Approximate formulas for expectation values using coherent states

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Received April 7, 2017; Revised August 22, 2017; Accepted August 26, 2017; Published October 24, 2017

For time-independent Hamiltonians, the dynamics of quantum expectation values of observables in coherent states $\bar{A}_T$ can be easily represented as an integral formula involving forward and backward propagators $K_\pm$. In the semiclassical regime, an approximate formula $\bar{A}_{sc}^T$ can be constructed via the replacement of $K_\pm$ by their semiclassical versions, followed by a consistent integration procedure. Alternatively, one can keep the original propagators and rewrite the integral formula for $\bar{A}_T$ as a truncated series expansion, thus introducing a new approximate formula $\bar{A}_{se}^T$. Yet a third approximation $\bar{A}_{cl}^T$ can be derived by use of a classical statistical approach based on the Liouville equation and Gaussian probability distributions. In the present paper, we develop these three approximate formulas for expectation values, apply them to simple systems, and evaluate their accuracy.

Subject Index A02, A60

1. Introduction

Semiclassical techniques applied to quantum dynamics are quite ubiquitous. Usually, their cornerstone is the propagator, written as a function of classical trajectories, an idea that was initially developed by van Vleck [1] and later improved by Gutzwiller [2]. Such a semiclassical propagator is an approximation for its quantum partner in the position representation and is widely known by the scientific community, including the nonspecialized part of it. Arguing, in a parallel manner, that coherent-states are more appropriate for semiclassical studies because of their natural connection with classical phase-space, and also considering that they have a simpler extension when, e.g., spin degrees of freedom are included, approximations for the quantum propagator in the coherent-state representation have been derived in the literature (Refs. [3–8]). These results have been shown to be very useful for the description of time-dependent phenomena, with direct application to propagation of wave-packets in a number of physical systems (Refs. [9–15]).

In this context, one should also mention other relevant expressions that are closely related to the coherent-state semiclassical propagator, namely, its initial value representations (Refs. [16–25]). Their most important advantage is that, while the propagator depends on classical trajectories with mixed (initial- and final-time) boundary conditions, the initial value representations avoid the so-called root search problem by means of an integration over classical trajectories determined exclusively by initial conditions.

Although this brief survey illustrates how important coherent-state-based semiclassical approaches are in describing dynamical behavior, there are only a few works using this machinery to deal with
expectation values (Refs. [26–33]). In particular, the methods used in all these articles essentially involve concepts related to initial value representations. As expectation values depend not only on the time-evolution operator, but also on its conjugate, backward (in time) trajectories naturally emerge from the formalism. The quantity of interest is therefore expressed essentially as the sum of contributions of combined forward–backward trajectories. In addition, it is important to mention other alternative semiclassical approaches in phase-space that also address the same issue. In, e.g., Refs. [34,35], using the Weyl–Wigner formalism, the authors have written expectation values of operators as an ℏ-series expansion and then evaluated the contribution of its first terms. In another approach (Ref. [36]), a proper association between the Ehrenfest theorem and Heller’s thawed Gaussian approximation was established in order to define average trajectories.

We point out that none of the above works on semiclassical expectation values explicitly identify a backward semiclassical coherent-state propagator in their methods. In the present paper, we employ both the backward and the forward semiclassical propagators to study quantum averages. We follow, to some extent, the mathematical framework put forward recently for the study of entanglement in the semiclassical regime (Refs. [15,37]). More precisely, our goal is to develop approximations for the dynamics of expectation values of arbitrary ordered operators \( \hat{A}_0 \equiv A_0(\hat{a}^\dagger, \hat{a}) \), assuming that the initial state of the (one-dimensional) system of interest is a coherent state \( |z_0\rangle \). The expression ordered operators means that, in each term of the polynomial function \( A_0 \), operators \( \hat{a}^\dagger \) are always disposed to the left side of \( \hat{a} \). Under the action of a time-independent Hamiltonian \( \hat{H} \), the mean value

\[
\bar{A}_T \equiv \langle z_0 | \exp(i\hat{H}T/\hbar) \hat{A}_0 \exp(-i\hat{H}T/\hbar) |z_0 \rangle ,
\]

with \( T \) the evolution time, can be written in terms of the forward (\( \xi = +1 \)) and backward (\( \xi = -1 \)) coherent-state quantum propagators

\[
K_\xi (z_\eta, z_\mu, T) \equiv \langle z_\eta | \exp (-i\xi \hat{H}T/\hbar) |z_\mu \rangle ,
\]

according to

\[
\bar{A}_T = \int d^2z_2 \frac{d^2z_1}{\pi} K_- (z_0, z_2, T) A_0(z_2^*, z_1) \langle z_2 | z_1 \rangle K_+ (z_1, z_0, T) ,
\]

where

\[
A_0(z_2^*, z_1) = \frac{\langle z_2 | \hat{A}_0 | z_1 \rangle}{\langle z_2 | z_1 \rangle} , \quad \text{with} \quad \langle z_2 | z_1 \rangle = \exp \left( -\frac{1}{2} |z_1|^2 + z_2^* z_1 - \frac{1}{2} |z_2|^2 \right) .
\]

Here the Hamiltonian \( \hat{H} \equiv H(\hat{a}^\dagger, \hat{a}) \) refers to one-dimensional systems, but extensions of the present formalism to greater degrees of freedom can be straightforwardly derived. To find the integral expression (3), we used the coherent-state completeness relation

\[
1 = \int \frac{d^2z}{\pi |z|} \langle z | z \rangle = \int \frac{d[\text{Re}(z)]}{\pi} \frac{d[\text{Im}(z)]}{\pi} |z| \langle z | z \rangle = \int \frac{dz dz^*}{2\pi i} |z| \langle z | z \rangle .
\]

Throughout the paper, we will use the following definitions for the annihilation and creation operators:

\[
\hat{a} = \frac{1}{\sqrt{2}} \left( \frac{\hat{q}}{b} + i \frac{\hat{p}}{c} \right) \quad \text{and} \quad \hat{a}^\dagger = \frac{1}{\sqrt{2}} \left( \frac{\hat{q}}{b} - i \frac{\hat{p}}{c} \right) ,
\]
where \( b = (\hbar/m\omega_0)^{1/2} \), \( c = (m\hbar\omega_0)^{1/2} \), \( \hat{q} \) and \( \hat{p} \) are the position and momentum operators, respectively, \( m \) is the mass of the particle under study, and \( \omega_0 \) is an independent parameter representing the frequency of the harmonic oscillator for which the coherent state is defined. There are a number of excellent textbooks studying these particular states, among which we suggest Refs. [38–40].

Equation (3) is the starting point for the derivation of two of our main results. The first one is achieved by replacing the exact propagators by their semiclassical versions in the integrand of Eq. (3), so that the integral becomes appropriate to be evaluated by the steepest descent method (Ref. [41]). As we will discuss opportunely, the resulting formula is excessively simple and similar to the Ehrenfest theorem. Actually, given the nature of the approximating method and since only one classical trajectory is involved in this formula, this approach can also be termed a kind of Gaussian approximation. Our second treatment for Eq. (3) consists of transforming it into a formal exact series expansion to be consistently truncated, thus giving rise to an alternative approximation. Finally, a conceptually different approximation is devised that makes use of a classical statistical formalism. It should be emphasized that such a classical treatment closely follows other initiatives in the literature developed to study different questions (Refs. [42–44]). All three approximate formulas are then compared with the exact quantum result for some emblematic physical systems.

The paper is organized as follows. In Sect. 2, we present the semiclassical formulas for the forward and backward coherent-state propagators, which will be used in our approximations of \( \bar{A}_T \). After that, in Sect. 3, the methods used to evaluate \( \bar{A}_T \) are discussed, while in Sect. 4, they are illustrated with some case studies. Section 5 is reserved for our final remarks.

2. Semiclassical coherent-state propagator

The semiclassical formula for both forward (\( \xi = +1 \)) and backward (\( \xi = -1 \)) quantum propagators in the coherent-state representation (2), as introduced in Refs. [15,37], is written as

\[
K_\xi(z^*, z_\mu, T) = \sum_{c.t.} \mathcal{P}_{\xi} \exp \left( \frac{i}{\hbar} \left( S_{\xi} + G_{\xi} \right) - \Lambda \right),
\]

where the sum runs over classical trajectories, which, in terms of the auxiliary variables \( u \) and \( v \), are solutions of the Hamilton equations

\[
\frac{\partial \tilde{H}}{\partial u} = -i\hbar \dot{v} \quad \text{and} \quad \frac{\partial \tilde{H}}{\partial v} = i\hbar \dot{u}.
\]

The semiclassical Hamiltonian is defined by \( \tilde{H}(v, u) \), with \( \tilde{H}(z^*, z) = \langle z|\tilde{H}|z \rangle \). In addition, trajectories contributing to Eq. (6) must satisfy the boundary conditions

\[
u' = z_\mu \quad \text{and} \quad v'' = z^*_\eta, \quad \text{for} \quad \xi = +1,
\]

\[
u' = z_\mu \quad \text{and} \quad v'' = z^*_\eta, \quad \text{for} \quad d\xi = -1,
\]

where single (double) prime refers to initial (final) time.

Before proceeding, some comments about the nature of the contributing trajectories are opportune. First, notice that Eqs. (7) and (8) completely define the trajectories to be considered in the sum of Eq. (6). Also, the independent variables of the problem are \( z^*_\eta, z_\mu, \) and \( T \). From them, classical trajectories are evaluated, which, used in Eq. (6), determine the value of \( K_\xi \). More than one trajectory may exist for a given set \( (z^*_\eta, z_\mu, T) \), which explains the existence of the sum in \( K_\xi \). Because in general \( u(t) \) and \( v(t) \) are not complex conjugates of each other, these solutions are said to be \textit{complex}.
trajectories. In some particular instances in which \( u(t) = v^*(t) \), these solutions constitute real trajectories, since we can conveniently change variables in such a way that they would live in a real phase-space. Contrarily, when \( u(t) \neq v^*(t) \), we can consider either a real phase-space whose dimension is twice the original one, or a complex phase-space. We also point out that \( u \) and \( v \) have no \( \xi \) index attached because the context in general implies no doubt about which propagator is being used. In case of potential confusion, their differences will be explicitly indicated.

The complex action \( S_\xi = S_\xi(z_\eta^*, z_\mu, T) \) and the function \( G_\xi = G_\xi(z_\eta^*, z_\mu, T) \) depend on the classical trajectories according to

\[
\frac{i}{\hbar} S_\xi = \xi \int_0^T \left[ \frac{1}{2} (u'v - v'u) - \frac{i}{\hbar} \dddot{H} \right] dt + \tilde{\Lambda} \quad \text{and} \quad \frac{i}{\hbar} G_\xi = \frac{\xi}{2} \int_0^T \left( i \frac{\partial^2 \dddot{H}}{\partial u \partial v} \right) dt. \tag{9}
\]

The elements \( \Lambda \), which account for the normalization, and \( \tilde{\Lambda} \), are given by

\[
\Lambda = \frac{1}{2} (|z_\eta|^2 + |z_\mu|^2) \quad \text{and} \quad \tilde{\Lambda} = \frac{1}{2} (u'v' + u''v'') . \tag{10}
\]

It should be emphasized that \( \mathcal{K}_\xi \) explicitly depends on \( z_\eta \) and \( z_\mu^* \) only by means of \( \Lambda \). That is, the nonnormalized semiclassical coherent-state propagator

\[
\kappa_\xi \equiv e^{\Lambda \mathcal{K}_\xi} \tag{11}
\]

is a function of \( z_\eta^* \) and \( z_\mu \) only. Lastly, we write the prefactor \( \mathcal{P}_\xi \) as

\[
\mathcal{P}_\xi = \left( \frac{i}{\hbar} \frac{\partial^2 S_\xi}{\partial z_\mu \partial z_\eta^*} \right)^{1/2}, \tag{12}
\]

which concludes the description of all terms appearing in formula (6).

Differentiating \( S_\xi \), we obtain a result that will prove important for the present work:

\[
\frac{i}{\hbar} \frac{\partial S_\xi}{\partial z_\mu} = \begin{cases} v' & \text{for } \xi = +1, \\ v' & \text{for } \xi = -1, \end{cases} \quad \text{and} \quad \frac{i}{\hbar} \frac{\partial S_\xi}{\partial z_\eta^*} = \begin{cases} u'' & \text{for } \xi = +1, \\ u' & \text{for } \xi = -1. \end{cases} \tag{13}
\]

It also follows that \( \frac{\partial S_\xi}{\partial T} = -\xi \dddot{H}(v', u') = -\xi \dddot{H}(v'', u'') \). Equation (13), in particular, allows us to write second derivatives of \( S_\xi \) in terms of elements of the stability matrix \( \mathbf{M} \), which is defined as

\[
\begin{pmatrix} \delta u'' \\ \delta v'' \end{pmatrix} = \mathbf{M} \begin{pmatrix} \delta u' \\ \delta v' \end{pmatrix} = \begin{pmatrix} M_{uu} & M_{uv} \\ M_{vu} & M_{vv} \end{pmatrix} \begin{pmatrix} \delta u' \\ \delta v' \end{pmatrix}, \tag{14}
\]

where \( \delta u' \) and \( \delta v' \) are arbitrarily small initial displacements around the classical trajectory, while \( \delta u'' \) and \( \delta v'' \) represent their propagation until the final time \( T \). It can be proved (Ref. [15]) that

\[
\mathcal{P}_\xi = \begin{cases} (M_{vv}^{-1})^{1/2} & \text{for } \xi = +1, \\ (M_{uu}^{-1})^{1/2} & \text{for } \xi = -1, \end{cases} \tag{15}
\]

which is clearly more appropriate for numerical studies. For completeness and future convenience, we write down other relations involving second derivatives of \( S_\xi \):

\[
\frac{i}{\hbar} \frac{\partial^2 S_+}{\partial z_\eta^* \partial z_\eta^*} = M_{uv} \quad \text{and} \quad \frac{i}{\hbar} \frac{\partial^2 S_-}{\partial z_\mu \partial z_\mu} = M_{uu}, \tag{16}
\]

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For the harmonic oscillator and free particle Hamiltonians, the results obtained from Eq. (6) are completely equivalent to those achieved via full quantum mechanical calculation. In what follows, we will briefly review the semiclassical propagators for these systems. More interestingly, we will discuss an application involving the quartic oscillator, in which case the results do not perfectly agree with the exact calculation. This study not only illustrates the modus operandi of Eq. (6), but also paves the way for the next calculations concerning expectation values.

2.1. Free particle

Using the definitions (5), one may write the free-particle Hamilton operator as

$$\hat{H}_{fp} = \frac{\hat{p}^2}{2m} = -\frac{\hbar \omega_0}{4} \left( \hat{a}^\dagger \hat{a}^\dagger + \hat{a} \hat{a} - 2 \hat{a}^\dagger \hat{a} - 1 \right).$$

The corresponding semiclassical Hamiltonian is simply

$$\tilde{H}_{fp} = \frac{-1}{4} \hbar \omega_0 (v^2 - 2uv + u^2 - 1).$$

The equations of motion (7) then become

$$\frac{\omega_0}{2} (u - v) = i \dot{v} \quad \text{and} \quad \frac{\omega_0}{2} (u - v) = i \dot{u}.$$  \hspace{1cm} (19)

Although the trajectories contributing to both $K_{\pm}$ are governed by the same equations of motion, their boundary conditions are distinct in general. As can be straightforwardly checked, for a given set $(z_\mu^*, z_\mu, T)$ only one trajectory contributes to $K_+$, while another one contributes to $K_-$. The sum appearing in Eq. (6), in this case, consists of only one term. Using these results, we find that

$$K_{fp}^{\xi}(z_\mu^*, z_\mu, T) = e^{-\Lambda} \frac{1}{(1 + \xi \alpha)^{1/2}} \exp \left\{ \frac{z_\mu}{2} \left( \frac{z_\mu + \xi \alpha z_\mu}{1 + \xi \alpha} \right) + \frac{z_\mu^*}{2} \left( \frac{z_\mu^* + \xi \alpha z_\mu^*}{1 + \xi \alpha} \right) \right\},$$

where $\alpha \equiv i \omega_0 T / 2$. This formula coincides with the exact one.

2.2. Harmonic oscillator

For the harmonic oscillator, the quantum and the semiclassical Hamiltonians are respectively given by

$$\hat{H}_{ho} = \frac{\hat{p}^2}{2m} + \frac{1}{2} m \omega_0 \hat{q}^2 = \hbar \omega_0 \left( \hat{a}^\dagger \hat{a} + \frac{1}{2} \right) \quad \text{and} \quad \tilde{H}_{ho} = \hbar \omega_0 \left( vu + \frac{1}{2} \right),$$

where the oscillation frequency is chosen to be the same as the parameter $\omega_0$ of the creation and annihilation operators (see Eq. (5)). Equations of motion (7) reduce to

$$-\omega_0 v = i \dot{v} \quad \text{and} \quad \omega_0 u = i \dot{u},$$

which can be easily solved. By imposing boundary conditions (8), we again find only one trajectory contributing to each propagator. It follows that

$$K_{ho}^{\xi}(z_\mu^*, z_\mu, T) = \exp \left\{ -\frac{i \omega_0 \xi T}{2} - \frac{1}{2} |z_\mu|^2 + z_\mu z_\mu^* \right\} \exp \left( -\frac{i \omega_0 \xi T}{2} - \frac{1}{2} |z_\mu|^2 \right).$$

As well as for the free particle model, the semiclassical propagator is equivalent to the exact one. In fact, for these two systems, this agreement could be anticipated since the Hamiltonians are at most
quadratic. Given that the expansions involved in the deduction of Eq. (6) are polynomials of second degree, the procedure turns out to be exact rather than approximate. The complete correspondence between the exact propagator $K_\xi$ and the semiclassical one $\mathcal{K}_\xi$ is not verified when nonlinear terms appear in the Hamiltonian, which is the case for the quartic model introduced next.

2.3. **Quartic oscillator**

The last model to be studied is the quartic oscillator, whose semiclassical regime has already been discussed in Refs. [14,45] with different approaches. Its Hamiltonian reads

$$\hat{H}_{qo} = \zeta \left( \frac{\hat{p}^2}{2m} + \frac{1}{2} m \omega^2_0 q^2 \right)^2 = \zeta \hbar^2 \omega^2_0 \left( \hat{a}^+ \hat{a}^+ \hat{a} \hat{a} + 2 \hat{a}^+ \hat{a} + c \right),$$

(24)

with $c = 1/4$ and $\zeta$ a parameter whose dimension is inverse energy. The semiclassical Hamiltonian to be used in the calculation is now given by

$$\tilde{\hat{H}}_{qo} = \frac{\hbar \omega}{2} \left[ (1 + uv)^2 + c - 1 \right],$$

(25)

where we introduce $\tilde{\omega} = 2 \xi \hbar \omega^2_0$. The equations of motion read

$$-\tilde{\omega}(1 + uv)v = i\dot{v} \quad \text{and} \quad \tilde{\omega}(1 + uv)u = i\dot{u},$$

(26)

which clearly render $uv$ constant. Then, we find

$$u_\pm(t) = A_\pm \exp (-i\tilde{\omega}(1 + A_\pm B_\pm)t) \quad \text{and} \quad v_\pm(t) = B_\pm \exp (+i\tilde{\omega}(1 + A_\pm B_\pm)t),$$

(27)

where $A_\pm$ and $B_\pm$ are arbitrary constants to be determined by the imposition of boundary conditions (8). In contrast to the last two examples, here one may find more than one trajectory for a given set $(\tilde{z}_n, \tilde{z}_\mu, T)$. To check this, we use Eq. (8) to conclude that $A_+ = \tilde{z}_\mu$ and $B_- = \tilde{z}_n^\ast$. However, finding $B_+$ and $A_-$ is more involved. They should satisfy

$$A_- \exp \left(-i\tilde{\omega}\tilde{z}_n^\ast A_- T\right) = \tilde{z}_\mu \exp (+i\tilde{\omega}T) \quad \text{and} \quad B_+ \exp \left(+i\tilde{\omega}\tilde{z}_\mu B_+ T\right) = \tilde{z}_n^\ast \exp (-i\tilde{\omega}T),$$

(28)

which are transcendental equations with many solutions, in general. Writing the numerical values of $A_-$ ($B_+$) obtained from the first (second) equation as $a_n (b_n^\ast)$, where each solution is labeled by $n$, we find that the trajectories contributing to Eq. (6) are formally given by

$$u_+^{(n)}(t) = \tilde{z}_\mu \exp \left(-i\tilde{\omega}(1 + \tilde{z}_\mu b_n^\ast)t\right) \quad \text{and} \quad v_+^{(n)}(t) = b_n^\ast \exp \left(+i\tilde{\omega}(1 + \tilde{z}_\mu b_n^\ast)t\right),$$

$$u_-^{(n)}(t) = a_n \exp \left(-i\tilde{\omega}(1 + a_n \tilde{z}_n^\ast)t\right) \quad \text{and} \quad v_-^{(n)}(t) = \tilde{z}_n^\ast \exp \left(+i\tilde{\omega}(1 + a_n \tilde{z}_n^\ast)t\right).$$

(29)

These expressions can be inserted in the functions $S_\xi$ and $G_\xi$. On the other hand, writing the prefactor $\mathcal{P}_\xi$ explicitly in terms of the trajectories is not straightforward. Through Eq. (28), we may consider that $b_n^\ast = b_n^\ast(\tilde{z}_n^\ast, \tilde{z}_\mu)$ and $a_n = a_n(\tilde{z}_n^\ast, \tilde{z}_\mu)$, so that their differentiation leads to

$$\frac{\partial b_n^\ast}{\partial \tilde{z}_n^\ast} = \frac{b_n^\ast}{\tilde{z}_n^\ast} \left( \frac{1}{1 + i\tilde{\omega} b_n^\ast T} \right), \quad \frac{\partial b_n^\ast}{\partial \tilde{z}_\mu} = \left( \frac{-i\tilde{\omega}(b_n^\ast)^2 T}{1 + i\tilde{\omega} b_n^\ast T} \right),$$

$$\frac{\partial a_n}{\partial \tilde{z}_\mu} = \frac{a_n}{\tilde{z}_\mu} \left( \frac{1}{1 - i\tilde{\omega} a_n^\ast T} \right), \quad \frac{\partial a_n}{\partial \tilde{z}_n^\ast} = \left( \frac{i\tilde{\omega} a_n^\ast T^2}{1 - i\tilde{\omega} a_n^\ast T} \right).$$

(30)
Using the last equation, the prefactor can be easily found by means of Eq. (12). Therefore,

\[ K_{\xi}^{q_{0}} = \exp \left( -\frac{i}{2} (c - 1) \xi \tilde{\omega} T - \Lambda \right) \]

\[ \times \sum_{n} \left[ \gamma_{n}^{\xi} \left( \frac{1}{z_{\mu}^{} z_{\eta}^{\xi}} \right) \right]^{1/2} \exp \left( \left[ \frac{i \tilde{\omega} T}{2} \gamma_{n}^{\xi} + (1 + i \xi \tilde{\omega} T) \right] \gamma_{n}^{\xi} \right), \]  

(31)

where \( \gamma_{n}^{+} \equiv z_{\mu} b_{n}^{*} \) and \( \gamma_{n}^{-} \equiv a_{n} z_{\eta}^{*} \). Before reporting the exact calculation, it is instructive to analyze the last expression in the limit \( T \to 0 \). In the extremal case \( T = 0 \), we have only one solution for Eq. (28), which implies \( \gamma_{n}^{\pm} = z_{\mu} z_{\eta}^{*} \), so that Eq. (31) clearly becomes \( \langle \gamma_{n}^{\xi} | z_{\mu} \rangle_{\xi} \), as expected. For finite but small \( T \), if we keep only terms of order \( T \) in Eq. (28), we find again just one solution for the transcendental equation, which implies \( \gamma_{n}^{\xi} = z_{\mu} z_{\eta}^{*} \left[ 1 - i \xi \tilde{\omega} \left( 1 + z_{\mu} z_{\eta}^{*} \right) T \right] + O(T^2) \). Inserting it into Eq. (31) we find

\[ K_{\xi}^{q_{0}} = \langle \gamma_{n}^{\xi} | z_{\mu} \rangle_{\xi} \exp \left( -i \xi \tilde{H} (z_{\mu}^{*}, z_{\mu}) T / \hbar \right) + O(T^2). \]  

(32)

This result can be shown to agree with the exact result. Then we can be assured that \( K_{\xi}^{q_{0}} \) is satisfactorily accurate for sufficiently short times.

Concerning the exact calculation, we can write \( K_{\xi}^{q_{0}} \) as the series

\[ K_{\xi}^{q_{0}} = \langle \gamma_{n}^{\xi} | z_{\mu} \rangle_{\xi} \exp \left( -\frac{i \xi \tilde{\omega} T (\hat{a}^{+} \hat{a}^{\xi} + \frac{1}{2})^{2} \right) |z_{\mu}\rangle \]

\[ = \exp \left( -\frac{i \xi \tilde{\omega} T}{2} - \Lambda \right) \sum_{m=0}^{\infty} \frac{(z_{\mu} z_{\eta}^{*})^{m}}{m!} \exp \left( -\frac{i \xi \tilde{\omega} T}{2} m (m + 1) \right), \]  

(33)

which cannot be resummed in general. In particular, by setting \( T = \tilde{T} \equiv 2\pi j / \tilde{\omega} \), with \( j \) integer, we can show that the last expression yields the periodicity relation \( |K_{\xi}^{q_{0}} (z_{\mu}^{*}, z_{\mu}, \tilde{T})| = |K_{\xi}^{q_{0}} (z_{\mu}^{*}, z_{\mu}, 0)| \). Clearly, numerical calculation is needed for a more precise comparison between \( K_{\xi}^{q_{0}} \) and \( K_{\xi}^{q_{0}} \). However, in what follows we will see that this step is not mandatory for the study of expectation values, which are the quantities of interest in the present paper.

### 3. Expectation values

#### 3.1. Quantum formula

To infer the quality of the approximate formulas to be developed in this work, we will make direct comparisons with the exact result. Thus, we start this section by explicitly stating what we regard as the exact quantum mean value. From now on, contrary to the procedure implemented in Sect. 2, the starting point is a classical Hamiltonian and an arbitrary function, whose quantum counterparts are derived via the following quantization rule.

Consider a canonically conjugated pair \((x, y)\), with quantum counterpart \((\hat{x}, \hat{y})\) and commutation relation \([\hat{x}, \hat{y}]\) resulting in a complex number. The quantum operator corresponding to a classical function \(x^{n} y^{m}\) is given by \(Q_{\xi,\hat{\xi}} [\hat{x}^{n} \hat{y}^{m}]\), where the quantizer

\[ Q_{\xi,\hat{\xi}} \equiv \exp \left( -\frac{1}{2} [\hat{x}, \hat{y}] \partial_{\hat{x}} \partial_{\hat{y}} \right) = \sum_{k=0}^{\infty} \left( -\frac{1}{2} [\hat{x}, \hat{y}] \right)^{k} \frac{\partial_{\hat{x}}^{k}}{k!} \frac{\partial_{\hat{y}}^{k}}{k!} \]  

(34)

is a differential operator that acts on \(\hat{x}^{n} \hat{y}^{m}\) without changing the ordering. As an example, consider the quantization of \(q^{2} p\). According to the above rule, the corresponding quantum operator is given
by $Q_{\hat{q}, \hat{p}}[\hat{q}^2 \hat{p}] = \hat{q}^2 \hat{p} - i\hbar \hat{q}$. It can be checked that this Hermitian operator corresponds to the ordered expression of the symmetrized version $\frac{1}{2} \left( \hat{q}^2 \hat{p} + \hat{p} \hat{q} \hat{p} + \hat{p} \hat{q}^2 \right)$ of $\hat{q}^2 \hat{p}$. (The interested reader is referred to Ref. [46] for further details and examples related to this quantization rule.)

Let $\hat{A}(q, p)$ be a function that does not depend explicitly on time. Because our approach is concerned with coherent states, it is convenient to work with the variables $(z^*, z)$ instead of $(q, p)$. We then use the parametrization

$$z(q, p) = \frac{1}{\sqrt{2}} \left( \frac{q}{(\hbar/m\omega_0)^{1/2}} + i \frac{p}{(\hbar/m\omega_0)^{1/2}} \right),$$

with the numerical choice $m\omega_0 = 1$, to establish the relation

$$\hat{A}(z^*, z) \equiv \hat{A}(q(z^*, z), p(z^*, z)).$$

Assume that the classical function can be expanded as

$$\hat{A}(z^*, z) = \sum_{n,m} a_{nm} z^{*n} z^m,$$

for $a_{nm} = a_{nm}^*$. Applying the quantizer $Q_{\hat{a}^\dagger, \hat{a}}$ to the above expression gives

$$\hat{A}(\hat{a}^\dagger, \hat{a}) \equiv Q_{\hat{a}^\dagger, \hat{a}}[\hat{A}(\hat{a}^\dagger, \hat{a})] = \sum_{n,m} a_{nm} \left[ \exp \left( \frac{i}{\pi} \delta_{\hat{a}^\dagger} \delta_{\hat{a}} \right) (\hat{a}^\dagger)^n \hat{a}^m \right].$$

Using the Heisenberg operators $(\hat{a}_T, \hat{a}_T^\dagger) = \hat{U}_T (\hat{a}, \hat{a}^\dagger) \hat{U}_T^\dagger$, with $\hat{U}_T = \exp (-iHT/\hbar)$, we finally write the exact formula for the quantum expectation value as

$$\langle z_0 | \hat{U}_T^\dagger \hat{A}(\hat{a}^\dagger, \hat{a}) \hat{U}_T | z_0 \rangle = \langle z_0 \left[ \exp \left( \frac{i}{\pi} \delta_{\hat{a}^\dagger} \delta_{\hat{a}} \right) \hat{A}(\hat{a}_T^\dagger, \hat{a}_T) \right] | z_0 \rangle.$$

The quantum Hamiltonian is obtained through the same quantization process. We apply the quantizer $Q_{\hat{a}^\dagger, \hat{a}}$ to $\mathcal{H}(z^*, z) = \sum_{n,m} h_{nm}(z)^n z^m$ to obtain

$$\hat{H} = Q_{\hat{a}^\dagger, \hat{a}}[\mathcal{H}(\hat{a}^\dagger, \hat{a})] = \exp \left( \frac{i}{\pi} \delta_{\hat{a}^\dagger} \delta_{\hat{a}} \right) \mathcal{H}(\hat{a}^\dagger, \hat{a}).$$

We are now ready to introduce the main contribution of this work. Next, we present a classical counterpart for the quantum expectation value (39), followed by the derivation of its two distinct approximate formulas.

### 3.2. Classical statistical approximation

Consider a classical time-independent Hamiltonian $\tilde{H}(q, p)$ inducing the time evolution of a generic phase-space point $(q, p)$ into $(Q, P)$, with $Q(q, p, T)$ and $P(q, p, T)$ solutions of the Hamilton equations with respective initial values $q = Q(q, p, 0)$ and $p = P(q, p, 0)$. Let $\tilde{A}(q, p)$ be a time-independent function. Its time evolution is governed by $d\tilde{A}/dT = \{\tilde{A}, \tilde{H}\}$, where $\{\mathcal{F}_1, \mathcal{F}_2\}$ denotes the Poisson brackets for functions $\mathcal{F}_1$ and $\mathcal{F}_2$ with respect to phase-space coordinates $q$ and $p$.

Now consider the time evolution of an ensemble of phase-space points described by the solution $\rho(q, p, T)$ of the Liouville equation $\partial_T \rho = \{\mathcal{H}, \rho\}$ with initial value

$$\rho(q, p, 0) = \frac{\exp \left[ -\frac{(q - q_0)^2}{\Delta_q^2} \right] \exp \left[ -\frac{(p - p_0)^2}{\Delta_p^2} \right]}{\left( \pi \Delta_q^2 \right)^{1/2} \left( \pi \Delta_p^2 \right)^{1/2}},$$

where $q_0$ and $p_0$ are initial values.
which is a Gaussian probability distribution centered at \((q_0, p_0)\). This choice, along with the identification \(z_0 = z(q_0, p_0)\), is intended to make the link with the coherent states. Also for this reason, the widths \(\Delta_{q,p}\) are chosen to be numerically equal to \(\sqrt{\hbar}\). The classical statistical mean value of \(\hat{A}(q,p)\) is then defined as the ensemble average

\[
\bar{A}_T^\text{cl} = \int dq \, dp \, \rho(q,p,T) \bar{A}(q,p) = \int dq \, dp \, \rho(q,p,0) \bar{A}_c(q,p,T),
\]

where

\[
\bar{A}_c(q,p,T) = \bar{A}(Q(q,p,T),P(q,p,T)).
\]

This function clearly includes information about the classical trajectory that departs from \((q,p)\) and reaches \((Q,P)\) after a time \(T\). The last integral, which can be derived from the fact that the Hamiltonian flow preserves the phase-space volume, i.e., \(dq \, dp = dQ \, dP\), can be expressed in terms of a series representation (see Appendix A for details). By direct application of the identity (A.5), we obtain our classical mean value formula

\[
\bar{A}_T^\text{cl} = \exp \left( \frac{\hbar}{2} \left( \partial_{q_0}^2 + \partial_{p_0}^2 \right) \right) \bar{A}_c(q_0,p_0,T).
\]

Using the parametrization (35), we may introduce

\[
\bar{A}_c(z^*,z,T) = \bar{A}_c(q(z^*,z),p(z^*,z),T),
\]

which allows us to express Eq. (43) as

\[
\bar{A}_T^\text{cl} = \exp \left( \frac{1}{2} \partial_{z^*}^2 \partial_{z_0} \right) \bar{A}_c(z^*_0,z_0,T),
\]

where \(z_0 = z(q_0,p_0)\). Notice that \(\mathcal{A}_c\), in analogy with \(\bar{A}_c\), takes into account the equations of motion of the problem. Also, we learn from the last equation that classical averages via Gaussian probability distributions depend exclusively on the trajectory followed by its central point \((z_0^*,z_0)\).

It is worth noticing that the result \(\bar{A}_T^\text{cl}\) can be derived through a conceptually different scheme. Take the initial function (37). Purely classical evolution leads to \(\mathcal{A}_c(z^*,z,T) = \sum_{n,m} a_{nm}(T)(z^*)^n z^m\), which, by action of \(Q_{\hat{a}^1,\hat{a}}\), is quantized as \(\hat{A}_c(T) = \sum_{n,m} a_{nm}(T) \exp \left( \frac{1}{\hbar} \partial_{\hat{a}^1}^2 \partial_{\hat{a}} \right) (\hat{a}^1)^n \hat{a}^m\). Since this operation preserves normal ordering, we can directly compute \(\langle z_0 | \hat{A}_c(T) | z_0 \rangle\), which turns out to fully reproduce Eq. (45). Thus, we see that the classical statistical mean value and the exact quantum result are obtained, respectively, by the procedures

\[
\begin{align*}
\mathcal{A}_c(z^*,z,T) & \quad \rightarrow \quad \hat{A}_c(T) = Q_{\hat{a}^1,\hat{a}}[\mathcal{A}_c(\hat{a}^1,\hat{a},T)] \\
\mathcal{A}_c(z^*,z,0) & \quad \rightarrow \quad \hat{A}_c(0) = Q_{\hat{a}^1,\hat{a}}[\mathcal{A}_c(\hat{a}^1,\hat{a},0)]
\end{align*}
\]

That is, evolving in time and then quantizing is just an approximation of quantizing and then evolving in time. This remark put in evidence a central difference between the classical statistical approximation and the quantum result.

### 3.3. Saddle point method

Our proposal here is the evaluation of the expectation value using the same kind of approximation involved in the derivation of the semiclassical propagators \(\mathcal{K}_\xi\) (Refs. [7,15]). To this end, we replace
the quantum propagators in Eq. (3) by their semiclassical versions (6), to obtain
\[
\tilde{A}_T^{sc} \equiv \exp \left( - \frac{1}{\hbar} |z_0|^2 \right) \times \int \frac{dz_2^* du''_\pm dv''_\pm dz_1}{2\pi i} A_0(z_2^*, z_1) P_-(z_0^*, u''_\pm, T) P_+(v''_\pm, z_0, T) \exp \left( \frac{1}{\hbar} \mathcal{F} \right), \tag{46}
\]
where
\[
\mathcal{F} \equiv \mathcal{F}(z_2^*, u''_\pm, v''_\pm, z_1, T)
= i h (z_2^* u''_\pm - z_2^* z_1 + v''_\pm z_1) + S_-(z_0^*, u''_\pm, T) + S_+(v''_\pm, z_0, T)
+ G_-(z_0^*, u''_\pm, T) + G_+(v''_\pm, z_0, T).
\]
In the last integral, for simplicity we omitted the sum over the trajectories contributing to \( \mathcal{K}_- \), and similarly to \( \mathcal{K}_+ \). Also, we renamed the original integration variables \( z_2 \) and \( z_1^* \) as \( u''_\pm \) and \( v''_\pm \), respectively, because of their clear interpretation in this framework. In addition, to establish a connection with the results of the previous section, in particular with the quantization process adopted, we should rewrite \( A_0(z_2^*, z_1) \) as
\[
A_0(z_2^*, z_1) = \exp \left( \frac{1}{2} \partial_{z_2^*} \partial_{z_1} \right) A(z_2^*, z_1). \tag{47}
\]
Integral (46) essentially means that, for each point \( (z_2^*, u''_\pm, z_1, v''_\pm) \) of the integration variables, forward and backward semiclassical propagators should be evaluated, so that its integrand can be calculated. Then, the result should be numerically summed over all integration points, implying in the semiclassical expectation value \( \tilde{A}_T^{sc} \). However, this is an extensive procedure that can be avoided by realizing that integral (46) can be approximated by the steepest descent method (Ref. [41]). Actually, as the semiclassical propagators themselves are built by the same method, their inherent inaccuracy makes exact and approximate integrations equivalent. As we will see in the following, the condition for the critical point of integral (46) couples trajectories of both propagators in such a way that the final result becomes a function of only the real trajectory.

The first step of the steepest descent method consists of finding the saddle point \( \tilde{r} = (z_2^*, \tilde{u}''_\pm, \tilde{z}_1, \tilde{v}''_\pm) \), which defines the critical trajectories to be considered in the evaluation of integral (46). Assuming as usual (Ref. [7]) that derivatives of the prefactors can be disregarded renders (46) as
\[
\left( \frac{\partial \mathcal{F}}{\partial z_2^*} \right) |_{\tilde{r}} \delta z_2^* + \left( \frac{\partial \mathcal{F}}{\partial u''_\pm} \right) |_{\tilde{r}} \delta u''_\pm + \left( \frac{\partial \mathcal{F}}{\partial v''_\pm} \right) |_{\tilde{r}} \delta v''_\pm + \left( \frac{\partial \mathcal{F}}{\partial z_1} \right) |_{\tilde{r}} \delta z_1 = 0. \tag{48}
\]
In addition, disregarding derivatives of \( G_\pm \) (Ref. [7]) and applying Eq. (13) we get
\[
\tilde{u}''_\pm = \tilde{z}_1, \quad \tilde{v}''_\pm = \tilde{z}_2^*, \quad \tilde{u}''_\pm = \tilde{z}_1, \quad \tilde{v}''_\pm = \tilde{z}_2^*.
\tag{49}
\]
These four equations imply that \( \tilde{u}''_\mp = \tilde{u}''_\pm = \tilde{z}_1 \) and \( \tilde{v}''_\mp = \tilde{v}''_\pm = \tilde{z}_2^* \), meaning that the final phase-space points of both critical trajectories should be identical. Because they are governed by the same equations of motion, the two trajectories turn out to be one and the same. Since the initial conditions are constrained to \( \tilde{u}_+ = z_0 \) and \( \tilde{v}_- = z_0^* \), the only way to satisfy all these conditions is by considering
a real trajectory, namely, the one defined by \( \bar{u}_+ = \bar{v}_+ = z_0 \) and \( \bar{v}_- = \bar{v}'_+ = z_0^* \). Proceeding with the method, we expand the integral up to second order around \( \bar{r} \) to find

\[
\bar{A}^{sc}_T = A_0 (\bar{v}'', \bar{u}'') \mathcal{P}_- (z_0^*, \bar{u}'', t) \mathcal{P}_+ (\bar{v}'', z_0, t) \int \frac{d[\delta z_2]}{2\pi i} \frac{d[\delta u'']}{2\pi i} \frac{d[\delta v'']}{2\pi i} \exp \left( \frac{1}{2} \delta^2 \mathcal{F} \right),
\]

(50)

where we have defined \( \delta^2 \mathcal{F} \equiv \delta r^T \cdot \mathbf{Q} \cdot \delta r \), with \( \delta r^T \equiv (\delta z_2^*, \delta u'', \delta v'', \delta z_1) \) and

\[
\mathbf{Q} = \begin{pmatrix}
0 & -1 & 0 & 1 \\
-1 & \frac{i \partial^2 S_-}{\hbar \partial u''^2} & 0 & 0 \\
0 & 0 & \frac{i \partial^2 S_+}{\hbar \partial v''^2} & 1 \\
1 & 0 & -1 & 0
\end{pmatrix}.
\]

(51)

The integral appearing in Eq. (50) is a Gaussian integral whose result is \( \left| \det \mathbf{Q} \right|^{-1/2} \exp (i\sigma) \), where \( \sigma \) represents the phase of the integral. Finally, using Eq. (16) and \( M_{uu}M_{vv} - M_{uv}M_{vu} = 1 \), which expresses volume conservation of phase-space flow, we conclude that \( \det \mathbf{Q} = (M_{vv}M_{uu})^{-1} \), so that

\[
\bar{A}^{sc}_T = A_0 (\bar{v}'', \bar{u}''),
\]

(52)

which, by Eq. (47), can be finally written as

\[
\bar{A}^{sc}_T = \exp \left( \frac{1}{2} \partial_{\bar{v}''}^2 \partial_{\bar{u}''} \right) A (\bar{v}'', \bar{u}'').
\]

(53)

Naturally, the question arises of whether one may express \( \bar{A}^{sc}_T \) in terms of the initial conditions \( \bar{v}' = z_0^* \) and \( \bar{u}' = z_0 \). By writing \( \bar{v}'' = \bar{u}'' (z_0^*, z_0, T) \) and \( \bar{v}'' = \bar{v}'' (z_0^*, z_0, T) \) and assuming their inverse, we find

\[
\bar{A}^{sc}_T = \exp \left( \frac{1}{2} \left( \frac{\partial \bar{v}''}{\partial z_0^*} \frac{\partial \bar{z}_0^*}{\partial z_0^*} + \frac{\partial \bar{v}''}{\partial z_0} \frac{\partial \bar{z}_0}{\partial z_0} \right) \right) \bar{A}_c (z_0^*, z_0, T),
\]

(54)

where \( \bar{A}_c (z_0^*, z_0, T) \equiv A (\bar{v}'' (z_0^*, z_0, T), \bar{v}'' (z_0^*, z_0, T)) \) may be different from \( \bar{A}_c (z_0^*, z_0, T) \) (see Eq. (44)), since the former is governed by the semiclassical Hamiltonian \( \hat{H} \), while the latter is governed by \( \mathcal{H} \). To make this difference explicit, we will keep using \( \bar{v}'' \) and \( \bar{u}'' (z''^*, \bar{z}''^*) \) for trajectories derived from \( \hat{H} \) (\( \mathcal{H} \)). Equation (53) is our semiclassical formula for the expectation value (39). As well as for the classical average (45), only the (real) trajectory starting at the central point \( (z_0^*, z_0) \) contributes to \( \bar{A}^{sc}_T \). To some extent, Eq. (54) can be viewed as an expression of the Ehrenfest theorem.

3.3.1. Semiclassical Husimi function

Before closing this section, it is instructive to make a brief digression on the application of the present formalism to the Husimi function. By considering in Eq. (1) the operator \( \hat{A}_0 \) as the operator \( \hat{h} \equiv |z \rangle \langle z| \), the mean value \( \bar{A}_T \) becomes the Husimi function

\[
\bar{h} (z, z_0, T) \equiv \langle z_0 | \exp \left( i\hat{HT} / \hbar \right) | z \rangle \langle z | \exp \left( -i\hat{HT} / \hbar \right) | z_0 \rangle = | K_+ (z, z_0, T) |^2.
\]

(55)

1 According to the Ehrenfest theorem \( m \frac{d^2 \hat{q}}{dt^2} (\hat{q}) = -\langle \partial_\hat{q} V (\hat{q}) \rangle \), the short-time dynamics of a particle of mass \( m \) subjected to an arbitrary potential \( V (\hat{q}) \) is approximately governed by Newton’s second law \( m \frac{d^2 \hat{q}}{dt^2} (\hat{q}) \equiv -\partial_\hat{q} V (\langle \hat{q} \rangle) \), whenever the initial state is sufficiently sharp. The bridge with our result (53) is made by setting \( \hat{A}(q, p) = q \), so that \( \langle \hat{q} \rangle (T) \approx \bar{A}^{sc}_T = \left( \frac{1}{2} \right)^{1/2} (v'' + u'') = q'' \).
For this particular case, our semiclassical formula (53) becomes completely useless because the semiclassical version of $h(z, z_0, T)$ is simply $|K_+(z^*, z_0, T)|^2$, which is an expression much richer than Eq. (53), since it generally includes contributions from more than one trajectory, as illustrated by Refs. [9,47].

The natural question then arises about the possibility of writing $\hat{h}$ in the polynomial form $\hat{A}_0 = \sum_{n,m} c_{n,m}(\hat{d}^\dagger)^n\hat{d}^m$, which a priori would imply the validity of Eq. (53) also for the semiclassical version of $h(z, z_0, T)$. Actually, we can investigate this issue by expressing matrix elements of $\hat{h}$ and $\hat{A}_0$ in the usual number basis,

$$\langle j | \hat{h} | k \rangle = \frac{z_j^* z_k^j}{j!k!} \exp (-|z|^2) \quad \text{and} \quad \langle j | \hat{A}_0 | k \rangle = \sum_{l=\mu}^k c_{j-k+l,l} j!l! k! \left(\frac{1}{(k-l)!}\right)^{\frac{1}{2}},$$

where $\mu$ is the maximum between 0 and $(k-j)$. If we now equate these terms, for any value of $j$ and $k$, we can, in principle, recursively\footnote{We can take $j = 0$ to find $c_{0,0}$, then we take $j = 1$ to find $c_{1,0}$, and so on.} find all coefficients $c_{n,m}$ for the polynomial form of $\hat{h}$. This suggests that $|K_+(z^*, z_0, T)|^2$ as well as Eq. (53) can be directly used as semiclassical approximations of $h(z, z_0, T)$. However, it is clear that the former is better than the latter, because $|K_+(z^*, z_0, T)|^2$ admits contributions from more than one trajectory.

Although the last paragraph seems to imply that Eq. (53) can be used to semiclassically approximate $\hat{h}$, we now argue that it is an inappropriate application. The point to be defended demonstrates that, for the operator $|z\rangle\langle z|$, the term $A_0(z_2^*, z_1)\langle z_2|z_1\rangle$ of Eq. (3) is indeed a separable function of $z_1$ and $z_2$, as expressed by Eq. (53) rewritten as

$$h(z, z_0, T) = \int \frac{d^2z_2}{\pi} \frac{d^2z_1}{\pi} K_-(z_0, z_2, T) \langle z_2|z\rangle \langle z_2|z_1\rangle K_+(z_1, z_0, T).$$

The semiclassical evaluation of this integral, via the saddle point method, clearly implies in critical finding critical trajectories, making it even harder.

3.4. Series representation

Now we develop a formal series expansion for the expectation value $\hat{A}_T$. We start by writing Eq. (3) as

$$\hat{A}_T = \exp (-|z_0|^2) \times \int \frac{d^2z_2}{\pi^2} \frac{d^2z_1}{\pi^2} \exp (-|z_1|^2 - |z_2^*|^2 + z_2^* z_1) A_0(z_2^*, z_1) k_-(z_0^*, z_2, T) k_+(z_1^*, z_0, T), \quad (56)$$
where \( k_\xi = e^{i \xi K_\xi} \) are nonnormalized quantum propagators corresponding to the exact versions of Eq. (11). Writing the integration variables as a function of the real and imaginary parts of \( z_1 \) and \( z_2 \) (see Eq. (35)) and defining

\[
\Phi \equiv A_0(z_1^*[q_2, p_2], z_1[q_1, p_1]) \: k_-(z_0^*, z_2[q_2, p_2], T) \: k_+(z_1^*[q_1, p_1], z_0, T) \\
\times \exp \left( z_2^*(q_2, p_2) \: z_1(q_1, p_1) \right),
\]

we have

\[
\tilde{A}_T = \exp \left( -|z_0|^2 \right) \\
\times \int \frac{dq_1 dq_2 dp_1 dp_2}{(2\pi \hbar)^2} \exp \left( -\frac{1}{2\hbar} \left( q_1^2 + p_1^2 + q_2^2 + p_2^2 \right) \right) \Phi(p_1, q_1, p_2, q_2, T).
\]

We now employ again the results proved in Appendix A. Direct application of Eq. (A.5) allows us to rewrite Eq. (58) as

\[
\tilde{A}_T = \exp \left( -|z_0|^2 \right) \left[ \exp \left( \frac{1}{2} \left( \partial_{z_1^*} \partial_{z_1} + \partial_{z_2^*} \partial_{z_2} \right) \right) \cdot k_-(z_0^*, z_2, T) \: k_+(z_1^*, z_0, T) \: \Phi(z_2^* z_1) \right]_{(p_1, q_1, p_2, q_2) = 0},
\]

which, in terms of the original variables, can be written as

\[
\tilde{A}_T^{\text{se}} = \exp \left( -|z_0|^2 \right) \\
\times \left[ \exp \left( \partial_{z_1^*} \partial_{z_1} \right) \exp \left( \partial_{z_2^*} \partial_{z_2} \right) \cdot k_-(z_0^*, z_2, T) \: k_+(z_1^*, z_0, T) \: \Phi(z_2^* z_1) \right]_{(p_1, q_1, p_2, q_2) = 0},
\]

with \( A_0(z_2^*, z_1) \) given by Eq. (47) and \( z = (z_2^*, z_2, z_1^*, z_1) \). Observe that in writing Eq. (60b) we have artificially introduced the integer \( N \) to truncate the series and thus obtain an approximate formula. In fact, had we kept \( N \to \infty \), then we would have just an alternative representation for the exact expectation value, i.e., \( \lim_{N \to \infty} A_T^{\text{se}} = \tilde{A}_T \). It follows that the quality of the approximation \( A_T^{\text{se}} \) must proportionally increase with \( N \).

Expression (60) can be further simplified by noticing that \( \partial_{z_1^*} \) and \( \partial_{z_2^*} \) act only on the nonnormalized propagators \( k_\pm \) whereas \( \partial_{z_1} \) and \( \partial_{z_2} \) act only on the term \( \exp \left( z_2^* z_1 \right) \cdot A_0(z_2^*, z_1) \). Then, by use of the identity \( \left[ \exp \left( \partial_{x} \partial_{y} \right) f(x) \: g(y) \right]_{x=0} = f(\partial_{y}) \: g(y) \), one shows that Eq. (60) can be written as

\[
\tilde{A}_T^{\text{se}} = \exp \left( -|z_0|^2 \right) \left[ \exp \left( \partial_{z_1^*} \partial_{z_1} \right) \: A_0(\partial_{z_2}, \partial_{z_2^*}) \: k_-(z_0^*, z_2, T) \: k_+(z_1^*, z_0, T) \right]_{(z_2^*, z_2) = 0},
\]

where it should be understood that \( \exp \left( \partial_{z_1^*} \partial_{z_1} \right) \approx \sum_{n=0}^{N} (\partial_{z_1^*} \partial_{z_1})^n / n! \), with a given truncation integer \( N \). As for the result (60), here we have that \( \lim_{N \to \infty} \tilde{A}_T^{\text{se}} = \tilde{A}_T \).

4. Applications

Formulas (39), (45), (53), and (60) define our machinery to study expectation values. Here we provide some instructive examples while discussing other defining features of our approach. For each physical system, we start with a classical Hamiltonian \( \mathcal{H}(q(z^*, z), p(z^*, z)) \), which generates the Hamilton operator \( \hat{H}(\hat{a}^\dagger, \hat{a}) \) through the action of \( \mathcal{Q}_{\hat{a}^\dagger, \hat{a}} \). Then, with pertinent choices of classical and quantum initial conditions, we compute all the aforementioned formulas. The comparison of the
results will be conducted for the following specific quantities:

(i) the position $q$, achieved by adopting $A(z^*, z) = (\hbar/2)^{1/2} (z^* + z)$, so that

$$
\langle q \rangle_{cl} = \left( \frac{\hbar}{2} \right)^{1/2} \exp \left( \frac{1}{2} \partial_{z_0} \partial_{\bar{z}_0} \right) (z''^* + z''),
$$

(ii) the quadratic function $q^2$, for which $A(z^*, z) = (\hbar/2)(z^* + z^2) + z + z^2$ and

$$
\langle q^2 \rangle_{cl} = \frac{\hbar}{2} \exp \left( \frac{1}{2} \partial_{z_0} \partial_{\bar{z}_0} \right) (z''^* + z'')^2,
$$

$$
\langle q^2 \rangle_{qm} = \frac{\hbar}{2} (z_0 | \hat{a}_T^+ + \hat{a}_T | z_0),
$$

$$
\langle q^2 \rangle_{sc} = \frac{\hbar}{2} \left[ (\bar{v}'' + \bar{u}'')^2 + 1 \right],
$$

(iii) the cubic function $q^3 p$, such that $A(z^*, z) = i \left( \hbar^3 / 8 \right)^{1/2} (z^* + z^2 - z^2 + z^3)$,

$$
\langle q^3 p \rangle_{cl} = \frac{i \sqrt{\hbar^3}}{2 \sqrt{2}} \left[ \exp \left( \frac{1}{2} \partial_{z_0} \partial_{\bar{z}_0} \right) (z''^* + z''^2 + z''^3),
$$

$$
\langle q^3 p \rangle_{qm} = \frac{i \sqrt{\hbar^3}}{2 \sqrt{2}} (z_0 | \hat{a}_T^+ \hat{a}_T \hat{a}_T^* + \hat{a}_T \hat{a}_T^* \hat{a}_T + \hat{a}_T \hat{a}_T^* \hat{a}_T^* | z_0),
$$

$$
\langle q^3 p \rangle_{sc} = \frac{i \sqrt{\hbar^3}}{2 \sqrt{2}} \left[ (\bar{v}'' + \bar{u}')^2 + (\bar{v}'' + \bar{u}')^3 + \bar{v}''^2 - \bar{u}'' \right],
$$

$$
\langle q^3 p \rangle_{se} = C \left[ (\partial_{z_2}^2 \partial_{z_1}^2 z_2^* - \partial_{z_2} \partial_{z_2} z_1^* - \partial_{z_2} \partial_{z_2} z_1^* - \partial_{z_2} \partial_{z_2} z_2^*) \exp \left( \partial_{z_1} \partial_{z_2} \right) \bar{k}_- \bar{k}_+ \right]_{z_1 = z_2 = 0}.
$$

In Eqs. (62d), (63d), and (64d), we introduced $\bar{k}_- \equiv k_- (z_0^*, z_2, T)$, $\bar{k}_+ \equiv k_+ (z_1^*, z_0, T)$, and the constant term $C \equiv i (\hbar/2)^{3/2} \exp (-|z_0|^2)$. Finally, recall that the series method prescribes that $\exp \left( \partial_{z_1} \partial_{z_2} \right) \cong \sum_{n=0}^N (\partial_{z_1} \partial_{z_2})^n / n!$, for a given truncation integer $N$.

4.1. Harmonic oscillator

Given the classical Hamiltonian $H_{cl} = \frac{p^2}{2m} + \frac{1}{2} m \omega_0^2 q^2 = \hbar \omega_0 z^2$, where Eq. (35) was used, we solve the corresponding equations of motion to find $z'' = z_0 \exp (-i \omega_0 T)$ and its complex conjugate. Because $\partial_{z_0} \partial_{\bar{z}_0} = \partial_{z''} \partial_{\bar{z}''}$, we can write Eq. (45) as

$$
\bar{A}_T^{cl} = \exp \left( \frac{1}{2} \partial_{z''} \partial_{\bar{z}''} \right) A(z''^*, z'').
$$
As far as the quantum result is concerned, we first apply the prescription (40) to the classical Hamiltonian $H_{ho}$ to obtain $\hat{H}_{ho} = \hbar \omega_0 (\hat{a}^\dagger \hat{a} + \frac{1}{2})$. Given that the Heisenberg solution for the dynamics is $\hat{a}_T = \hat{a} \exp (-i\omega_0 T)$, we obtain from Eq. (39) that

$$\bar{A}_T = \bar{A}_T^{cl}. \quad (66)$$

For the semiclassical result, since $H_{ho}$ and $\tilde{H}_{ho}$ differ only by a constant term, we have $\tilde{u}'' = z''$ and $\tilde{v}'' = z''^*$. Then, it follows from Eq. (53) that

$$\bar{A}_T^{sc} = \bar{A}_T. \quad (67)$$

Finally, as far as the series approximation (60) is concerned, we have used the propagators (23) and performed numerical calculations for several values of $\hbar$ and $N$. These studies have shown that $\bar{A}_T^{se}$ succeeded in reproducing $\bar{A}_T$ with arbitrarily high accuracy, for all quantities investigated, whenever the number $N$ of terms in the series was taken to be sufficiently large, which roughly means that $N$ should increase with $\hbar^{-1}$ (in agreement with the criteria (A.8) discussed in Appendix A). That is, the smaller the numerical value of $\hbar$ the greater $N$ has to be in order for the series approximation to yield a good mimic of the quantum expectation value. The same behavior was observed for other systems, as we will illustrate later.

To a certain extent, the good agreement among the results is not surprising, since expectation values in coherent states constitute a privileged framework for the harmonic oscillator dynamics. In any case, this was a necessary consistency test for our approach.

4.2. Free particle

For this case study, it is instructive to start with a function $A_{nm} \equiv z^n z^m$, where $n$ and $m$ are integers, which can be thought of as the $n$th term of the series expansion of a generic function $A(z^*, z)$. Taking the classical Hamiltonian $H_{fp} = \frac{p^2}{2m} = -\frac{1}{4} \hbar \omega_0 (z^* - z)^2$, we can show that

$$z'' = (1 - \alpha) z_0 + \alpha z^*_0 \quad \text{and} \quad z''^* = (1 + \alpha) z_0^* - \alpha z_0, \quad (68)$$

where $\alpha = i\omega_0 T/2$. From Eq. (45) it follows that

$$\bar{A}_T^{cl} = \exp \left( \frac{1}{2} \partial_{z_0}^* \partial_{z_0} \right) \left[ (1 + \alpha) z_0^* - \alpha z_0 \right]^n \left[ (1 - \alpha) z_0 + \alpha z_0^* \right]^m, \quad (69)$$

which turns out to be identical to the quantum result (39), as we demonstrate in Appendix B. On the other hand, since $H_{fp}$ and $\tilde{H}_{fp}$ differ from each other by only a constant term, $\tilde{v}'' = z''^*$ and $\tilde{u}'' = z''$, and the semiclassical expression (53) reads

$$\bar{A}_T^{sc} = \exp \left( \frac{1}{2} \left[ \alpha (1 - \alpha) \partial_{z_0}^2 + (1 - 2\alpha^2) \partial_{z_0} \partial_{z_0} - \alpha (1 + \alpha) \partial_{z_0}^2 \right] \right)$$

$$\times \left[ (1 + \alpha) z_0^* - \alpha z_0 \right]^n \left[ (1 - \alpha) z_0 + \alpha z_0^* \right]^m. \quad (70)$$

Except for $T = 0$, for an arbitrary pair $(n, m)$, $\bar{A}_T^{sc}$ is clearly different from $\bar{A}_T^{cl} = \bar{A}_T$. Concerning the formula (60), we have made an effort to compare it (in the limit $N \to \infty$) with the analytical results.
given above. In Appendix C (Eq. (C.6)) we present the detailed algebra that allows us to write

\[
\lim_{N \to \infty} \tilde{A}_T^\text{sc} = \exp\left(-|z_0|^2 - \frac{\alpha z_0^2}{2(1-\alpha)} + \frac{\alpha z_0^2}{2(1+\alpha)}\right) \frac{1}{(1-\alpha^2)^{1/2}} \exp\left(\frac{1}{2} \left[ \alpha(1+\alpha)\partial_{z_0}^2 - \alpha(1-\alpha)\partial_{z_0}^2 \right] \right)
\times \exp\left(\frac{|z_0|^2}{1-\alpha}\right) \exp\left(\frac{1}{2}(1-\alpha^2)\partial_{z_0}^2 \frac{z_0^n}{(1-\alpha)^n} \frac{z_0^m}{(1+\alpha)^m}\right),
\]

which does not show any apparent equivalence with either \(\tilde{A}_T = \tilde{A}_T^\text{cl}\) or \(\tilde{A}_T^\text{sc}\).

On closer inspection, we found a scenario in which the semiclassical approximation becomes very accurate. Consider the short time regime \(\left(|z_0| = \frac{|q_0 + \omega_0|}{\sqrt{2\hbar}} \ll 1 \text{ or, equivalently, } \hbar \to 0\right)\). In this case, we can neglect second-order terms such as \(\alpha \partial_{\tilde{z}_0}^2\), \(\alpha \partial_{\tilde{z}_0}^2\), and \(\alpha \partial_{\tilde{z}_0} \partial_{\tilde{z}_0}\) in the above expressions and then show that \(\tilde{A}_T^\text{sc} \cong \tilde{A}_T^\text{cl} = \tilde{A}_T\). The series approximation, though, is different. Setting \(n = m\), for simplicity, we can further manipulate the expressions to obtain

\[
\tilde{A}_T = \tilde{A}_T^\text{cl} = \tilde{A}_T^\text{sc} \cong \exp\left(\frac{1}{2} \partial_{\tilde{z}_0}^2 \partial_{\tilde{z}_0} \right) \left[ |z_0|^2 \exp\left(\alpha \left(\frac{z_0}{z_0} - \frac{z_0}{z_0^2}\right) \right) \right]^m,
\]

\[
\lim_{N \to \infty} \tilde{A}_T^\text{sc} \cong \exp\left(\alpha |z_0|^2 \left[ 1 - \frac{1}{2} \left(\frac{z_0}{z_0} - \frac{z_0}{z_0^2}\right) \right] \right) \exp\left(\frac{1}{2} \partial_{\tilde{z}_0}^2 \partial_{\tilde{z}_0} \right) |z_0|^{2m},
\]

which reveal some peculiarities of \(\tilde{A}_T^\text{sc}\) in relation to the other formulas. In particular, given that the initial function now reads \(\tilde{A}_n = |z|^{2m}\), we see differences on the sequence of application of the time evolution and the Gaussian smoothing \(\exp\left(\frac{1}{2} \partial_{\tilde{z}_0}^2 \partial_{\tilde{z}_0}\right)\).

To further illustrate the differences among the methods, in Fig. 1, for an initial configuration \(z_0 = (1 + i)/\sqrt{\hbar}, \omega_0 = 1\), and \(\hbar = 0.3\), we show the dynamics of expectation values for \(q, q^2\), and \(\alpha^2 \rho\) (in panels (a), (b), and (c), respectively), as defined in Eqs. (62)–(64). We verify that, while the semiclassical mean position reproduces its equivalent quantum result for all shown values of \(T\) (Fig. 1a), averages over the other functions deteriorate with \(T\) (Figs. 1b and 1c). In general, numerics has shown that the semiclassical approximation \(\tilde{A}_T^\text{sc}\) is very accurate for short times but gets increasingly worse as time runs, in agreement with the analysis conducted above. Figure 1 also shows the behavior of \(\tilde{A}_T^\text{sc}\) for \(N = 65\), i.e., we have kept only the first 65 terms in the series expansion of \(\exp\left(\partial_{\tilde{z}_0}^2 \partial_{\tilde{z}_0}\right)\) (see Eqs. (62d), (63d), and (64d)). Clearly, the approximation is very accurate for short times but rapidly becomes worthless, which signals that the truncation integer \(N\) is not large enough for providing a good description in this time scale.

To check the \(\hbar\)-dependence of our approximations, we present in Fig. 2 numerical calculations of \(\langle q^2 \rho \rangle_{\text{se}}\) for \(\hbar = 0.7\) and \(\hbar = 0.07\) (in panels (a) and (b), respectively). As expected, the semiclassical approximation improves as \(\hbar\) diminishes. On the other hand, the series approximation gets worse, which is not surprising since the simulations have been performed with \(N\) fixed. As discussed previously in Sect. 3.4, the series representation is more likely to succeed for \(N\) increasing with \(\hbar^{-1}\). This behavior is also analyzed in Appendix A, where Eq. (A.8) in particular clearly stresses this question. In panel (c), we illustrate this point by fixing \(\hbar = 0.3\) and comparing \(\langle q^2 \rho \rangle_{\text{qm}}\) with \(\langle q^2 \rho \rangle_{\text{se}}\) for different values of \(N\).

Before closing this case study, a final comment is in order. With regard to \(\tilde{A}_T^\text{sc}\), its discrepancies with the exact results seem to be, a priori, surprising, since there is no reason why the saddle point method should imply any deviation from the exact formula for the null potential. However, we recall
Fig. 1. Free-particle expectation value as a function of time $T$ for (a) $q$, (b) $q^2$, and (c) $q^2p$. The black solid line refers to the exact quantum result $\bar{A}_T = \bar{A}_{T}^{qm}$ (which coincides with the blue dashed curve in panel (a)), while the approximate formulas $\bar{A}_{T}^{sc}$ and $\bar{A}_{T}^{se}$ are given by the blue dashed and green dot-dashed lines, respectively. To evaluate the latter, we set $N = 65$ in Eqs. (62d), (63d), and (64d). The initial configuration amounts to $z_0 = (1 + i)/\sqrt{\hbar}$. Also, we used $\omega_0 = 1$ and $\hbar = 0.3$. All physical quantities are plotted in arbitrary units throughout the paper.

Fig. 2. Free-particle expectation value as function of time $T$ for the cubic function $q^2p$, for (a) $\hbar = 0.7$ and (b) $\hbar = 0.07$. Other relevant parameters are $z_0 = (1 + i)/\sqrt{\hbar}$ and $\omega_0 = 1$. Black solid, blue dashed, and green dot-dashed lines refer respectively to $\langle q^2p \rangle_{qm}$, $\langle q^2p \rangle_{sc}$, and $\langle q^2p \rangle_{se}$. Again, we used $N = 65$ to evaluate $\langle q^2p \rangle_{se}$. In panel (c), adopting $\hbar = 0.3$, we compare $\langle q \rangle_{qm}$ (black solid line) with $\langle q \rangle_{se}$, for $N = 45$ (green dot-dashed), $N = 55$ (violet dashed), and $N = 65$ (red dotted).

that, in the approach of Sect. 3.3, the prefactor appearing in integral (46) was taken as a constant term. This procedure is generally acceptable because any gain from its precise treatment would dissipate due to the inaccuracy inherited from the exponential terms of the integral (Ref. [41]). But, as there is no such exponential error for the free particle case (see Sect. 2.2), one may conclude that the exact treatment of the prefactor would render perfect agreement with $\bar{A}_{T}^{qm}$. Indeed, we have verified that this is precisely what happens when we perform the complete calculation (omitted due to its very particular character).

4.3. Quartic oscillator

Finally, we examine the quartic oscillator model, whose classical Hamiltonian reads

$$\mathcal{H}_{qo} = \zeta \left( \frac{p^2}{2m} + \frac{1}{2}m\omega_0^2q^2 \right) = \zeta \hbar^2 \omega_0^2 z^2 + \frac{\zeta}{2} \hbar \omega_0^2 z.$$

(72)

Following our prescription, we obtain the Hamilton operator for this system:

$$\hat{\mathcal{H}}_{qo} = \zeta \hbar^2 \omega_0^2 \left( \hat{a}^\dagger \hat{a}^\dagger \hat{a} \hat{a} + 2 \hat{a}^\dagger \hat{a} + \frac{1}{2} \right),$$

(73)

which differs from that studied in Sect. 2.3 only by a constant factor. The semiclassical Hamiltonian $\hat{\mathcal{H}}_{qo}$, which here also differs from $\mathcal{H}_{qo}$, is given by Eq. (25) with $c = \frac{1}{2}$. Trajectories contributing to
the classical expectation value $\tilde{A}_T^{cl}$ are given by

$$z'' = z_0 \exp\left(-i\tilde{\omega}|z_0|^2 T\right) \quad \text{and} \quad z''^* = z_0^* \exp\left(+i\tilde{\omega}|z_0|^2 T\right),$$

while those contributing to $\tilde{A}_T^{se}$ read

$$\tilde{u}'' = z_0 \exp\left(-i\tilde{\omega}(1 + |z_0|^2) T\right) \quad \text{and} \quad \tilde{v}'' = z_0^* \exp\left(+i\tilde{\omega}(1 + |z_0|^2) T\right),$$

where $\tilde{\omega} = 2\zeta \hbar \omega_0^2$. For the term $A_{nm} \equiv z^n z^m$ of the series expansion of a generic function $A(z^n, z)$, we have

$$\tilde{A}_T^{se} = \exp\left(\frac{1}{2} \partial_{z_0} \partial_{z_0}^*\right) \{\tilde{\omega}''(\tilde{u}'')^m \exp (2\nu(1 + |z_0|^2)) \exp \left(\frac{1}{2} \partial_{z_0} \partial_{z_0}^*\right) z_0^n z_0^m\}.$$  (77)

Concerning the quantum result, we can write annihilation and creation operators in the Heisenberg picture as

$$\hat{a}_T = \exp\left(-i\tilde{\omega}(1 + \hat{a}_T^\dagger \hat{a}_T) T\right) \hat{a} \quad \text{and} \quad \hat{a}_T^\dagger = \hat{a}^\dagger \exp\left(+i\tilde{\omega}(1 + \hat{a}_T^\dagger \hat{a}_T) T\right),$$  (78)

so that Eq. (39) for the function $A(\hat{a}_T^\dagger, \hat{a}_T) = (\hat{a}_T^\dagger)^n (\hat{a}_T)^m$ reduces to

$$\tilde{A}_T = \exp \left(|z_0|^2 (1 - \exp (2\nu)) + \nu(n + m + 1)\right) \exp \left(\frac{1}{2} \exp (-2\nu) \partial_{z_0} \partial_{z_0}^*\right) z_0^n z_0^m.$$  (79)

Finally, from this expression we obtain the series approximation $\tilde{A}_T^{se}$ by expanding $\exp \left(\frac{1}{2} \exp (-2\nu) \partial_{z_0} \partial_{z_0}^*\right)$ in power series up to the $N$th term.

For an effective comparison among Eqs. (76), (77), (79), and $\tilde{A}_T^{se}$, a numerical calculation is convenient. Again, we restrict our analysis to the expectation values presented in Eqs. (62), (63), and (64), which can be computed with the help of the expressions provided above. In Fig. 3, we show the mean values as functions of time for $q$ (panels (a) and (b)), $q^2$ (panel (c)), and $q_T^2 p$ (panel (d)). For their calculation, the initial configuration is characterized by $z_0 = (1 + i)/\sqrt{T}$, with $\epsilon_0 = \zeta = 1$ and $\hbar = 0.3$. We see that the quantum mean values are characterized by oscillating structures that vanish and eventually reappear. This quantum recurrence (visible in panels (b), (c), and (d) for $T \approx 10$, $T \approx 5$, and $T \approx 3$, respectively) is due to wave-packet interference, a phenomenon that cannot be described with single-trajectory-based classical theories (Refs. [9,14,47]). In this regard, the results indeed show that even though both $\tilde{A}_T^{cl}$ and $\tilde{A}_T^{se}$ are rather good approximations to $\tilde{A}_T$ for very short times, the classical one being satisfactory even for relatively longer times, they clearly fail to reproduce the quantum recurrence. The performance of $\tilde{A}_T^{se}$, on the other hand, is shown to be highly satisfactory even for $N = 20$. Notice that this value is considerably smaller than the one used in the free-particle problem ($N = 65$). No visible difference from the exact result was observed within the time scale investigated and even the quantum recurrence was perfectly reproduced.

Finally, in Fig. 4 we show that both $\tilde{A}_T^{cl}$ and $\tilde{A}_T^{se}$ get better and better as $\hbar$ decreases. As for the previous figure, the classical approximation is accurate for longer times but neither $\tilde{A}_T^{cl}$ nor $\tilde{A}_T^{se}$ is able...
Fig. 3. Expectation values for the quartic oscillator as a function of time $T$ for position $q$ (panels (a) and (b)), its square $q^2$ (panel (c)), and the cubic function $q^2p$ (panel (d)). The black solid line refers to the exact quantum result $\hat{A}_T$, which in this case is indistinguishable from $\hat{A}_T^{se}$ evaluated with $N = 20$ (see Eqs. (62d), (63d), and (64d)). The approximate formulas $\hat{A}_T^{cl}$ and $\hat{A}_T^{sc}$ are given by the dotted red and dashed blue lines, respectively. The initial configuration for these calculations amounts to $z_0 = (1 + i)/\sqrt{\hbar}$. Also, we used $\omega_0 = 1$ and $\hbar = 0.3$.

Fig. 4. Expectation values for the quartic oscillator as a function of time $T$ for the cubic function $q^2p$, for (a) $\hbar = 0.03$ and (b) $\hbar = 0.003$. Other relevant parameters are $z_0 = (1 + i)/\sqrt{\hbar}$ and $\omega_0 = 1$. Black solid, red dotted, and blue dashed lines refer respectively to $\langle q^2p \rangle_{qm}$, $\langle q^2p \rangle_{cl}$, and $\langle q^2p \rangle_{sc}$.

to reproduce the quantum recurrence (not shown in the figure). It is also interesting to note that while the semiclassical shape does not change appreciably as $\hbar$ decreases, the shape of both the quantum and the classical statistical curves tend to the semiclassical one. This is because all these quantities coalesce to a classical Hamiltonian function as $\hbar \to 0$. We explicitly verified that this is indeed the case by computing the classical trajectories $q(T)$ and $p(T)$ directly from the Hamiltonian (72) with
\[ \zeta = \omega_0 = m = 1 \text{ and } q_0 = p_0 = \sqrt{2}. \] We found that

\[ \lim_{\hbar \to 0} \langle q^2 p \rangle_{qm} = \lim_{\hbar \to 0} \langle q^2 p \rangle_{se} = \lim_{\hbar \to 0} \langle q^2 p \rangle_{cl} = \lim_{\hbar \to 0} \langle q^2 p \rangle_{sc} = q^2(T)p(T), \tag{80} \]

and similarly for the quantities \( q \) and \( q^2 \). Actually, we expect this to be the case for all expectation values and all physical systems that admit the classical formulation.

5. Final remarks

In this work, based on the coherent state representation, we investigated the dynamics of general quantum expectation values \( \bar{A}_T \). Essentially, we studied three approximate expressions for this quantity. First, we presented a classical statistical formula \( \bar{A}_T^{cl} \), by use of the Liouville formalism equipped with a classical Hamiltonian \( \mathcal{H} \) and a Gaussian probability distribution. We showed that \( \bar{A}_T^{cl} \) depends on the trajectory defined by the time evolution induced by \( \mathcal{H} \) for the center of the initial distribution.

Second, a semiclassical approximation \( \bar{A}_T^{sc} \) was achieved by implementing the limit \( \hbar \to 0 \) through the saddle point method. The resulting formula depends exclusively on the trajectory described by the center of the state, governed by a semiclassical Hamiltonian \( \tilde{H} \). Third, we rewrote \( \bar{A}_T \) as a series expansion that, upon appropriate truncation, became our series approximation \( \bar{A}_T^{se} \).

In order to evaluate the quality of the approximate formulas, we made comparisons with the exact quantum expectation value \( \bar{A}_T \) for some emblematic physical models, namely (i) the harmonic oscillator, (ii) the free particle, and (iii) the quartic oscillator. The classical statistical formula \( \bar{A}_T^{cl} \), which is conceptually based on an ensemble of classical trajectories, was perfect in describing systems (i) and (ii) and relatively successful for the short-time regime in (iii). It presents itself as a good approximation for dynamics that do not involve any sort of exclusively quantum effects, such as quantum recurrence. The semiclassical formula \( \bar{A}_T^{sc} \), which exhibits a simple formulation in terms of a single trajectory, also performed perfectly for (i) and rather accurately for (ii). However, for the nonlinear dynamics of (iii), it proved accurate only for very short times and, therefore, was unable to reproduce quantum recurrence. Its main advantage relies on the fact that \( \bar{A}_T^{sc} \) demands the simplest calculation of all formulas, so it figures as the best candidate for quick estimates. The series approximation \( \bar{A}_T^{se} \) in turn performed rather accurately in reproducing quantum recurrence even for a relatively small number of terms in the series. Also, because it is actually just a different representation of the exact quantum result, it will always work as long as we take a sufficiently large number of terms in the series. Typically, \( N \) should increase with \( \hbar^{-1} \) and, presumably, also with \( T^{-1} \) in more general cases. A drawback of this method in relation to the other two is that it is more demanding computationally, although its formulation is given in terms of derivatives only.

With regard to \( \bar{A}_T^{sc} \), it is worth mentioning that, according to the literature (see, e.g., Refs. [9,14,47]), the semiclassical approximations employed in this work can eventually account for interference phenomena provided more than one trajectory is involved. This observation delineates a clear framework for improving the semiclassical formula and constitutes, therefore, a fruitful idea for future work.

Acknowledgements

R.M.A. and A.D.R. acknowledge financial support from the National Institute for Science and Technology of Quantum Information (INCT-IQ/CNPq). We are also grateful to an anonymous referee for pointing out the need for a better understanding of the eventual application of our results to the Husimi function.
Appendix A. Series representation of an integral

Consider a Gaussian smoothing of some function \( f(x) \), i.e.,

\[
I_1(x_c) = \int_{-\infty}^{\infty} dx \frac{\exp \left( \frac{-(x-x_c)^2}{a} \right)}{\sqrt{\pi a}} f(x),
\]

(A.1)

with \( a \) a positive real number. Expanding \( f(x) \) in Taylor series around \( x_c \) gives

\[
I_1(x_c) = \sum_{n=0}^{\infty} \left[ \int_{-\infty}^{\infty} dx \frac{\exp \left( \frac{-(x-x_c)^2}{a} \right)}{\sqrt{\pi a}} \frac{(x-x_c)^n}{n!} \right] \frac{\partial^n f(x_c)}{\partial x^n}.
\]

(A.2)

Noticing that only even terms survive within the sum, we immediately arrive at

\[
I_1(x_c) = \left[ \exp \left( \frac{a^2}{4} \right) f(x) \right]_{x=x_c}.
\]

(A.3)

The generalization for multiple integrals is straightforward. Consider the \( n \)-dimensional smoothing

\[
I_n(\vec{x}_c) = \int d^n\vec{x} \frac{\exp \left( \frac{-(\vec{x}-\vec{x}_c)^2}{a} \right)}{(\pi a)^{n/2}} f(\vec{x}),
\]

(A.4)

where \( \vec{x} = (x_1, \ldots, x_n) \) is an \( n \)-dimensional real vector, \( d^n\vec{x} = dx_1 \ldots dx_n \), and \( f(\vec{x}) \) is some analytic function. Given that all integration variables are mutually independent, we just apply the Gaussian smoothing (A.3) successively to obtain

\[
I_n(\vec{x}_c) = \left[ \exp \left( \frac{a^2}{4} \nabla^2 \right) f(\vec{x}) \right]_{\vec{x}=\vec{x}_c},
\]

(A.5)

which constitutes a formal expression for the action of an infinite power series of the Laplacian \( \nabla^2 \equiv \partial^2_{x_1} + \ldots + \partial^2_{x_n} \) on the function \( f(\vec{x}) \).

It is clear from Eq. (A.3) that if \( f(x) \) is a polynomial function, then the application of \( \exp \left( \frac{a^2}{4} \partial^2_{x} \right) \) exactly results in a finite series. However, the usefulness of the formula (A.3) extends to more general functions. The crux here is that when \( a \) is sufficiently small, we can expand the differential operator \( \exp \left( \frac{a^2}{4} \partial^2_{x} \right) \) in power series, retain only the leading terms, and thus still get a finite series. Of course, this will be possible only if the series converges. To assess the convergence of the infinite series associated with the formula (A.3), we write \( I_1(x_c) = \sum_n \frac{1}{n!} \left( \frac{a^2}{4} \right)^n f(x_c) \equiv \sum_n s_n(x_c) \) and apply the ratio test

\[
\lim_{n \to \infty} \left| \frac{s_n}{s_{n-1}} \right| < 1.
\]

From this, we conclude that the series will converge only if

\[
n > \left| \frac{a}{4} \right| \left. \frac{\partial^2 f(x)}{\partial x^2} \right|_{x=x_c}.
\]

(A.6)

Of particular interest to this work is the exponential function \( f(x) = \exp \left( \frac{x^2}{b} \right) \), which helps us to understand a defining feature of the series approximation as applied to the calculation of expectation values. As far as the criterion (A.6) is concerned, we may introduce the dimensionless coordinate
Appendix B. Free-particle quantum expectation values

With them, it is straightforward to show that

\[
  n > \frac{a^2}{\hbar^2} x_c^2 \quad \text{for } x_c \to \infty,
\]

\[
  n > (n - \frac{1}{2}) \frac{|a|}{|b|} \quad \text{for } x_c \to 0.
\]

Typically, in applications involving coherent states and the propagator, one has that \( a = b = \hbar \) (see, e.g., Eq. (60)), in which case the above formulas can be written

\[
  n > \frac{x_c^2}{\hbar} \quad \text{for } h \to 0,
\]

\[
  n > n - \frac{1}{2} \quad \text{for } h \to \infty.
\]

Thus, while for large \( h \) the series will generally converge, for small \( h \) (semiclassical regime) the series will converge only if the number of its terms is greater than \( O(h^{-1}) \). Therefore, in this regime we had better not truncate the series to a smaller number of terms.

Appendix B. Free-particle quantum expectation values

The Heisenberg creation and annihilation operators for the free-particle model read

\[
  \hat{a}_T^\dagger = \beta^* \hat{a}_T^\dagger + \alpha^* \hat{a} \quad \text{and} \quad \hat{a}_T = \beta \hat{a} + a \hat{a}_T^\dagger,
\]

where \( \alpha \equiv i \omega_0 T/2 \) and \( \beta \equiv 1 - \alpha \). To evaluate Eq. (39) for the function \( \mathcal{A}_{nm} \equiv z^n z_m^* \), we write

\[
  \exp \left( \frac{1}{2} \partial_{\hat{a}_T} \partial_{\hat{a}_T^\dagger} \right) (\hat{a}_T^\dagger)^n (\hat{a}_T)^m = \sum_{k=0}^{\min[n,m]} \frac{n!m!}{2^k(n-k)!(m-k)!} (\alpha \hat{a}_T^\dagger + \beta \hat{a})^{n-k} (\alpha^* \hat{a}_T + \beta^* \hat{a})^k.
\]

Since we want to compute the average of this operator with the coherent state \( |z_0\rangle \), it is convenient to write it in normal ordering. To this end, we employ the following identities. First, we have

\[
  (\alpha \hat{a}_T^\dagger + \beta \hat{a})^{m-k} = \sum_{s=0}^{m-k} \frac{(m-k)!}{(m-k-s)!s!} \frac{\alpha^{m-k-s} \beta^s}{(m-k-s)!} \exp \left( \frac{1}{2} \partial_{\hat{a}_T} \partial_{\hat{a}_T^\dagger} \right) (\hat{a}_T^\dagger)^{m-k-s} \hat{a}^s
\]

and the analogous for \( (\beta^* \hat{a}_T^\dagger + \alpha^* \hat{a})^{n-k} \). Second, it is useful to write

\[
  \hat{a}_T^\dagger (\hat{a}_T^\dagger)^n = \exp \left( \partial_{\hat{a}_T^\dagger} \partial_{\hat{a}_T} \right) (\hat{a}_T^\dagger)^n \hat{a}_T^\dagger.
\]

With them, it is straightforward to show that the expectation value

\[
  \langle z_0 | \exp \left( \frac{1}{2} \partial_{\hat{a}_T} \partial_{\hat{a}_T^\dagger} \right) (\hat{a}_T^\dagger)^n (\hat{a}_T)^m | z_0 \rangle
\]

can be written as

\[
  \langle z_0 | \exp \left( \frac{1}{2} \partial_{\hat{a}_T} \partial_{\hat{a}_T^\dagger} \right) (\hat{a}_T^\dagger)^n (\hat{a}_T)^m | z_0 \rangle
  = n!m! \times \sum_{k=0}^{\min[n,m]} \frac{1}{2^k k!} \times \sum_{r=0}^{\min[n-k,r]} \frac{1}{2^r r!} \times \sum_{j=0}^{\min[n-k-r,j]} \frac{1}{2^j j!} \times \sum_{s=0}^{\min[k-m-k-s,s]} \frac{1}{2^s s!}
  \times \left[ \partial_{z_0}^s (\beta^* z_0^* )^r \right] \left[ \partial_{z_0}^{r+p} (\alpha^* z_0)^m \right] \left[ \partial_{z_0}^{l+p} (\alpha z_0^*)^{n-k-s} \right] \left[ \partial_{z_0}^l (\beta z_0)^s \right]
  \times \frac{1}{(n-k-r)!(m-k-s)!}.
\]
By summing first on the indexes $j$ and $l$, and then on $r$ and $s$, we have

$$
\tilde{A}_{TM}^{nm} = \sum_{k=0}^{\min[n,m]} \sum_{p=0}^{\infty} \left[ \exp \left( \frac{1}{2} \partial_{z^0} \partial_{\bar{z}^0} \right) \partial_{z^n} \partial_{\bar{z}^m} \left( z^{n'} \right)^n \right] \left[ \exp \left( \frac{1}{2} \partial_{z^0} \partial_{\bar{z}^0} \right) \partial_{z'^n} \partial_{\bar{z}^m} \left( z^{m'} \right)^m \right] \frac{1}{2^k k!}.
$$

where $z^{n'}$ and $z^{m'}$ are given by Eq. (68). It is convenient now to write $\partial_{z^0} = \beta \partial_{z^0} + \alpha^* \partial_{z^0*}$ and $\partial_{z^0*} = \alpha \partial_{z^0} + \beta^* \partial_{z^0*}$, so that a simple manipulation leads us to

$$
\tilde{A}_{TM}^{nm} = \exp \left( \frac{1}{2} \partial_{z^0} \partial_{\bar{z}^0} \right) z^{n'} z_{m'}^{m'},
$$

which is completely equivalent to the classical average (69).

**Appendix C. Free-particle expectation values using the series expansion**

For the free-particle model, the nonnormalized propagators are written

$$
k^{\text{fp}}_T(z^\eta, z^\mu, T) = \frac{1}{(1 + \xi \alpha)^{1/2}} \exp \left\{ \frac{z_\mu}{2} \left( \frac{z_\eta^* + \xi \alpha z_\mu}{1 + \xi \alpha} \right) + \frac{z_\eta^*}{2} \left( \frac{z_\mu + \xi \alpha z_\eta^*}{1 + \xi \alpha} \right) \right\},
$$

where we recall that $\xi = \pm 1$ and $\alpha = i\omega_0 T/2$. Applying them directly to Eq. (61) and considering $A(z^*, z) = z^n z^m$, we find

$$
\check{A}_T^{\text{sc}} = \sum_{k=0}^{N} \sum_{l=0}^{\min[n,m]} \frac{A_p}{2^l l!} \frac{n!}{(n - l)!} \frac{m!}{(m - l)!} \left[ \partial_{z^2}^{k+n-l} \exp (a z^2 + b z_0^2) \right] \left[ \partial_{z_1}^{k+m-l} \exp (a^* z_1^* + b^* z_1^*) \right] \Bigg|_{z_2 = z_1^* = 0},
$$

where

$$
A_p \equiv \exp \left( -|z_0|^2 + b z_0^2 + b^* z_0^2 \right) \left( 1 - \alpha^2 \right)^{-1/2}, \quad a \equiv \frac{z_0^*}{1 - \alpha}, \quad \text{and} \quad b \equiv \frac{-\alpha}{2(1 - \alpha)}.
$$

Notice that the terms in parentheses are derivatives of a function $f^{(0)}(x) = \exp \left( \eta x + \nu x^2 \right)$, where $\eta$ and $\nu$ are arbitrary constants. Writing $f^{(n)}(x) \equiv \frac{d^n}{dx^n} f^{(0)}(x) = f_n(x) f^{(0)}(x)$, we can show that

$$
f_n(x) = \left\{ \sum_{j=0}^{\left\lfloor n/2 \right\rfloor} \frac{n! f_1(x) n! - 2(2
\nu)^j}{(n - 2j)!! (2j)!!} \right\} f^{(0)}(x),
$$

where $f_1(x) \equiv \frac{d}{dx} f^{(0)}(x) = \eta + 2 \nu x$. Inserting this result into Eq. (C.2), we get

$$
\check{A}_T^{\text{sc}} = \sum_{k=0}^{N} A_p \frac{k!}{(2r)!!} \partial_{a^r} \left( \sum_{s=0}^{\infty} \left( \frac{2 b^* \nu^s}{(2s)!!} \partial_{a^r} \right) \right) a^k a^{m-k} \sum_{l=0}^{\min[n,m]} \frac{1}{2^l l!} \frac{n! a^{n-l} m! a^{m-l}}{(n - l)! (m - l)!},
$$

which is a convenient formula for numerical studies. After rearrangement of terms, Eq. (C.5) becomes

$$
\lim_{N \to \infty} \check{A}_T^{\text{sc}} = A_p \exp \left( b \partial_{a^2} \right) \exp \left( b^* \partial_{a^2} \right) \exp \left( |a|^2 \right) \exp \left( \frac{1}{2} \partial_{a^*} \partial_{a} \right) a^n a^{m^n}.
$$

(C.6)
For the numerical applications presented in the main text, we need to evaluate the above equation for some specific pairs \((n, m)\) and pertinent finite-series representations (truncated at the \(N\)th order) for the differential operators \(\exp\left(b \partial^2_0\right)\), \(\exp\left(b^* \partial^2_\alpha\right)\), and \(\exp\left(\frac{1}{2} \Delta \partial^2\right)\). Then, renaming Eq. \((C.5)\) as \(\tilde{A}_{nm}^{se}\) in order to make explicit the values of those exponents, we have

\[
\tilde{A}_{n0}^{se} = \sum_{k=0}^{N} \frac{A_p}{k!} \sum_{r=0}^{\left[\frac{k}{2}\right]} \sum_{s=0}^{\left[\frac{k}{2}\right]} \frac{(2b)^r (2b^*)^s (k + n)! a^{k+n-2r} a^{k-2s}}{(2r)!! (2s)!! (k + n - 2r)! (k - 2s)!}.
\]

\[
\tilde{A}_{11}^{se} = \sum_{k=0}^{N} \frac{A_p}{k!} \sum_{r=0}^{\left[\frac{k+1}{2}\right]} \sum_{s=0}^{\left[\frac{k+1}{2}\right]} \frac{(2b)^r (2b^*)^s (k + 1)^2 k! a^{k+1-2r} a^{k+1-2s}}{(2r)!! (2s)!! (k + 1 - 2r)! (k + 1 - 2s)!} + \tilde{A}_{00}^{se},
\]

\[
\tilde{A}_{21}^{se} = \sum_{k=0}^{N} \frac{A_p}{k!} \sum_{r=0}^{\left[\frac{k+2}{2}\right]} \sum_{s=0}^{\left[\frac{k+2}{2}\right]} \frac{(2b)^r (2b^*)^s (k + 2)(k + 1)^2 k! a^{k+2-2r} a^{k+1-2s}}{(2r)!! (2s)!! (k + 2 - 2r)! (k + 1 - 2s)!} + \tilde{A}_{10}^{se},
\]

and also \(\tilde{A}_{n0}^{se} = (\tilde{A}_{n0}^{se})^*\) and \(\tilde{A}_{21}^{se} = (\tilde{A}_{12}^{se})^*\).

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