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Initial or final values for semiclassical evolutions in the Weyl–Wigner representation

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Abstract

Initial value representations are constructed to avoid the search for trajectories that are only defined in semiclassical approximations by their boundary conditions. We show how to incorporate these procedures within the full Weyl representation, so that quantum expectation values are given by phase space integrals over the evolving Wigner function. Spurious semiclassical singularities at caustics are cancelled, even though there is no increase in the number of trajectories, as compared to usual semiclassical formulae. The whole construction remains exact in the case of quadratic Hamiltonians. The evolution of (density) operators depends on either a forward and backward trajectory, given by an initial value, or else on a pair of trajectories, propagating backwards from their final value. The latter option reduces numerical errors in the computation of trajectories. The general scheme also leads to analogous algorithms for evolving the quantum fidelity, which can be approximated perturbatively with a single trajectory, reducing to the 'dephasing representation' for small times. The theory is developed within a generalized 'Maslov method', based on semiclassical Fourier transforms, in order to avoid singularities in the limit of small times.

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(Some figures may appear in colour only in the online journal)

1. Introduction

The marked distinction between the structures of classical and quantum mechanics accounts for the difficulties in the practical implementation of semiclassical (SC) approximations. The uncertainty principle obstructs the natural specification of relevant classical trajectories by their initial values, so that the orbits in SC propagators need to be specified variationally by boundary conditions at both ends. Unlike the unique trajectory emanating from an initial value, there may be multiple variational solutions that coalesce along caustics. This is sometimes referred to as the *root search problem*.

The caustics themselves may have complex configurations where amplitudes are indeed high, but not singular as in the simpler SC formulae, which must be substituted by elaborate *uniform approximations,* depending on the different types of local *catastrophe* [1]. The fact that a caustic may always be obtained as the projection of a manifold in a higher space left open the possibility that they could be avoided if the framework of SC approximations was entirely cast in phase space itself, instead of relying on the position representation. However, it turned out that the Wigner function [2, 3], its Fourier transform (the *chord function* or the *quantum characteristic function*) and the Weyl representation of the evolution operator are all bedevilled by caustics in their own right [4–7]. Furthermore, the higher dimensionality of the space generates the need to accommodate higher generic singularities within the theory.

The hazard in dealing with such rich structures justifies to some extent the continued use of simulations, that rely on purely classical molecular dynamics, for a variety of physical processes within the quantum realm. The more satisfactory alternative is to employ the traditional SC approximations within integrals and then to juggle for a change of variables, from a final boundary condition to an initial value. Remarkably, there are contexts where the Jacobian of this transformation exactly cancels off the spurious SC singularities, thus avoiding the need for sophisticated uniform approximations along caustics. Such initial value representations (IVRs) were initially introduced by Miller [8, 9] for the standard Van Vleck propagator in the position representation [10, 11]. The alternative IVR for the coherent state propagator, proposed by Hermann and Kluk [12] and Kay [13], is even more used in simulations. However, it is obtained from the Van Vleck propagator by smoothing [14] and is not quite satisfactory from a theoretical point of view [15].

Can one implement the IVR program for the Wigner function? After all, it allows one to calculate quantum expectation values as if with a probability distribution in phase space and it is a part of the full Weyl–Wigner representation of quantum mechanics, for which SC approximations are available, as reviewed in [7]. Even so, the same difficulties with root searches for trajectories, as well as caustics, also arise in SC approximations for this phase space representation. Recently, an IVR has been introduced by Vaníček [18] for the evolution of the fidelity (or quantum Loschmidt echo) in terms of the Wigner function. It was shown in [25] that this corresponds to a first-order classical perturbation within a standard SC formula involving an integral over the Weyl propagator. However, this extra approximation has not hampered efficient and successful applications [20–24, 26], just as in the case of the Herman–Kluk propagator. Otherwise, the Weyl representation seems to be invoked only for approximations in which a linearization of the evolution in the neighbourhood of a classical trajectory may be in order, so that the exact propagation of Wigner functions for quadratic Hamiltonians can be invoked [9, 29].

Our objective here is to show how the IVR program fits perfectly within the general framework of the Weyl representation, if one includes both the Wigner function and the Weyl propagator, defined in terms of a basis of reflection operators and their Fourier transforms, with their basis of translation operators [16, 17, 7]. As a first illustration, we derive IVRs for the Fourier integrals of the propagators themselves, thus avoiding caustics that are also present in this representation. However, it is in the combination of the propagators with the density operator, or observables, that the distinct advantage of the Weyl representation manifests itself. Indeed, disposing of a basis composed of operators within the same family as the unitary operators that are responsible for the evolution, one can combine a product of operators so as to form a (basis-dependent) compound unitary operator within a single IVR. There is no extra smoothing, so that the formulae remain exact in the case of linear classical evolution that is generated by quadratic Hamiltonians.

The task of deriving suitable integrals for the full evolution of density operators, or for the observables, is nontrivial. The direct SC approximation in [31] demands a root search and it cannot be applied either in the neighbourhood of caustics nor for coherent states, unless complex trajectories are allowed. Pure states of any kind can be transported by Wigner function propagators, whose SC form has been presented by Dittrich *et al* [32]. However, it is then this propagator itself that has trajectories defined indirectly by boundary conditions and the region near the dominant classical trajectory is invariably marred by a caustic. The alternative of mixed propagators taking the Wigner function into its Fourier transform [33], or vice versa, does circumvent this vicious caustic, but parallel numerical work to this paper reveals that caustics still hover around and constitute a problem.

Therefore, a new IVR integral that evolves a Wigner function or chord function, without caustics, or root search, while avoiding any extra integration steps, is most welcome. It turns out that one needs no recourse to the IVR formulae for the propagators themselves. Again, it is the interplay between the usual Weyl representation and its Fourier transform that leads to the simplest SC algorithm, as in [33]. One can opt between two alternatives. One is to define a pair of final values, and thus a pair of trajectories travelling back for a time t, in effect a final value representation (FVR). Another possibility is to take an initial value, travel forward for a time t, then travel backwards along a related trajectory. The disadvantage of this option is that numerical errors in the integration of the trajectory then build up exponentially for a time $2t$.

Both these methods can be immediately adapted to provide a full IVR or FVR for an evolving quantum fidelity. Furthermore, in all cases, we obtain exact results if the driving Hamiltonian is quadratic. Evolved density operators can then be inserted in classical-like expressions for expectation values. In the examples cited in [29], this further step merely limits the range of values for which the evolving Wigner function (or chord function) needs to be calculated.

The following section is devoted to the review of both the Weyl and chord representations from the perspective of reflection and translation operators. Then, the discussion of the SC form of the evolution operators and their new IVR is presented in section 3. There follows the theory for either the IVR or the FVR that describes the evolution of the density (or other arbitrary) operators in section 4. In the case of the quantum fidelity, treated in section 5, we also present a comparison of the result of our exact IVR with the dephasing approximation for oscillators of variable frequency. The discussion of the full form of expectation values is then presented in section 6.

2. Review

Let us recall that $\mathbf{R}^{2N}$ stands for a $2N$-dimensional classical phase space, $\{\boldsymbol{x} = (\mathbf{p}, \mathbf{q})\}$ with its *skew product*,

$$\boldsymbol{x} \wedge \boldsymbol{x}' = \sum_{l=1}^{N} (p_l q_l' - q_l p_l') = \mathbf{J}\,\boldsymbol{x} \cdot \boldsymbol{x}', \tag{2.1}$$

which also defines the skew-symplectic matrix $\mathbf{J}$. We shall here use a distinct notation for the *centre* of a pair of points, $\mathbf{x} = (\boldsymbol{x}^+ + \boldsymbol{x}^-)/2$, whereas the *chords*, $\boldsymbol{\xi} = (\xi_p, \xi_q) = \boldsymbol{x}^+ - \boldsymbol{x}^-$, are the conjugate variables to the *centres* $\mathbf{x}$ and correspond to tangent vectors in phase space, as in the scheme for a Legendre transform. Each of these chords labels a uniform translation of phase space points $\boldsymbol{x}_0 \in \mathbf{R}^{2N}$ by the vector $\boldsymbol{\xi} \in \mathbf{R}^{2N}$, i.e. $\boldsymbol{x}_0 \mapsto \boldsymbol{x}_0 + \boldsymbol{\xi}$. Likewise, each centre, $\mathbf{x}$, labels a reflection of phase space $\mathbf{R}^{2N}$ through the point $\mathbf{x}$, i.e. $\mathbf{x}_0 \mapsto 2\mathbf{x} - \mathbf{x}_0$.

Corresponding to the classical translations, one defines *translation operators*:

$$\hat{T}_{\boldsymbol{\xi}} = \exp\left\{\frac{\mathrm{i}}{\hbar}\,\boldsymbol{\xi} \wedge \hat{\mathbf{x}}\right\}, \tag{2.2}$$

also known as displacement operators, or Heisenberg operators. The chord representation of an operator $\hat{A}$ on the Hilbert space $L^2(\mathbf{R}^N)$ is defined via the decomposition of $\hat{A}$ as a linear (continuous) superposition of translation operators. In this way,

$$\hat{A} = \frac{1}{(2\pi\hbar)^N}\int \mathrm{d}\boldsymbol{\xi}\,\tilde{A}(\boldsymbol{\xi})\,\hat{T}_{\boldsymbol{\xi}} \tag{2.3}$$

and the expansion coefficient, a function on $\mathbf{R}^{2N}$, is the *chord symbol* of the operator $\hat{A}$:

$$\tilde{A}(\boldsymbol{\xi}) = \mathrm{tr}\,\left[\hat{T}_{-\boldsymbol{\xi}}\,\hat{A}\right]. \tag{2.4}$$

The Fourier transform of the translation operators defines the *reflection operators*,

$$2^N\,\hat{R}_{\mathbf{x}} = \frac{1}{(2\pi\hbar)^N}\int \mathrm{d}\boldsymbol{\xi}\,\exp\left\{\frac{\mathrm{i}}{\hbar}\,\mathbf{x} \wedge \boldsymbol{\xi}\right\}\,\hat{T}_{\boldsymbol{\xi}}, \tag{2.5}$$

such that each of these corresponds classically to a reflection of phase space $\mathbf{R}^{2N}$ through the point $\mathbf{x}$. The same operator $\hat{A}$ can then be decomposed into a linear superposition of reflection operators

$$\hat{A} = 2^N\int \frac{\mathrm{d}\mathbf{x}}{(2\pi\hbar)^N}\,A(\mathbf{x})\,\hat{R}_{\mathbf{x}}, \tag{2.6}$$

thus defining the *centre symbol or Weyl symbol* of operator $\hat{A}$,

$$A(\mathbf{x}) = 2^N\,\mathrm{tr}\,\left[\hat{R}_{\mathbf{x}}\,\hat{A}\right]. \tag{2.7}$$

It follows that the centre and chord symbols are always related by a Fourier transform:

$$\tilde{A}(\boldsymbol{\xi}) = \frac{1}{(2\pi\hbar)^N}\int \mathrm{d}\mathbf{x}\,\exp\left\{\frac{\mathrm{i}}{\hbar}\,\mathbf{x} \wedge \boldsymbol{\xi}\right\} A(\mathbf{x}), \tag{2.8}$$

$$A(\mathbf{x}) = \frac{1}{(2\pi\hbar)^N}\int \mathrm{d}\boldsymbol{\xi}\,\exp\left\{\frac{\mathrm{i}}{\hbar}\,\boldsymbol{\xi} \wedge \mathbf{x}\right\}\tilde{A}(\boldsymbol{\xi}). \tag{2.9}$$

In particular, one obtains the reciprocal representations of the reflection operator and the translation operator as

$$2^N\,\tilde{R}_{\mathbf{x}}(\boldsymbol{\xi}) = \exp\left\{\frac{\mathrm{i}}{\hbar}\,\mathbf{x} \wedge \boldsymbol{\xi}\right\} \quad \text{or} \quad T_{\boldsymbol{\xi}}(\mathbf{x}) = \exp\left\{-\frac{\mathrm{i}}{\hbar}\,\mathbf{x} \wedge \boldsymbol{\xi}\right\}. \tag{2.10}$$

These expressions are ideally suited for use in SC approximations. The direct representations are

$$2^N\,\tilde{R}_{\mathbf{x}}(\mathbf{x}') = \delta(\mathbf{x}' - \mathbf{x}) \quad \text{or} \quad T_{\boldsymbol{\xi}}(\boldsymbol{\xi}') = \delta(\boldsymbol{\xi}' - \boldsymbol{\xi}). \tag{2.11}$$

In the case of the density operator, $\hat{\rho}$, it is convenient to normalize its chord symbol, so that we define the *chord function* as

$$\chi(\boldsymbol{\xi}) = \frac{1}{(2\pi\hbar)^N}\mathrm{tr}\,\left[\hat{T}_{-\boldsymbol{\xi}}\,\hat{\rho}\right] = \frac{\tilde{\rho}(\boldsymbol{\xi})}{(2\pi\hbar)^N}, \tag{2.12}$$

whose Fourier transform is the *Wigner function*,

$$W(\mathbf{x}) = \frac{1}{(2\pi\hbar)^N}\int \mathrm{d}\boldsymbol{\xi}\,\exp\left\{\frac{\mathrm{i}}{\hbar}(\boldsymbol{\xi} \wedge \mathbf{x})\right\}\,\chi(\boldsymbol{\xi}), \tag{2.13}$$

or alternatively [17]

$$W(\mathbf{x}) = \frac{1}{(\pi\hbar)^N} \mathrm{tr}\left[\hat{R}_{\mathbf{x}}\,\hat{\rho}\right]. \tag{2.14}$$

From the general expression for the trace of a product of operators,

$$\mathrm{tr}(\hat{A}\,\hat{B}) = \int \frac{\mathrm{d}\mathbf{x}}{(2\pi\hbar)^N}\, A(\mathbf{x})\, B(\mathbf{x}) \; = \int \frac{\mathrm{d}\boldsymbol{\xi}}{(2\pi\hbar)^N}\, \tilde{A}(\boldsymbol{\xi})\, \tilde{B}(-\boldsymbol{\xi}), \tag{2.15}$$

one obtains the expectation values

$$\langle\hat{A}\rangle = \mathrm{tr}(\hat{\rho}\,\hat{A}) = \int \mathrm{d}\mathbf{x}\, A(\mathbf{x})\, W(\mathbf{x}) \; = \int \mathrm{d}\boldsymbol{\xi}\, \tilde{A}(\boldsymbol{\xi})\, \chi(-\boldsymbol{\xi}). \tag{2.16}$$

The normalization condition reads

$$1 = \mathrm{tr}\;\hat{\rho} = \int \mathrm{d}\mathbf{x}\, W(\mathbf{x}) = (2\pi\hbar)^N \chi(\mathbf{0}). \tag{2.17}$$

The Weyl–Wigner representation and its Fourier transform have a long history. The authors of [3, 16, 17, 19] cover most aspects, with unavoidable variations in the notation and interpretation. Our presentation is largely based on the review [7].

3. SC Weyl propagators and their IVR

The *Weyl propagator* for the unitary operators, $\widehat{U}$, that correspond classically to symplectic transformations, $\boldsymbol{x} \mapsto \boldsymbol{x}' = \mathbf{M}\boldsymbol{x}$ (i.e. $\mathbf{M}$ is a symplectic matrix), is [7]

$$U(\mathbf{x}) = \frac{2^N}{|\det(\mathbf{I}+\mathbf{M})|^{1/2}} \;\exp\left[\frac{\mathrm{i}}{\hbar}\left(S(\mathbf{x}) + \frac{\hbar\pi\sigma}{2}\right)\right]. \tag{3.1}$$

This group of *metaplectic* unitary transformations includes all motions generated by quadratic Hamiltonians. The action is then also a quadratic form, $S(\mathbf{x}) = \mathbf{x}\mathbf{B}\mathbf{x}$, where the symmetric matrix $\mathbf{B}$ is one of the Cayley parametrizations of $\mathbf{M}$:

$$\mathbf{M} = [\mathbf{I}+\mathbf{J}\mathbf{B}]^{-1}[\mathbf{I}-\mathbf{J}\mathbf{B}] = [\mathbf{I}-\mathbf{J}\tilde{\mathbf{B}}]^{-1}[\mathbf{I}+\mathbf{J}\tilde{\mathbf{B}}]. \tag{3.2}$$

The action specifies the canonical transformation indirectly through [7]

$$\boldsymbol{\xi} = -\mathbf{J}\frac{\partial S}{\partial \mathbf{x}}, \quad \boldsymbol{x}' = \mathbf{x} + \frac{\boldsymbol{\xi}}{2}, \quad \boldsymbol{x} = \mathbf{x} - \frac{\boldsymbol{\xi}}{2}. \tag{3.3}$$

Within this restricted class of transformations, the amplitude in (3.1) is a constant with respect to $\mathbf{x}$, but, for a continuous evolution in time, an eigenvalue of $\mathbf{M}$ (or a pair of eigenvalues) may eventually equal -1. This is not a spurious singularity: at this instant, the divergent form of (3.1) is substituted by a Dirac δ-function and, beyond it, the integer (Maslov) index σ may change (signifying a switch of metaplectic sheet). The passage through caustics of metaplectic operators, in the context of the position representation, is described by Littlejohn [34], but has only now been worked out for the Weyl representation [35][3].

No such discontinuity occurs at this instant for the *chord propagator*,

$$\tilde{U}(\boldsymbol{\xi}) = \frac{1}{|\det(\mathbf{I}-\mathbf{M})|^{1/2}} \;\exp\left[\frac{\mathrm{i}}{\hbar}\left(\tilde{S}(\boldsymbol{\xi}) + \frac{\hbar\pi\tilde{\sigma}}{2}\right)\right], \tag{3.4}$$

for the same quantum evolution, $\widehat{U}$, and, hence, the same classical symplectic matrix, $\mathbf{M}$. In this case, the classical chord action generates a canonical transformation through [7]

$$\mathbf{x} = \mathbf{J}\frac{\partial \tilde{S}}{\partial \boldsymbol{\xi}}, \quad \boldsymbol{x}' = \mathbf{x} + \frac{\boldsymbol{\xi}}{2}, \quad \boldsymbol{x} = \mathbf{x} - \frac{\boldsymbol{\xi}}{2}, \tag{3.5}$$

[3] The index $\sigma = 0$ in the neighbourhood of the identity that has no caustics.

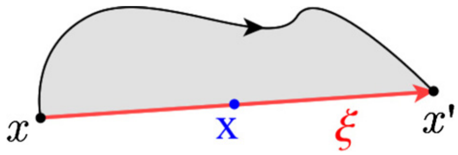

Figure 1. Sketch of the chord–centre variables in terms of the initial $\boldsymbol{x}$ and $\boldsymbol{x}'$ variables for a continuous evolution.

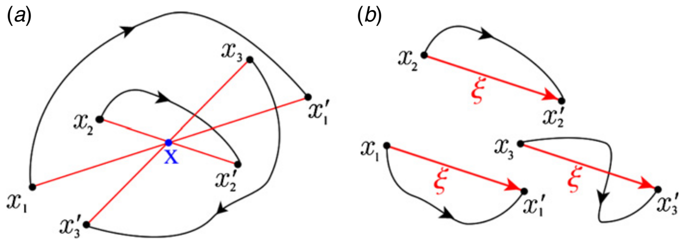

Figure 2. Multiplicity of trajectories for a given centre $\mathbf{x}$ or a chord $\boldsymbol{\xi}$. In each case, the trajectories have different initial values.

and the quadratic form for the action becomes $\tilde{S}(\boldsymbol{\xi}) = (1/4)\boldsymbol{\xi}\tilde{B}\boldsymbol{\xi}$, where $\tilde{B}$ is the alternative Cayley parametrization for $\mathbf{M}$ in (3.2). For a continuous time evolution, it is when $\mathbf{M}$ has a pair of unit eigenvalues that the index $\tilde{\sigma}$ changes parity, at which point (3.4) is replaced by a δ-function.

SC approximations of the Weyl and chord propagators for general unitary transformations [30, 7] have the same form as (3.1) and (3.4). However, the Weyl action, $S(\mathbf{x})$, and the chord action, $\tilde{S}(\boldsymbol{\xi})$, are no longer quadratic; they are related by Legendre transforms [7]. The geometry for a continuous trajectory, resulting from Hamiltonian evolution, is illustrated in figure 1. The geometric part of the Weyl action, $S(\mathbf{x})$, is just the symplectic area between the trajectory and the chord, $\boldsymbol{\xi} = \boldsymbol{x}' - \boldsymbol{x}$, joining its endpoints. From this, one subtracts $-Et$, where E is the energy of the trajectory. The symplectic matrix $\mathbf{M}$ is now only defined locally by the linearization of the canonical transformation that is specified implicitly by (3.3) or (3.5), so that, henceforth, we write $\mathbf{M}(\mathbf{x})$ or $\mathbf{M}(\boldsymbol{\xi})$. There may be multiple solutions to the variational problem that identifies trajectories with a given centre, $\mathbf{x}$, or a given chord, $\boldsymbol{\xi}$, as shown in figure 2, so the actions may have many branches and these branches meet along caustics where the SC amplitude diverges. On crossing a caustic, the index $\sigma(\mathbf{x})$ or $\tilde{\sigma}(\boldsymbol{\xi})$ switches parity[4].

The IVR alternative is to describe the propagator as an integral over trajectories. Counterbalancing the vast increase in the number of trajectories to be computed, each of these is determined directly by its initial value. In all the foregoing sections, one casts the function to be calculated as the trace of a product of operators. Here, these are just the operator $\widehat{U}$, itself, together with the chosen basis operator, $\widehat{R}_{\mathbf{x}}$ or $\widehat{T}_{-\boldsymbol{\xi}}$. Then, from expressions (2.4), (2.7), (2.10) and (2.15), one obtains

$$U(\mathbf{x}) = 2^N \mathrm{tr}\left[\hat{R}_{\mathbf{x}}\,\hat{U}\right] = \int \frac{\mathrm{d}\boldsymbol{\xi}}{(2\pi\hbar)^N}\,\tilde{U}(\boldsymbol{\xi})\,\exp\left(-\frac{\mathrm{i}}{\hbar}\mathbf{x}\wedge\boldsymbol{\xi}\right) \tag{3.6}$$

[4] Then, $U(\mathbf{x})$ or $\tilde{U}(\boldsymbol{\xi})$ become a sum of terms of the form (3.1) or (3.4).

and

$$\tilde{U}(\boldsymbol{\xi}) = \mathrm{tr}\left[\hat{T}_{-\boldsymbol{\xi}}\,\hat{U}\right] = \int \frac{\mathrm{d}\mathbf{x}}{(2\pi\hbar)^N}\,U(\mathbf{x})\,\exp\left(\frac{\mathrm{i}}{\hbar}\mathbf{x}\wedge\boldsymbol{\xi}\right). \tag{3.7}$$

In this instance, one thus retrieves the expressions of $U(\mathbf{x})$ in (2.8) and $\tilde{U}(\boldsymbol{\xi})$ in (2.9) as reciprocal Fourier transforms.

Inserting the SC approximations, (3.1) or (3.4), for the integrand in a region without caustics, one notes that the Jacobian for the change of integration variable to the initial value is

$$\det\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}\boldsymbol{x}} = \det\left(\frac{\mathbf{I}+\mathbf{M}}{2}\right) \quad \text{or} \quad \det\frac{\mathrm{d}\boldsymbol{\xi}}{\mathrm{d}\boldsymbol{x}} = \det(\mathbf{I}-\mathbf{M}). \tag{3.8}$$

Hence, we obtain the IVRs for the propagators

$$U(\mathbf{x}) = \int \frac{\mathrm{d}\boldsymbol{x}}{(2\pi\hbar)^N}\sqrt{|\det(\mathbf{I}-\mathbf{M}(\boldsymbol{x}))|}\,\exp\left[-\frac{\mathrm{i}}{\hbar}\left(\tilde{S}(\boldsymbol{\xi}(\boldsymbol{x})) + \mathbf{x}\wedge\boldsymbol{\xi}(\boldsymbol{x}) + \frac{\tilde{\sigma}(\boldsymbol{x})\pi\hbar}{2}\right)\right] \tag{3.9}$$

and

$$\tilde{U}(\boldsymbol{\xi}) = \int \frac{\mathrm{d}\boldsymbol{x}}{(2\pi\hbar)^N}\sqrt{|\det(\mathbf{I}+\mathbf{M}(\boldsymbol{x}))|}\,\exp\left[\frac{\mathrm{i}}{\hbar}\left(S(\mathbf{x}(\boldsymbol{x})) - \mathbf{x}(\boldsymbol{x})\wedge\boldsymbol{\xi} + \frac{\sigma(\boldsymbol{x})\pi\hbar}{2}\right)\right]. \tag{3.10}$$

Here, the absence of a sum over contributing trajectories is no longer a sleight of hand, as in (3.1) and (3.4) for general evolutions. Indeed, the possible multiplicity of trajectories that share a given centre (or a given chord) has different initial values, $\boldsymbol{x}$, and each of these is the source of an unique trajectory (see figure 2).

No smoothing has been introduced to obtain these IVRs. By reversing the exact change of variable, $\mathbf{x} \mapsto \boldsymbol{x}$ or $\boldsymbol{\xi} \mapsto \boldsymbol{x}$, one performs the complex Gaussian integrals in the case of metaplectic transformations, thus retrieving the exact propagators (3.1) and (3.4), for which the amplitude is constant. For general nonlinear transformations, nodal surfaces of $\det(\mathbf{I}\pm\mathbf{M})$ are no longer spurious singularities of the respective propagators, but the integrand still changes phase with $\sigma(\boldsymbol{x})$ or $\tilde{\sigma}(\boldsymbol{x})$.

4. Evolution of operators: final and initial values

We now implement the same procedure that generated IVRs for the propagators to describe directly the Weyl and chord representations of arbitrary operators, $\widehat{A}$, undergoing Heisenberg evolution:

$$\widehat{A}(t) = \widehat{U}(t)^\dagger\,\widehat{A}\,\widehat{U}(t). \tag{4.1}$$

The important case of density operators, which undergo Liouville–Von Neumann evolution, is special in that the time is reversed, that is, their forward time evolution will be denoted as

$$\widehat{\rho}(t) = \widehat{U}(t)\,\widehat{\rho}\,\widehat{U}(t)^\dagger, \tag{4.2}$$

so that the corresponding evolution of the Wigner function is

$$\begin{aligned} W_t(\mathbf{x}') &= \frac{\mathrm{tr}\left[\widehat{\rho}(t)\,\widehat{R}_{\mathbf{x}'}\right]}{(\pi\hbar)^N} = \frac{\mathrm{tr}\left[\widehat{\rho}\,\widehat{R}_{\mathbf{x}'}(t)\right]}{(\pi\hbar)^N} \\ &= \int \frac{\mathrm{d}\mathbf{x}}{(\pi\hbar)^N}\,W(\mathbf{x})\,R_{\mathbf{x}'}(\mathbf{x},t) = \int \frac{\mathrm{d}\boldsymbol{\xi}}{(\pi\hbar)^N}\,\chi(\boldsymbol{\xi})\,\tilde{R}_{\mathbf{x}'}(\boldsymbol{\xi},t). \end{aligned} \tag{4.3}$$

Here, one recognizes the direct *centre–centre propagator* of Wigner functions [32] as $R_{\mathbf{x}'}(\mathbf{x},t)$, that is, the Weyl representation of the Heisenberg-evolved reflection operator, whereas its chord

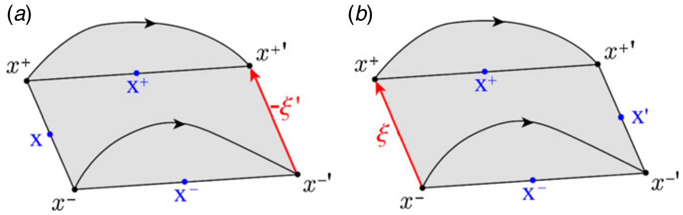

Figure 3. SC phase space structure of the evolved translation and reflection operators: (*a*) $T_{-\boldsymbol{\xi}'}(\boldsymbol{x}, t)$ and (*b*) $R_{\mathbf{x}'}(\boldsymbol{\xi}, t)$.

representation $\tilde{R}_{\mathbf{x}'}(\boldsymbol{\xi}, t)$ can be identified as the *mixed chord–centre propagator*, introduced in [33]. The evolution of the chord function follows suit:

$$\chi_t(\boldsymbol{\xi}') = \frac{\mathrm{tr}\big[\widehat{\rho}(t)\,\widehat{T}_{\boldsymbol{\xi}'}\big]}{(2\pi\hbar)^N} = \frac{\mathrm{tr}\big[\widehat{\rho}\,\widehat{T}_{\boldsymbol{\xi}'}(t))\big]}{(2\pi\hbar)^N}$$

$$\chi_t(\boldsymbol{\xi}') = \int \frac{\mathrm{d}\mathbf{x}}{(2\pi\hbar)^N}\, W(\mathbf{x})\, T_{-\boldsymbol{\xi}'}(\mathbf{x}, t) = \int \frac{\mathrm{d}\boldsymbol{\xi}}{(2\pi\hbar)^N}\, \chi(\boldsymbol{\xi})\, \tilde{T}_{\boldsymbol{\xi}'}(-\boldsymbol{\xi}, t), \tag{4.4}$$

so that the chord representation of the Heisenberg-evolved translation operator $\tilde{T}_{\boldsymbol{\xi}'}(-\boldsymbol{\xi}, t)$ is the direct *chord–chord propagator*, while $T_{-\boldsymbol{\xi}'}(\mathbf{x}, t)$ is the *mixed centre–chord propagator*[5]. Similar formulae describe the chord and centre representations of Heisenberg-evolved operators by merely reversing $t \mapsto -t$. The mixed propagators, related by [33] $\tilde{R}_{\mathbf{x}}(\boldsymbol{\xi}', t) = T_{-\boldsymbol{\xi}'}(\mathbf{x}, -t)$, have the advantage over the direct propagators that $\tilde{R}_{\mathbf{x}}(\boldsymbol{\xi}', 0)$ and $T_{\boldsymbol{\xi}}(\mathbf{x}', 0)$, as given by (2.10), are already in their standard SC form, whereas the corresponding direct representations (2.11) are not.

The crucial point is that the basis that has been adopted is composed entirely of unitary operators, be they reflections or translations. Thus, the evolving operator, $\widehat{R}_{\mathbf{x}}(t)$ or $\widehat{T}_{\boldsymbol{\xi}}(t)$, can be considered as a single unitary operator, corresponding classically to a compound canonical transformation, in which a phase space reflection or translation is sandwiched by a pair of trajectories of the Hamiltonian, so as to constitute a single piecewise smooth trajectory. Let us first consider the component classical trajectories entering the SC Weyl representation of $\widehat{U}(t) = \widehat{T}_{-\boldsymbol{\xi}'}(t)$, namely it is considered as an instance of the general form (3.1), i.e. $U(\mathbf{x}, t) = T_{-\boldsymbol{\xi}'}(\mathbf{x}, t)$. An initial point $\boldsymbol{x}^-$ evolves to $\boldsymbol{x}^{-\prime}(\boldsymbol{x}^-, t)$; then it is translated, i.e. $\boldsymbol{x}^{-\prime} \mapsto (\boldsymbol{x}^{-\prime} - \boldsymbol{\xi}' = \boldsymbol{x}^{+\prime})$ and finally evolves back to $\boldsymbol{x}^+(\boldsymbol{x}^{+\prime}, -t)$. This full compound trajectory, shown in figure 3(*a*), determines the phase and amplitude of the SC approximation (3.1), evaluated at the point $\mathbf{x} = (\boldsymbol{x}^- + \boldsymbol{x}^+)/2$. Indeed, the intermediate step is just a translation, which does not alter the neighbourhood of $\boldsymbol{x}^{-\prime} \mapsto \boldsymbol{x}^{+\prime}$, so that the symplectic matrix for the full evolution $\boldsymbol{x}^- \mapsto \boldsymbol{x}^+$ is defined as

$$\mathbf{M}_{-\boldsymbol{\xi}'}(\mathbf{x}) = [\mathbf{M}(\mathbf{x}^+)]^{-1}\, \mathbf{I}\;\; \mathbf{M}(\mathbf{x}^-), \tag{4.5}$$

given that the pair of symplectic matrices $\mathbf{M}(\mathbf{x}^\pm)$ accounts for the linearized motion near the pair of trajectories that have centres $\mathbf{x}^\pm = (\boldsymbol{x}^\pm + \boldsymbol{x}^{\pm\prime})/2$. It is important to note that the insertion of a translation between the pair of symplectic evolutions, corresponding to $\mathbf{M}(\mathbf{x}^\pm)$, does not alter the parity σ for the full transformation, according to the analysis in [35].

[5] Both mixed propagators were defined in [33] in terms of appropriate Lagrangian double phase space surfaces evolving forward in time, whereas here they arise from the backward motion of the surfaces corresponding to the final centre $\mathbf{x}'$ or the final chord $\boldsymbol{\xi}'$.

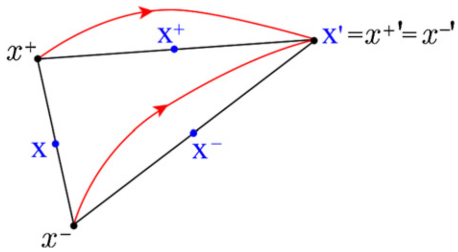

Figure 4. Phase space scheme for the fidelity. It is the same as in figure 3(*a*), for the limit of $\boldsymbol{\xi} \to 0$, i.e. when the translation operator tends to the identity operator. Note that the paths are driven by different Hamiltonians, i.e. the path departing from $\boldsymbol{x}^+$ ($\boldsymbol{x}^-$) is driven by H_+ (H_-).

The action $S_{-\boldsymbol{\xi}'}(\mathbf{x})$ in (3.1) has an energy term and a geometric term, which is the symplectic area of the curvilinear quadrangle in figure 3(*a*). Thus, according to [7], the action can be decomposed as

$$S_{-\boldsymbol{\xi}'}(\mathbf{x}) = \Delta_4 + S(\mathbf{x}^-) - S(\mathbf{x}^+) + (E^+ - E^-)\, t + \tfrac{1}{2}(x^{+\prime} + x^{-\prime}) \wedge \boldsymbol{\xi}', \tag{4.6}$$

where $S(\mathbf{x}^\pm)$ are the (centre) actions for both smooth trajectory segments, $E^\pm$ are their energies and the symplectic area of the straight-sided quadrilateral in figure 3(*a*) is

$$\Delta_4 = \tfrac{1}{2}[-\boldsymbol{x}^+ \wedge \boldsymbol{x}^{+\prime} + \boldsymbol{x}^- \wedge \boldsymbol{x}^{-\prime} - \boldsymbol{x}^{+\prime} \wedge \boldsymbol{x}^{-\prime} + \boldsymbol{x}^+ \wedge \boldsymbol{x}^-]. \tag{4.7}$$

A similar compound trajectory determines the SC chord representation of $\widehat{R}_{\mathbf{x}'}(t)$, i.e. a special case of the general unitary operator (3.4). The difference is that here the point $\boldsymbol{x}^{-\prime}(\boldsymbol{x}^-, t)$ is then reflected through the given centre $\mathbf{x}'$, i.e. $\boldsymbol{x}^{-\prime} \mapsto (\boldsymbol{x}^{+\prime} = -\boldsymbol{x}^{-\prime} + 2\mathbf{x}')$, before evolving back to $\boldsymbol{x}^+$. This reflection simply reverses the sign of the symplectic matrix, so that here the matrix in the amplitude of (3.4) is defined as

$$\mathbf{M}_{\mathbf{x}'}(\boldsymbol{\xi}) = [\mathbf{M}(\mathbf{x}^+)]^{-1}\ [-\mathbf{I}]\ \ \mathbf{M}(\mathbf{x}^-). \tag{4.8}$$

The chord action is the Legendre transform of the centre action for any given trajectory, so that, evaluating $S_{\mathbf{x}'}(\mathbf{x})$ just as in (4.6), but without the $\boldsymbol{\xi}'$-dependent term, we then have

$$\tilde{S}_{\mathbf{x}'}(\boldsymbol{\xi}) = \boldsymbol{\xi} \wedge \mathbf{x} - S_{\mathbf{x}'}(\mathbf{x}) = \boldsymbol{x}^+ \wedge \boldsymbol{x}^- - S_{\mathbf{x}'}\left(\frac{\boldsymbol{x}^+ + \boldsymbol{x}^-}{2}\right). \tag{4.9}$$

Notwithstanding the overall similarity for calculating $\tilde{S}_{\mathbf{x}'}(\boldsymbol{\xi})$ and $S_{-\boldsymbol{\xi}'}(\mathbf{x})$, there is a subtlety concerning the overall phase $\tilde{\sigma}$ for the chord propagator: The product of a metaplectic transformation by a reflection changes its sign (i.e. $\tilde{\sigma}$ gains a phase π) if it is elliptic, but does not if it is hyperbolic, according to [35]. In the hyperbolic case, the transformation switches between straight hyperbolic and hyperbolic with inversion, but there is no overall change of phase.

So far, we have determined the contribution of a specific compound trajectory that will be relevant for some centre argument of the Wigner function or some chord argument of the chord function, to be discovered *a posteriori*, because it depends on the chosen initial value. However, nothing prevents us from treating this unitary operator in the same way as in the previous section, that is, one can change the integration variable precisely to this initial value $\mathbf{x} \mapsto \boldsymbol{x}^-$ in the first integral in (4.4), with the Jacobian

$$\det \frac{\mathrm{d}\mathbf{x}}{\mathrm{d}\boldsymbol{x}^-} = \det\left(\frac{\mathbf{I} + \mathbf{M}_{-\boldsymbol{\xi}'}(\mathbf{x})}{2}\right) = \det\left(\frac{\mathbf{I} + [\mathbf{M}(\mathbf{x}^+)]^{-1}\mathbf{M}(\mathbf{x}^-)}{2}\right). \tag{4.10}$$

Otherwise, one changes the integration variable $\boldsymbol{\xi} \mapsto \boldsymbol{x}^-$ in the second integral in (4.3), with the Jacobian

$$\det \frac{\mathrm{d}\boldsymbol{\xi}}{\mathrm{d}\boldsymbol{x}^-} = \det(\mathbf{I} - \mathbf{M}_{\mathbf{x}'}(\boldsymbol{\xi})) = \det(\mathbf{I} + [\mathbf{M}(\mathbf{x}^+)]^{-1}\mathbf{M}(\mathbf{x}^-)). \tag{4.11}$$

Thus, the evolved Wigner function in (4.3) becomes

$$W_t(\mathbf{x}') = \int \frac{\mathrm{d}\boldsymbol{x}^-}{(2\pi\hbar)^N} \sqrt{|\det(\mathbf{I} + [\mathbf{M}(\mathbf{x}^+)]^{-1}\mathbf{M}(\mathbf{x}^-))|} \times \exp\left\{-\frac{\mathrm{i}}{\hbar}\left[\tilde{S}_{\mathbf{x}'}(-(\boldsymbol{x}^+ - \boldsymbol{x}^-)) + \frac{\hbar\tilde{\sigma}\pi}{2}\right]\right\} \chi(\boldsymbol{x}^+ - \boldsymbol{x}^-), \tag{4.12}$$

while the evolving chord function becomes

$$\chi_t(\boldsymbol{\xi}') = \int \frac{\mathrm{d}\boldsymbol{x}^-}{(2\pi\hbar)^N} \sqrt{|\det(\mathbf{I} + [\mathbf{M}(\mathbf{x}^+)]^{-1}\mathbf{M}(\mathbf{x}^-))|} \times \exp\left\{\frac{\mathrm{i}}{\hbar}\left[S_{-\boldsymbol{\xi}'}\left(\frac{\boldsymbol{x}^+ + \boldsymbol{x}^-}{2}\right) + \frac{\hbar\sigma\pi}{2}\right]\right\} W\left(\frac{\boldsymbol{x}^+ + \boldsymbol{x}^-}{2}\right). \tag{4.13}$$

Thus, one obtains the same amplitude of propagation for a given initial value for both representations of the evolution.

In the general case where each compound trajectory can only be computed numerically, the need of integrating it forward and then backwards in time can magnify computational errors. There is then a considerable advantage in making an alternative change of variable to the complementary variable of the representation employed. Thus, in the case of the evolved Wigner function, where the final centre $\mathbf{x}'$ is given, we adopt the final chord $\boldsymbol{\xi}'$ as the integrand. One then integrates both trajectories, starting at $\boldsymbol{x}'_\pm = \mathbf{x}' \pm \boldsymbol{\xi}'/2$, backwards to $\boldsymbol{x}_\pm = (\boldsymbol{x}'_\pm, -t)$. The fact that the matrices $\mathbf{M}(\mathbf{x})$ all have unit determinants then implies that the Jacobian,

$$\det \frac{\mathrm{d}\boldsymbol{\xi}}{\mathrm{d}\boldsymbol{\xi}'} = \det[\mathbf{M}(\mathbf{x}^+) + \mathbf{M}(\mathbf{x}^-)] = \det[\mathbf{I} - \mathbf{M}_{\mathbf{x}'}(\mathbf{x})], \tag{4.14}$$

is again what is needed to cancel eventual caustics. Hence, the FVR for the evolving Wigner function is

$$W_t(\mathbf{x}') = \int \frac{\mathrm{d}\boldsymbol{\xi}'}{(2\pi\hbar)^N} \sqrt{|\det[\mathbf{M}(\mathbf{x}^+) + \mathbf{M}(\mathbf{x}^-)]|} \times \exp\left[-\frac{\mathrm{i}}{\hbar}\left[\tilde{S}_{\mathbf{x}'}(-(\boldsymbol{x}^+ - \boldsymbol{x}^-)) + \frac{\hbar\tilde{\sigma}\pi}{2}\right]\right] \chi(\boldsymbol{x}^+ - \boldsymbol{x}^-). \tag{4.15}$$

Likewise, for an evolved chord function evaluated at $\boldsymbol{\xi}'$, one can adopt the complementary centre $\mathbf{x}'$ as the new integration variable, so that again the trajectories travel backwards from $\boldsymbol{x}'_\pm = \mathbf{x}' \pm \boldsymbol{\xi}'/2$. The Jacobian for the coordinate transformation is then

$$\det \frac{\mathrm{d}\mathbf{x}}{\mathrm{d}\mathbf{x}'} = \det\left(\frac{\mathbf{M}(\mathbf{x}^+) + \mathbf{M}(\mathbf{x}^-)}{2}\right) = \det\left(\frac{\mathbf{I} + \mathbf{M}_{-\boldsymbol{\xi}'}(\mathbf{x})}{2}\right), \tag{4.16}$$

so that the FVR for the evolved chord function becomes

$$\chi_t(\boldsymbol{\xi}') = \int \frac{\mathrm{d}\mathbf{x}'}{(2\pi\hbar)^N} \sqrt{|\det[\mathbf{M}(\mathbf{x}^+) + \mathbf{M}(\mathbf{x}^-)]|} \times \exp\left[\frac{\mathrm{i}}{\hbar}\left[S_{-\boldsymbol{\xi}'}\left(\frac{\boldsymbol{x}^+ + \boldsymbol{x}^-}{2}\right) + \frac{\hbar\sigma\pi}{2}\right]\right] W\left(\frac{\boldsymbol{x}^+ + \boldsymbol{x}^-}{2}\right). \tag{4.17}$$

It is remarkable that both these IVRs and FVRs are derived directly, without any recourse to the extra integration, which would arise from the intermediate use of the IVRs for the propagators themselves at each step, as presented in the previous section. Just as in those simple examples, all singularities at caustics are replaced by nodal lines (or nodal surfaces) along which the integrand switches sign. Again, these IVRs and FVRs are exact changes of variable for exact expressions, in the case of evolution generated by quadratic Hamiltonians: the evolution is simply the classical Liouville evolution of the Wigner function or the chord function, which is Fourier transformed (in the beginning or the end) because we are here using mixed propagators. Equivalent IVRs for the Heisenberg evolution of other sorts of operators result in analogous equations, except for the exchange $t \mapsto -t$.

5. IVR or FVR for the quantum fidelity

The evolution of the quantum fidelity may also be obtained from the trace of two operators. First, we define the *echo operator* as the modification of the Heisenberg evolution of the identity operator, by having different forward and backward propagations [25],

$$\widehat{I}_L(t) = \widehat{U}_+(t)^\dagger\, \widehat{I}\, \widehat{U}_-(t) = \exp\left(\frac{\mathrm{i}}{\hbar}\widehat{H}_+ t\right)\, \widehat{I}\, \exp\left(-\frac{\mathrm{i}}{\hbar}\widehat{H}_- t\right), \tag{5.1}$$

with the Weyl representation $I_L(\mathbf{x}, t)$ so that the echo is the intensity of

$$L(t) = \mathrm{tr}\left[\widehat{\rho}\, \widehat{I}_L(t)\right] = \int \frac{\mathrm{d}\mathbf{x}}{(\pi\hbar)^N}\; W(\mathbf{x}) I_L(\mathbf{x}, t). \tag{5.2}$$

Evidently, one deals with the same structure as in the previous section. Indeed, the identity operator is a special ($\boldsymbol{\xi} = 0$) translation operator, so that (5.2) is a particular evolution of the chord function, albeit for a non-Heisenberg evolution. The difference between the operators $\widehat{U}_\pm$ is responsible for the identity operator evolving nontrivially, rather than remaining invariant. The classical trajectory scheme corresponding to $I_L(\mathbf{x}, t)$, shown in figure 5, replaces the curvilinear rectangle of figure 3(a) by a triangle. Furthermore, one must now distinguish the symplectic matrices $\mathbf{M}_\pm(\mathbf{x})$ for the linearized motions near the trajectories generated by the pair of Hamiltonians $H_\pm$ that are centred on a given $\mathbf{x}$. According to [35], there will be no change of overall phase beyond that contributed by the pair of factor operators if both are of the same type, either both elliptic or both hyperbolic.

It follows that all the SC ingredients can be defined in exact analogy to the previous section, leading to the FVR

$$L(t) = \int \frac{\mathrm{d}\mathbf{x}'}{(2\pi\hbar)^N} \sqrt{|\det[\mathbf{M}_+(\mathbf{x}^+) + \mathbf{M}_-(\mathbf{x}^-)]|} \times \exp\left\{\frac{\mathrm{i}}{\hbar}\left[S_0\left(\frac{\boldsymbol{x}^+ + \boldsymbol{x}^-}{2}\right) + \frac{\hbar\sigma\pi}{2}\right]\right\} W\left(\frac{\boldsymbol{x}^+ + \boldsymbol{x}^-}{2}\right), \tag{5.3}$$

where $\boldsymbol{x}^\pm(\mathbf{x}', -t)$ are the ends of both the backward classical trajectories generated by the pair of Hamiltonians $H_\pm(\boldsymbol{x})$. The action $S_0(\mathbf{x})$ is given by (4.6) with $\boldsymbol{\xi}' = 0$. The alternative is to start at the arbitrary point $\boldsymbol{x}^-$, evolve forward along the trajectory generated by $H_-(\boldsymbol{x})$ and then reverse the motion with $H_+(\boldsymbol{x})$, thus obtaining the IVR:

$$L(t) = \int \frac{\mathrm{d}\boldsymbol{x}^-}{(2\pi\hbar)^N} \sqrt{|\det(\mathbf{I} + [\mathbf{M}_+(\mathbf{x}^+)]^{-1}\, \mathbf{M}_-(\mathbf{x}^-))|} \times \exp\left\{\frac{\mathrm{i}}{\hbar}\left[S_0\left(\frac{\boldsymbol{x}^+ + \boldsymbol{x}^-}{2}\right) + \frac{\hbar\sigma\pi}{2}\right]\right\} W\left(\frac{\boldsymbol{x}^+ + \boldsymbol{x}^-}{2}\right). \tag{5.4}$$

It is the approximate evaluation of $S_0(\mathbf{x})$ by classical perturbation theory that leads to a simple IVR with a single trajectory, as obtained in [25]. The amplitude of $I_L(\mathbf{x}, t)$ will then be small if $(H_+ - H_-)t$ is small, so that, if this is neglected, one obtains Vanicek's *dephasing representation* (DR) [18]. Here, one need not make such assumptions and, in the case of the

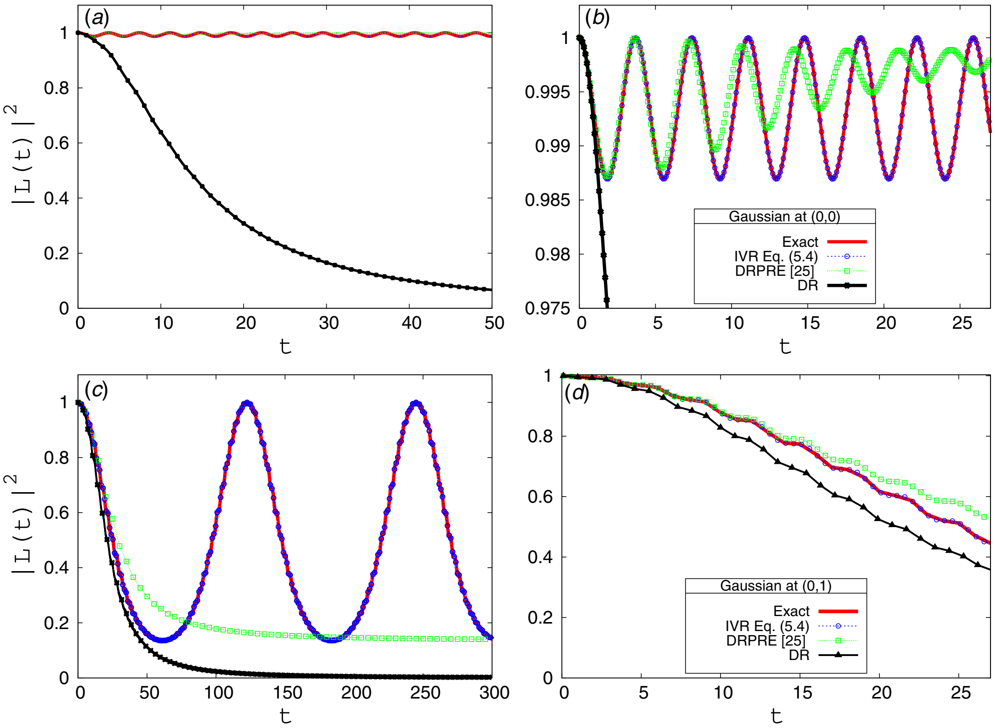

Figure 5. Fidelity of a coherent state driven by a pair of harmonic oscillators with frequencies 1 and $\sqrt{0.9}$. The centre of the initial states is (a) at the origin and (c) at (0, 1). Panels (b) and (d) are magnifications of (a) and (c), respectively. One observes that the IVR (5.4) reproduces the exact quantum fidelity. The DR [18] and the version of DR with a prefactor [25] are presented for comparison. Here, $\hbar = 1$.

FVR (5.3), the trajectories are calculated for the same time as in the DR, so there is no growth of numerical errors due to doubling the integration time, as in (5.4).

Even in the case of quadratic Hamiltonians, the evolution of the fidelity is not trivial because of the difference in the forward and backward motions. In figure 5, we display the fidelity amplitude for $\widehat{H}_{\pm} = \frac{1}{2}(p^2 + k_{\pm}q^2)$, i.e. a pair of harmonic oscillators with different frequencies, and compare it with the DR, as well as the corrected DR developed in [25]. We can observe that equation (5.4) is essentially equal to the exact quantum calculation, as expected.

The usual picture for fidelity decay has two components: the decay of classical overlaps and the decay of dephasing [27, 18]. The DR approximation only takes into account the dephasing part; thus, it successfully describes the quantum-mechanical decays for complex systems but it fails in systems with recurrences or *revivals* of the fidelity. The more rigorous approach in [25] includes a short time correction for the amplitude, which as shown in figures 5(a) and (b), compensates this decay and furnishes more accurate evaluation for fidelity at small times (see figures 5(b) and (d)).

Summarizing this section, formulae (5.3) and (5.4) evaluate the fidelity amplitude with the simplicity of the DR prefactor but with a higher accuracy. In the present example, where both Hamiltonians are quadratic, the trajectories are known analytically, so there is no increase of numerical effort with respect to the perturbation approach in [25]. We remark that for higher dimensional systems, the propagation of the monodromy matrices can be considered a challenge, for which some strategies are developed in the literature; see, e.g., [28, 26].

6. IVR or FVR for evolving expectation values

SC evolution of expectation values for observables or general quantum operators may also be evaluated by means of a direct IVR or FVR. All one needs is to exchange variables in

$$\langle \hat{A}\rangle(t) = \mathrm{tr}(\hat{\rho}(t)\,\hat{A}) = \int \frac{\mathrm{d}\mathbf{x}}{2\pi\hbar}\, A(\mathbf{x})\, \mathrm{tr}(\widehat{\rho}(t)\,\widehat{R}_{\mathbf{x}}) = \int \frac{\mathrm{d}\boldsymbol{\xi}}{2\pi\hbar}\, \tilde{A}(\boldsymbol{\xi})\, \mathrm{tr}\Big(\widehat{\rho}(t)\,\widehat{T}_{-\boldsymbol{\xi}}\Big), \tag{6.1}$$

that is, there is just an extra integral on top of (4.3) or (4.4). This becomes especially symmetric in the case of the FVR:

$$\langle \hat{A}\rangle(t) = 2^N \int \frac{\mathrm{d}\mathbf{x}'\,\mathrm{d}\boldsymbol{\xi}'}{(2\pi\hbar)^{2N}} \sqrt{|\det[\mathbf{M}(\mathbf{x}^+)+\mathbf{M}(\mathbf{x}^-)]|} \times \exp\left[\frac{\mathrm{i}}{\hbar}\left[S_{-\boldsymbol{\xi}'}\left(\frac{\boldsymbol{x}^+ + \boldsymbol{x}^-}{2}\right) + \frac{\hbar\sigma\pi}{2}\right]\right] \tilde{A}(-\boldsymbol{\xi}') W\left(\frac{\boldsymbol{x}^+ + \boldsymbol{x}^-}{2}\right) \tag{6.2}$$

or

$$\langle \hat{A}\rangle(t) = 2^N \int \frac{\mathrm{d}\mathbf{x}'\,\mathrm{d}\boldsymbol{\xi}'}{(2\pi\hbar)^{2N}} \sqrt{|\det[\mathbf{M}(\mathbf{x}^+)+\mathbf{M}(\mathbf{x}^-)]|} \times \exp\left[-\frac{\mathrm{i}}{\hbar}\left[\tilde{S}_{\mathbf{x}'}(-(\boldsymbol{x}^+ - \boldsymbol{x}^-)) + \frac{\hbar\tilde{\sigma}\pi}{2}\right]\right] A(\mathbf{x})\,\chi(\boldsymbol{x}^+ - \boldsymbol{x}^-). \tag{6.3}$$

One can immediately recognize that here the integrals are carried out over the full double phase space variables, that is, the final values for the returning trajectories $\boldsymbol{x}^{\pm\prime}$ in which terms we have

$$\langle \hat{A}\rangle(t) = 2^N \int \frac{\mathrm{d}\boldsymbol{x}^{+\prime}\,\mathrm{d}\boldsymbol{x}^{-\prime}}{(2\pi\hbar)^{2N}} \sqrt{|\det[\mathbf{M}(\mathbf{x}^+)+\mathbf{M}(\mathbf{x}^-)]|} \times \exp\left[\frac{\mathrm{i}}{\hbar}\left[S_{-\boldsymbol{\xi}'}\left(\frac{\boldsymbol{x}^+ + \boldsymbol{x}^-}{2}\right) + \frac{\hbar\sigma\pi}{2}\right]\right] \tilde{A}(\boldsymbol{x}^- - \boldsymbol{x}^+) W\left(\frac{\boldsymbol{x}^+ + \boldsymbol{x}^-}{2}\right) \tag{6.4}$$

or

$$\langle \hat{A}\rangle(t) = 2^N \int \frac{\mathrm{d}\boldsymbol{x}^{+\prime}\,\mathrm{d}\boldsymbol{x}^{-\prime}}{(2\pi\hbar)^{2N}} \sqrt{|\det[\mathbf{M}(\mathbf{x}^+)+\mathbf{M}(\mathbf{x}^-)]|} \exp\left[\frac{\mathrm{i}}{\hbar}\left[\tilde{S}_{\mathbf{x}'}(-(\boldsymbol{x}^+ - \boldsymbol{x}^-)) + \frac{\hbar\tilde{\sigma}\pi}{2}\right]\right] A\left(\frac{\boldsymbol{x}^- + \boldsymbol{x}^-}{2}\right) \chi(\boldsymbol{x}^+ - \boldsymbol{x}^-). \tag{6.5}$$

Thus, in both cases, the endpoints of the pair of backward trajectories specify the chord, for the chord representation of $\widehat{A}$, or the centre, for the Weyl representation of $\widehat{\rho}$, or vice versa. In any case, all trajectory integrations are carried out for a time t, rather than $2t$. We have here privileged the density operator, but similar formulae follow for arbitrary $\mathrm{tr}(\widehat{A}\,\widehat{B}(t))$[6].

The choice between the alternative FVRs for evolving expectation values (6.4) or (6.5) depends on the operators involved. It should be recalled that the chord function is immediately obtained from the Wigner function, within a phase factor and a change of scale, if the state has a centre of symmetry [41], which is the case of coherent states and the eigenstates of the harmonic oscillator. Besides the obvious *classical observables* that are suitably symmetrized polynomial functions of momenta and positions, choices such as $\delta(\widehat{p} - p_0)$ or $\delta(\widehat{q} - p_0)$ may be physically relevant [29]. Evidently, the integrals in (6.4) and (6.5) are greatly simplified in these instances.

[6] Curiously, these are generally referred to as *correlations* in the chemical literature, even though the statistical sense only arises for the density operator, where they are just expectation values.

7. Discussion

It is a formal possibility to work directly with a centre–centre propagator, i.e. the propagator for the Wigner function in (4.3), instead of the mixed centre–chord or chord–centre formulae that we have presented. Besides the difficulty with the limits of small time and quadratic Hamiltonians, one should note that though the region of the direct trajectory is then no longer a caustic, because of the switch of variables, it has instead a nodal line in the amplitude. Thus, even when it should work, there must be some overall compensation for omitting that which should be the dominant classical contribution, with very dangerous effects for numerical convergence for the IVR or the FVR integrals. It may still be interesting to investigate whether sensible results can be obtained in this direct approach, but, for the moment, we are confining to numerical investigations for the Kerr Hamiltonian [36], within the theory developed here.

It is certainly illuminating to translate this entire theory into double phase space. Following [37], this is the basis for the presentation of mixed propagators in [33]. The advantage is that pairs of trajectories become a single trajectory driven by an appropriate double Hamiltonian. The SC theory for evolving unitary operators is then reduced to ordinary WKB theory, i.e. Van Vleck evolution in double phase space. Nonetheless, the emphasis here has been on obtaining usable formulae with the least theoretical investment and the interested reader should have no difficulty in adapting the discussion in [33].

The doubling of phase space does become indispensible for the SC treatment of motion for open quantum systems [38, 39] because dissipation destroys the decomposition of a double phase space trajectory into trajectory pairs in a single phase space [40]. The possibility of extending the present theory for Markovian open systems may turn the SC approximations of open systems into a viable future computational tool.

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