( q, p \) variables for complex and real trajectories. In particular, we show that

\[ i\frac{\partial^2 S}{\hbar \partial z_0 \partial z^*_f} = \frac{1}{M_{uv}}. \]  

Before we end this subsection we define the scaled coordinates and momenta \( \bar{q} = q/b \) and \( \bar{p} = pb/\hbar \). Defining the scaled Hamiltonian

\[ \bar{H}(\bar{q}, \bar{p}) = \frac{1}{\hbar} H(bq, h\bar{p}/b) \]  

it is easy to check that the semiclassical expressions in terms of \( \bar{q}, \bar{p} \) and \( \bar{H} \) become identical to the original expressions with \( b \) and \( \hbar \) replaced by 1. Therefore, from now one we shall use these scaled variables, which amounts to set \( b = \hbar = 1 \), but will omit the bar to make the notation simpler. The original variables will be recovered later in the examples.
3.2 The calculation of complex trajectories

For analytic Hamiltonian functions $H(q,p)$ it is possible to rewrite the equations of motion for the complex variables $q$ and $p$ in terms of real trajectories of an auxiliary Hamiltonian system with twice as many degrees of freedom, or as we call it, the double phase space. The definitions [34,35]

$$q = Q_1 + iP_2, \quad p = P_1 + iQ_2$$  \hspace{1cm} (19)

and

$$H(q,p) = H_1(Q_1, Q_2, P_1, P_2) + iH_2(Q_1, Q_2, P_1, P_2),$$  \hspace{1cm} (20)

where $H_1$ and $H_2$ are real functions, allows to show easily that Hamilton’s equations for $q$ and $p$ are equivalent to

$$\dot{Q}_i = \frac{\partial H_1}{\partial P_i}, \quad \dot{P}_i = -\frac{\partial H_1}{\partial Q_i}, \quad i = 1, 2.$$  \hspace{1cm} (21)

Note that $H_2$ is also a constant of the motion. The separation of variables in (19) may look unusual because it mixes $q$’s and $p$’s, but this is the proper combination to get the correct signs in Hamilton’s equations. These separation of variables also look natural when the form of equation (13) is considered.

For the case $|\psi(0)\rangle = |z_0\rangle$, the real trajectory starting from the center of the wavepacket plays an important role, and we shall use it as a reference. Therefore the integration over $q_1$ and $p_1$ in the CIVR will be centered on $q_0$ and $p_0$ and only a limited region around this point is expected to significantly contribute to the propagation. In this way we write

$$q_1 = q_0 + \Delta q, \quad p_1 = p_0 + \Delta p$$  \hspace{1cm} (22)

and the initial conditions (13) reduce to

$$Q_1(0) = q_0 + \Delta q/2 \quad Q_2(0) = \Delta q/2$$

$$P_1(0) = p_0 + \Delta p/2 \quad P_2(0) = -\Delta p/2.$$  \hspace{1cm} (23)
In accordance with Eq. (19), \( q(0) = q_0 + w, \ p(0) = p_0 + iw \) with \( w = (\Delta q - i\Delta p)/2 \), which is exactly the variable used in a search procedure developed in ref. [9].

All the tangent matrix elements appearing in equations (38) and (39) can be readily computed from the tangent matrix of the real trajectory in the double phase space. This procedure eliminates the need to work with complex trajectories and also the so called root search problem, involved in finding trajectories with mixed initial-final conditions.

### 3.3 The connection between initial and final displacements

The connection between the initial and final displacements can be established as follow. Initially by comparing equations (19) with (13) we see that

\[
\begin{align*}
Q_1(0) &= \frac{1}{2}(q_0 + q_1) \\
Q_2(0) &= \frac{1}{2}(q_1 - q_0) \\
P_1(0) &= \frac{1}{2}(p_0 + p_1) \\
P_2(0) &= \frac{1}{2}(p_0 - p_1)
\end{align*}
\]

(24)

which also leads to \( q_1 = Q_1(0) + Q_2(0) \) and \( p_1 = P_1(0) - P_2(0) \). It turns out to be convenient to extend this definition to

\[
\begin{align*}
q_1(t) &= Q_1(t) + Q_2(t) \\
p_1(t) &= P_1(t) - P_2(t). \\
\end{align*}
\]

(25)

Because of the filtering functions in (15) and (16) (smoothed or sharp) the relevant contributions to the integrals over \( q_1 \) and \( p_1 \) come from the vicinities of \( \tilde{q}_1 \) and \( \tilde{p}_1 \), that should also be close to \( q_0 \) and \( p_0 \). For this particular trajectory \( v(T) = z_f^* \):

\[
[Q_1(T) + iP_2(T)] - i[P_1(T) + iQ_2(T)] = q_f - iq_f
\]

(26)

or, according to (25), \( q_1(T) = q_f \) and \( p_1(T) = p_f \).
For neighboring trajectories we may expand the final values of $q_1(T)$ and $p_1(T)$ around $q_f$ and $p_f$ as:

$$q_1(T) \approx q_f + \frac{\partial q_1(T)}{\partial q_1}(q_1 - \tilde{q}_1) + \frac{\partial q_1(T)}{\partial p_1}(p_1 - \tilde{p}_1)$$

$$p_1(T) \approx p_f + \frac{\partial p_1(T)}{\partial q_1}(q_1 - \tilde{q}_1) + \frac{\partial p_1(T)}{\partial p_1}(p_1 - \tilde{p}_1)$$

or

$$\begin{pmatrix} q_1(T) - q_f \\ p_1(T) - p_f \end{pmatrix} = \begin{pmatrix} \frac{\partial q_1(T)}{\partial q_1} & \frac{\partial q_1(T)}{\partial p_1} \\ \frac{\partial p_1(T)}{\partial q_1} & \frac{\partial p_1(T)}{\partial p_1} \end{pmatrix} \begin{pmatrix} q_1 - \tilde{q}_1 \\ p_1 - \tilde{p}_1 \end{pmatrix} \equiv \Lambda \begin{pmatrix} q_1 - \tilde{q}_1 \\ p_1 - \tilde{p}_1 \end{pmatrix}. \quad (27)$$

It follows that

$$\delta(q_1 - \tilde{q}_1)\delta(p_1 - \tilde{p}_1) = |\det \Lambda| \delta(q_1(T) - q_f)\delta(p_1(T) - p_f). \quad (28)$$

In appendix B, equation (B.6), we show that $|\det \Lambda| = |M_{vv}|^2$.

### 3.4 Sudden complex initial value representation

In the case of sharp delta functions we can use equation (28) to write down the first of our formulas, that we term sudden CIVR. Since

$$\frac{1}{\sqrt{2}}(q_1(T) - ip_1(T)) = v(T) \quad (29)$$

and defining

$$\delta^2(v(T) - z_f^*) = 2\pi \delta(q_1(T) - q_f)\delta(p_1(T) - p_f) \quad (30)$$

we obtain

$$\psi(z_f^*, T) = \int |M_{vv}|^{3/2} e^{i(S+I)} - \frac{i}{2} (|z_f^*|^2 + |z_0|^2)^{3/2} \psi(z_0^*, 0) \delta^2(v(T) - z_f^*) \frac{d^2z_0}{\pi} \frac{d^2v_1}{\pi} \quad (31).$$
where $\xi$ is the phase of $M_{vv}$. Each pair of phase space points $q_0, p_0$ and $q_1, p_1$ define a complex trajectory with initial conditions

\[
q(0) = \frac{1}{2}(q_0 + q_1) + i\frac{1}{2}(p_0 - p_1) \\
p(0) = \frac{1}{2}(p_0 + p_1) + i\frac{1}{2}(q_0 - q_1).
\] (32)

The contribution of these trajectories to the final result are filtered by the delta function. The integration measures are defined as usual as $d^2z_0/\pi = dq_0 dp_0/2\pi$ and $d^2v_1/\pi = dq_1 dp_1/2\pi$.

Notice that the arguments of $S$ and $I$ in (31), which were originally $(z^*_f, z_0, T)$, can be replaced by $(v(T), z_0, T)$, so that both $S$ and $I$ are computed for the trajectories defined by (32). Also important is the fact that $M_{vv}$ in the pre-factor has moved from the denominator to the nominator so that divergences at caustics are replaced by non-contributing trajectories. This is a well known property of IVR’s constructed in this way.

### 3.5 Smooth complex initial value representation

If the delta functions in the CIVR are replaced by Gaussian functions a more well behaved approximation is obtained. Following Filinov [36] and Makri [37] we replace the filtering integrals of trajectories according to

\[
\int \delta(v_1 - \tilde{v}) \frac{d^2v_1}{\pi} \rightarrow \int e^{-\frac{1}{2a^2|M_{vv}|^2}[(q_1(\tilde{q}_1))^2 + (p_1(\tilde{p}_1))^2]} \frac{d^2v_1}{\pi a^2} \\
\approx \int e^{-\frac{1}{2a^2|M_{vv}|^2}[(q_1(\tilde{q}_1)-q_f)^2 + (p_1(\tilde{p}_1)-p_f)^2]} \frac{d^2v_1}{\pi a^2} \\
= \int |M_{vv}|^2 e^{-\frac{|v(T) - z^*_f|^2}{\alpha^2}} \frac{d^2v_1}{\pi \alpha^2},
\] (33)

where we have used equation (27) in the second line and defined the re-scaled width

\[
\alpha = a|M_{vv}|.
\] (34)

The use of smooth filters seems appropriate to coherent state propagation. It implies that not only the trajectories satisfying the exact boundary conditions (10) are
considered, but also their neighborhood as defined by the parameter $a$. In this case the action $S(z_f^*, z_0, T)$ in equation (15) cannot be simply replaced by $S(v(T), z_0, T)$, but has to be expanded around each initial value trajectory up to second order. The result is

$$
S(z_f^*, z_0, T) \approx S(v(T), z_0, T) + \frac{\partial S}{\partial v(T)}(z_f^* - v(T)) + \frac{1}{2} \frac{\partial^2 S}{\partial v(T)^2}(z_f^* - v(T))^2 \\
\approx S(v(T), z_0, T) - iu(T)(z_f^* - v(T)) - i\frac{M_{uv}}{2M_{vv}}(z_f^* - v(T))^2,
$$

(35)

where once again we have resorted to expressions derived in appendix B.

The smooth CIVR can then be obtained by using equations (33) and (35) in (16):

$$
\psi(z_f^*, T) = \int |M_{vv}|^{3/2} \exp \left\{ \phi - \frac{|v(T) - z_f^*|^2}{\alpha^2} \right\} \psi(z_0^*, 0) \frac{d^2z_0}{\pi} \frac{d^2v_1}{\pi\alpha^2},
$$

(36)

where

$$
\phi = i(S + I) + u(T) \left( z_f^* - v(T) \right) + \frac{M_{uv}}{2M_{vv}} \left( z_f^* - v(T) \right)^2 - \frac{|z_f|^2}{2} - \frac{|z_0|^2}{2} - i\frac{\xi}{2}.
$$

(37)

If the initial state to be propagate is itself a coherent state, equation (15), the smooth CIVR simplifies to

$$
K(z_f^*, z_0, T) = \int |M_{vv}|^{3/2} \exp \left\{ \phi - \frac{|v(T) - z_f^*|^2}{\alpha^2} \right\} \frac{d^2v_1}{\pi\alpha^2},
$$

(38)

with

$$
\phi = i(S + I) + u(T)z_f^* + \frac{M_{uv}}{2M_{vv}} \left( z_f^* - v(T) \right)^2 - \frac{|z_f|^2}{2} - \frac{|z_0|^2}{2} - i\frac{\xi}{2}.
$$

(39)

In this paper we shall discuss an example of this simple case only.

### 3.6 Filtering out non-contributing trajectories

It is well known that not all trajectories satisfying the boundary conditions (10) should be included in the semiclassical propagator. The trajectories for which the
real part of the exponent \( \phi \) in (39) is positive must be discarded as they give rise to divergent contributions in the semiclassical limit. These trajectories are probably associated with forbidden deformations of the integration contours that are necessary to derive the semiclassical approximation (4).

For the harmonic oscillator it can be checked explicitly that not only equations (38) and (39) give exact results but also that \( \text{Re}(\phi) \leq 0 \) for all complex trajectories. In our calculations trajectories satisfying

\[
\text{Re}(\phi) > c \hbar,
\]

where \( c \) is a constant, are neglected. We discuss the importance of the cutoff value of \( c \) in the next section.

4 Example

As a simple application of the smooth CIVR we consider the system

\[
\dot{H} = \frac{1}{2} \dot{p}^2 + \Omega^2 q^2 + \frac{\lambda}{4} \dot{q}^4.
\] (41)

It has been studied also in [14] by directly computing the relevant complex trajectories. The parameters are set to \( \Omega = 1, \lambda = 0.4 \) and \( \hbar = 1 \). For these values the ground state energy is \( E_0 \approx 0.559 \) and the first two excited states have \( E_1 \approx 1.770 \) and \( E_2 \approx 3.319 \). For the initial wavepacket we choose \( q_0 = 0, p_0 = -2.0 \), and \( b = 1.0 \). This gives \( E = H(q, p) = 2.0 \) for the energy of the central trajectory, \( \tau \approx 4.7 \) for its period, and \( X_{\text{turn}} \approx \pm 1.6 \) for its turning points. Figure 1(c) shows a plot of the potential function and indicates also the central trajectory energy.

We momentarily restore the original un-scaled variables to illustrate both the computation of the classical Hamiltonian and the scaling process. The classical Hamiltonian function is

\[
H = \frac{1}{2} p^2 + \frac{1}{2} \left( \frac{\Omega^2 + 3\lambda b^2}{4} \right) q^2 + \frac{\lambda}{4} q^4 + \left( \frac{\hbar^2}{4b^2} + \frac{\Omega^2 b^2}{4} + \frac{3\lambda b^4}{16} \right),
\] (42)
where $b$ is the width of the wavepacket. In terms of scaled variables (see equation (18)) the Hamiltonian becomes

$$\bar{H} = \omega \left[ \frac{1}{2} \bar{p}^2 + \frac{1}{2} \nu^2 \bar{q}^2 + \frac{1}{4} \bar{q}^4 + \frac{1}{4} \left( 1 + \nu^2 + \frac{3\bar{\lambda}}{16} \right) \right],$$

(43)

where $\omega = \hbar/b^2$, $\nu = \Omega/\omega$, $\bar{\lambda} = \lambda \hbar/\omega^3$ and $\bar{\nu}^2 = \nu^2 + 3\bar{\lambda}/2$. For the present values we have $\omega = \nu = 1$, $\bar{\lambda} = 0.4$ and $\bar{\nu}^2 = 1.6$.

Figure 1 shows five snapshots of the wavepacket (left column) and the corresponding regions of the $q_1, p_1$ plane where trajectories contribute significantly to the propagation. In these figures we have fixed the constant $c = 1.0$ (see equation (40)), except for figure 1(a), where $c = 2.5$. The width $a$ of the smoothing Gaussian was adjusted to get the best results for each propagation time, starting at $a = 1.5$ for $T = 1.0$ and decreasing to $a = 0.4$ for $T = 8.5$ (see caption for all values). The integration over $q_1$ and $p_1$ was performed using a regular grid with 30 points in $q_1$, varying from $-3$ to $3$, and 40 points in $p_1$ varying from $-4$ to $4$. The computational time for the present calculation is as fast as the split-operator method, well known for being efficient and accurate for one dimensional problems. For $T = 8.5$ the calculations take about 3 seconds in a Core 2 Quad PC with 2.4GHz.

The wavefunctions in figure 1 were calculated using the simple discretization

$$\psi(x, T) = \sum_{n,m} \langle x | z_{nm} \rangle K(z_{nm}^*, z_0, T) \frac{\Delta q \Delta p}{2\pi}$$

(44)

where $n$ and $m$ represent the grid in phase-space centered on the origin. We used a total of 40 and 60 points in the $q$ and $p$ directions respectively, with $-4 < q_n < +4$ and $-6 < p_m < +6$.

In spite of the accuracy of our results, specially as compared to previous calculations using root search procedures [14], several details remain to be understood and improved. The main problem is the sensitivity of the method to the choice of the width $a$ and the lack of a theory on how to choose it properly and automatically. A possible way out of this difficulty might to be the procedure devised in [37], where the width is chosen to minimize the oscillations of the integrand. Another problem is that the propagated wavepackets turn out not to be properly normalized, and the
amount by which normalization is lost also depends on the width $a$. In figure 1 the wave-functions have been re-normalized by hand after the propagation.

Despite these problems the method improves the results obtained by direct computation of the contributing trajectories and is much faster and simple to program. The next step is an application of the method to multidimensional systems, where the integrations over the initial conditions may be performed by Monte Carlo techniques. The difficulties just mentioned are currently under investigation.

### A Tangent matrices

In this appendix we use the scaled units where $\hbar = b = 1$. In the $u$ and $v$ variables the tangent matrix is defined by

\[
\begin{pmatrix}
\delta u(T) \\
\delta v(T)
\end{pmatrix} =
\begin{pmatrix}
M_{uu} & M_{uv} \\
M_{vu} & M_{vv}
\end{pmatrix}
\begin{pmatrix}
\delta u(0) \\
\delta v(0)
\end{pmatrix}
\tag{A.1}
\]

where $\delta u(0)$ and $\delta v(0)$ are small displacements at the initial point of the trajectory and $\delta u(T)$ and $\delta v(T)$ are the corresponding final deviations. The action $S(v'', u', T)$ for the trajectory with $u(0) = u'$ and $v(T) = v''$ satisfies

\[
u(T) \equiv u'' = i \frac{\partial S}{\partial v''}, \quad v(0) \equiv v' = i \frac{\partial S}{\partial u'}.
\tag{A.2}
\]

From the differentiation of (A.2) keeping the variable $T$ constant, we can obtain the connection between initial and final displacements. In matrix form it is

\[
\begin{pmatrix}
\delta u(T) \\
\delta v(0)
\end{pmatrix} = i
\begin{pmatrix}
S_{uu} & S_{uv} \\
S_{vu} & S_{vv}
\end{pmatrix}
\begin{pmatrix}
\delta u(0) \\
\delta v(T)
\end{pmatrix}
\tag{A.3}
\]

where $S_{uv} = \frac{\partial^2 S}{\partial u' \partial v''}$, etc. Comparing with eq. (A.1) we find

\[
S_{uv} = -i M_{vv}^{-1}, \quad S_{ev} = -i \frac{M_{uv}}{M_{vv}}.
\tag{A.4}
\]
Using the definition of $u$ and $v$ in terms of $q$ and $p$ (notice that all these variables are complex) it is easy to show that

\[
M_{uu} = \frac{1}{2}(m_{qq} + m_{pp} + im_{pq} - im_{qp})
\]
\[
M_{uv} = \frac{1}{2}(m_{qq} - m_{pp} + im_{pq} + im_{qp})
\]
\[
M_{vu} = \frac{1}{2}(m_{qq} - m_{pp} - im_{pq} - im_{qp})
\]
\[
M_{vv} = \frac{1}{2}(m_{qq} + m_{pp} - im_{pq} + im_{qp}),
\]

where $m$ is the tangent matrix in the $q, p$ system. Finally, using the definition of the real variables $Q_1, Q_2, P_1, P_2$ and defining its corresponding $4 \times 4$ tangent matrix $n$ we can show that

\[
m_{qq} = n_{11} - in_{14}
\]
\[
m_{qp} = n_{13} - in_{12}
\]
\[
m_{pq} = n_{24} + in_{21}
\]
\[
m_{pp} = n_{22} + in_{23}.
\]

Therefore, by working directly with the real trajectories in the double phase space we can compute $n$ and reconstruct the matrices $m$ and $M$ using simple linear transformations.

B Calculation of $\det \Lambda$

If $v(T)$ in equation (29) is an analytic function of the initial condition $v_1$, then, by the Cauchy-Riemann conditions we have

\[
\frac{\partial q_1(T)}{\partial q_1} = \frac{\partial p_1(T)}{\partial p_1}, \quad \frac{\partial q_1(T)}{\partial p_1} = -\frac{\partial p_1(T)}{\partial q_1}.
\]

By the definition of $\Lambda$, equation (27),

\[
\det \Lambda = \left(\frac{\partial q_1(T)}{\partial q_1}\right)^2 + \left(\frac{\partial q_1(T)}{\partial p_1}\right)^2.
\]
On the other hand we also have,

\[
\frac{\partial v(T)}{\partial v_1} = \frac{1}{\sqrt{2}} \left( \frac{\partial}{\partial q_1} + i \frac{\partial}{\partial p_1} \right) \frac{1}{\sqrt{2}} (q_1(T) - ip_1(T)) \\
= \frac{1}{2} \left( \frac{\partial q_1(T)}{\partial q_1} + \frac{\partial p_1(T)}{\partial p_1} \right) + i \frac{1}{2} \left( \frac{\partial q_1(T)}{\partial p_1} - \frac{\partial p_1(T)}{\partial q_1} \right) \\
= \frac{\partial q_1(T)}{\partial q_1} + i \frac{\partial q_1(T)}{\partial p_1} 
\]

(B.3)

and, therefore,

\[
\det \Lambda = \left| \frac{\partial v(T)}{\partial v_1} \right|^2. 
\]

(B.4)

Finally, using the second of equations (A.2) with \( v' = v_1 \), and differentiating with respect to \( v(T) \),

\[
\frac{\partial v_1}{\partial v(T)} = i \frac{\partial^2 S}{\partial v' \partial v(T)} 
\]

(B.5)

which implies

\[
\det \Lambda = \left| i \frac{\partial^2 S}{\partial v' \partial v(T)} \right|^2 = |M_{vv}|^2 
\]

(B.6)

by equation (A.4).

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Figure Caption:

Figure 1. (color online) The right panels show the exact and semiclassical wavefunctions for several values of $T$. The thin continuous line (red) displays the exact result obtained via split operator method; the thick solid line is the CIVR approximation and the dashed line (green) shows the result obtained in ref. [14] by direct computation of contributing trajectories. For $T = 2.5$ we also show the potential ($V(x)/10$) and the energy $E = 2.0$ of the central trajectory (shown as $E/10$). The left panel shows the contributing and non-contributing initial trajectories as white and dark areas respectively. The star indicates the positions $q_0$ and $p_0$ of the initial wavepacket.
