Nonlinear semiclassical dynamics of open systems

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A semiclassical approximation for an evolving density operator, driven by a ‘closed’ Hamiltonian and ‘open’ Markovian Lindblad operators, is reviewed. The theory is based on the chord function, i.e. the Fourier transform of the Wigner function. It reduces to an exact solution of the Lindblad master equation if the Hamiltonian is a quadratic function and the Lindblad operators are linear functions of positions and momenta. The semiclassical formulae are interpreted within a (real) double phase space, generated by an appropriate classical double Hamiltonian. An extra ‘open’ term in the double Hamiltonian is generated by the non-Hermitian part of the Lindblad operators in the general case of dissipative Markovian evolution. Decoherence narrows the relevant region of double phase space to the neighbourhood of a caustic for both the Wigner function and the chord function. This difficulty is avoided by the definition of a propagator, here developed in both representations. Generalized asymptotic equilibrium solutions are thus presented for the first time.

Keywords: decoherence; quantum Markovian systems; phase-space representations; semiclassical mechanics

1. Introduction

The most general description of the state of a system in quantum mechanics is the density operator $\hat{\rho}$, also called the ‘state operator’, normalized by $\text{tr} \hat{\rho} = 1$. If we have complete knowledge about the system in the quantum-mechanical sense, then the state operator $\hat{\rho}$ is a projector $\hat{\rho} = |\psi\rangle\langle\psi|$ and the state is said to be pure, i.e. its von Neumann entropy, $S = -\text{tr} \ln \hat{\rho}$, is null, and its purity $\text{tr} \hat{\rho}^2 = 1$. If we have incomplete knowledge about the system, then the state operator $\hat{\rho}$ is not a projector any more, so the state, with $S > 0$, is said to be in a statistical mixture and $\text{tr} \hat{\rho}^2 < 1$.

Basic quantum theory presupposes that the system is isolated, so that the evolution is unitary and preserves the state’s purity. However, generally, in practical situations that certainly hold for mesoscopic systems, they inevitably interact to some extent with an environment. Thus, an initially pure state will

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One contribution of 17 to a Theme Issue ‘Nonlinear dynamics in meso and nano scales: fundamental aspects and applications’.

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undergo a non-unitary evolution that will not preserve purity; one is in the paradigm of quantum open systems. The consequences are threefold. Decoherence corresponds to the vanishing of the off-diagonal terms of the density operator. Albeit this is a purely quantum process, its outcome is to generate a statistical distribution that can be interpreted classically. Dissipation corresponds to the loss or gain of energy, and is usually considered as much slower than decoherence, especially for large systems. Of course, this process is shared by classical open systems, as is diffusion, i.e. the spatial broadening of the probability distribution for finding the system.

The general evolution of $\hat{\rho}(t)$ for an open system is a practical issue in many experimental situations, already well established in quantum optics [1], also in atomic and nuclear physics, and more recently in the physics of quantum information, where it is of crucial importance to control the interaction of the system with its environment, in order to avoid decoherence. To construct theoretical models with the maximum of generality, it is generally admitted that such an evolution should satisfy at least three basic requirements: preservation of Hermiticity ($\text{tr} \hat{\rho} \hat{A} \in \mathcal{R}$), trace ($\text{tr} \hat{\rho} = 1$) and positivity ($\text{tr} \hat{\rho} |j\rangle \langle j| \geq 0$).

Two main approaches have been explored to obtain explicit dynamics of an open quantum system. The first is to consider that the open system is part of a larger closed system, which itself obeys a unitary evolution, and then to trace over the environment, i.e. over all the degrees of freedom that are not directly concerned with the system under study. Such an approach leads to the Bloch–Redfield equations [2,3]. The second is to assume that, beyond the general requirements previously introduced, the time evolution should obey a semigroup law, that is, a forward translational time invariance. Then, the most general equation was derived by Lindblad [4] (see also [5–7]). The great advantage of this latter approach, which is adopted here, is its great generality, but it is most reliable in the case where the coupling to the environment is weak.

The Lindblad master equation describes the general evolution for Markovian open systems under the weakest possible constraint. Given the internal Hamiltonian, $\hat{H}$, and the Lindblad operators, $\hat{L}_k$, which account for the action of the random environment, the evolution of the density operator may be reduced to the canonical form

$$
\frac{\partial \hat{\rho}}{\partial t} = -\frac{i}{\hbar} [\hat{H}, \hat{\rho}] + \frac{1}{\hbar} \sum_k \left( \hat{L}_k \hat{\rho} \hat{L}_k^\dagger - \frac{1}{2} \hat{L}_k^\dagger \hat{L}_k \hat{\rho} - \frac{1}{2} \hat{\rho} \hat{L}_k^\dagger \hat{L}_k \right),
$$

so that, in the absence of the environment ($\hat{L}_k = 0$), the motion is governed by the Liouville–von Neumann equation appropriate for unitary evolution.

A typical example is based on the Jaynes–Cummings model, which describes the interaction of a two-level atom with a single mode of the optical field in a cavity. The statistically independent arrival of atoms leads to the damped harmonic oscillator equation for the photon field,

$$
\frac{\partial \hat{\rho}}{\partial t} = -\frac{i}{\hbar} [\hat{a}^\dagger \hat{a}, \hat{\rho}] + \frac{A}{\hbar} (v + 1) \left( \hat{a}^\dagger \hat{\rho} \hat{a} - \frac{1}{2} \hat{a}^\dagger \hat{a} \hat{\rho} - \frac{1}{2} \hat{\rho} \hat{a}^\dagger \hat{a} \right) + \frac{A}{\hbar} v \left( \hat{a}^\dagger \hat{\rho} \hat{a} - \frac{1}{2} \hat{a}^\dagger \hat{a} \hat{\rho} - \frac{1}{2} \hat{\rho} \hat{a}^\dagger \hat{a} \right),
$$

$\textit{Phil. Trans. R. Soc. A}$ (2011)
where we identify the pair of Lindblad operators as proportional to the annihilation operator \( \hat{a} = (\hat{q} + i\hat{p})/\sqrt{2} \) and the creation operator \( \hat{a}^\dagger = (\hat{q} - i\hat{p})/\sqrt{2} \) for photons in the field mode (e.g. [8,9] and references therein). To simplify the notation, we will restrict the formulae in this review to the case of a single Lindblad operator.

The case where the Lindblad operators are all self-adjoint has deserved special attention. It is known that the corresponding Lindblad equation describes decoherence, or dephasing, as well as diffusion, but no dissipation [7]. Since the latter is usually a much slower process, it is often useful to simplify the evolution by considering only the self-adjoint part of the \( \hat{L}_j \)'s when studying the decoherence process, as in the semiclassical theory proposed in Ozorio de Almeida [10]. However, most physical processes for an open system such as equation (1.2) are dissipative. It is, therefore, desirable to develop a semiclassical theory for the evolution of the density operator that combines the description of both the initial decoherence process and the more classical development of diffusion and dissipation.

In this paper, we review the formalism for treating the semiclassical limit of evolving density operators subject to equation (1.1), including the cases where the Lindblad operators are not self-adjoint [11]. By semiclassical, we mean generalized Wentzel, Kramers and Brillouin (WKB) expansions (e.g. [12]), as opposed to simple power expansions in \( \bar{\hbar} \). The present theory expands on our phase–space treatment for the semiclassical evolution of closed systems in Rios & Ozorio de Almeida [13] and of non-dissipative open Markovian systems in Ozorio de Almeida [10]. In so doing, we now establish contact with the semiclassical theory for the propagator of Wigner functions that has been developed by Dittrich et al. [14]. Indeed, we present here a generalization of their propagator for Markovian systems.

The basic modification of WKB semiclassical theory, which is required for treating Markovian dissipation, is that it is necessary to work in double phase space: \( (x, \xi) \in \mathbb{R}^{2N} \times \mathbb{R}^{2N} \). This is a natural setting for the corresponding description of the semiclassical evolution of the density operator [15,16], or indeed, for the representation of general operators acting on the Hilbert space of quantum states, considered as superpositions of \( |ket \rangle \langle bra | \) elements. Just as an evolving quantum state, \( |\psi \rangle \), corresponds to an evolving surface in simple phase space, \( x \in \mathbb{R}^{2N} \), the unitary evolution of a pure state density operator in a closed system, that is, a projector, \( |\psi \rangle \langle \psi | \), corresponds to the evolution of a surface in double phase space. We thus obtain a formal generalization of the WKB framework, where an approximate oscillating solution of the Schrödinger equation is built from a classically evolving solution [12,17,18]. However, even in the standard case of a closed system and hence unitary quantum evolution, it becomes necessary to make a strong restriction on the allowed form of the corresponding classical double Hamiltonian [19,20].

The crucial point is that an additional term in the double Hamiltonian, which accounts for dissipation, is produced naturally by the semiclassical treatment of the open terms in the master equation. This new term depends exclusively on the Lindblad operators and cancels in the special case where these are self-adjoint. As it should be, the resulting description of the full semiclassical evolution again coincides with the exact solution of the master equation in the quadratic case.
The adaptation for Markovian systems has been achieved for both the real and the complex forms of WKB semiclassical theory, in Ozorio de Almeida et al. [11] and in Brodier & Ozorio [21], respectively. The latter is more complete, and it can be used to propagate local coherent states and their superpositions (Schrödinger cat states) as well as the usual semiclassical states that are supported by surfaces in phase space. Furthermore, it is shown in [21] that the real version can be obtained by applying classical perturbation theory to the complex formalism. Even so, there is no denying the more intuitive aspects of the real theory. Another reason for choosing the real approach in this article is that we shall concentrate on the propagators that correspond to initially flat surfaces in the real double phase space.

The emphasis in this article is to present clearly the results of a henceforth rather abstract theory so they can be readily applied. For this reason, all subtle points concerning the derivations and discussion of domains of validity are left to the original papers. Nonetheless, our presentation of the semiclassical propagators has several new features and the approach to equilibrium in this context is discussed here for the first time.

2. Lindblad equation in the Weyl formalism

The Weyl representation maps every quantum operator onto a phase-space function, that is, a function of the vector \( x = (p, q) \) [22,23]. For an operator \( \hat{A} \), the Weyl symbol \( A \) is defined as

\[
A(x) = 2 \mathcal{N} \int \exp \left( -\frac{i}{\hbar} pQ \right) \left( q + \frac{Q}{2} |\hat{A}|q - \frac{Q}{2} \right) \, dQ = \text{tr} (2\hat{R}_x \hat{A}),
\]

with \( \mathcal{N} = 1/(2\pi \hbar) \) if there is only one degree of freedom, which will be assumed to simplify the notation. The second equation involves, \( \hat{R}_x \), the operator for reflection through the point \( x \) [24,25], which is the Fourier transform of the more familiar translation (or displacement) operator

\[
\hat{T}_\xi = \exp \left\{ \frac{i}{\hbar} (\xi \wedge \hat{x}) \right\}.
\]

Here, the wedge product of two vectors \( x = (p, q) \) and \( x' = (p', q') \) is defined by \( x \wedge x' = pq' - p'q = Jx \cdot x' \), which also defines the skew matrix \( J = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \). The Weyl symbol of the state operator \( \hat{\rho} \) is the Wigner function [26]

\[
W(x) = \mathcal{N} \int \exp \left( -\frac{i}{\hbar} pQ \right) \left( q + \frac{Q}{2} |\hat{\rho}|q - \frac{Q}{2} \right) \, dQ,
\]

while its Fourier transform, the chord function \( \chi(\xi) \), one of the quantum characteristic functions, is

\[
\chi(\xi) = \mathcal{N} \int \exp \left( -\frac{i}{\hbar} \xi \wedge x \right) W(x) \, dx.
\]
One can obtain the chord symbol directly from the quantum operator through the formula

\[
\chi(\xi) = N \int \exp \left( -\frac{i}{\hbar} \xi_p q \right) \left( q + \frac{\xi_q}{2} \hat{\rho} | q - \frac{\xi_q}{2} \right) dq = \frac{1}{2\pi \hbar} \text{tr} (\hat{T}_- \hat{\rho}).
\]  

(2.5)

We call the space of all \(x\) the centre space, and the space of all \(\xi\) the chord space.

In the chord space, by using product rules for the product of operators [22,27], the Lindblad equation is represented by a partial differential equation. In the case where the Lindblad operators are linear functions of \(\hat{p}\) and \(\hat{q}\), that is,

\[
\hat{L} = \mathbf{l}' \cdot \hat{x} + i \mathbf{l}'' \cdot \hat{p},
\]  

(2.6)

with \(\mathbf{l}'\) and \(\mathbf{l}''\) real vectors, the master equation can be written

\[
\frac{\partial \chi}{\partial t}(\xi, t) = -\frac{i}{\hbar} N \int \left[ H(x + \frac{1}{2} \xi, t) - H(x - \frac{1}{2} \xi, t) \right] \times \exp \left( \frac{i}{\hbar} (\xi' - \xi) \cdot x \right) \chi(\xi', t) d\xi' dx 
- \gamma \xi \cdot \frac{\partial \chi}{\partial \xi} (\xi, t) - \frac{1}{2\hbar} \left( (\mathbf{l}' \cdot \xi)^2 + (\mathbf{l}'' \cdot \xi)^2 \right) \chi(\xi, t).
\]  

(2.7)

The dissipation coefficient,

\[
\gamma = \mathbf{l}'' \cdot \mathbf{l}',
\]  

(2.8)

is null for a Hermitian Lindblad operator (\(\mathbf{l}'' = 0\)), and we then have a purely diffusive case. \(H\) is the Weyl representation of the Hamiltonian of the isolated system and coincides with the corresponding classical Hamiltonian, up to corrections coming from non-commutativity of \(\hat{p}\) and \(\hat{q}\). Its arguments in equation (2.7) are the pair of remarkable points \(x_+ = x + \frac{\xi}{2}\) and \(x_- = x - \frac{\xi}{2}\), which can be considered as both tips of a chord \(\xi\), centred on \(x\). Although this chord \(\xi = (\xi_p, \xi_q)\) can be interpreted as an auxiliary conjugate variable of \(x\), in the current approach, it is actually more convenient to write the solution in terms of \(y = J \xi = (-\xi_q, \xi_p)\) (in order to respect the symplectic structure of the double phase space). The direct sum of these conjugate spaces can be interpreted as a double phase space, where \(x\) formally plays the role of the position \(q\), and \(y\) the role of its Fourier conjugate, the momentum \(p\). Then, the above equation becomes

\[
\frac{\partial \chi}{\partial t}(y, t) = -\frac{i}{\hbar} N \int \left[ H \left( x - \frac{1}{2} J y, t \right) - H \left( x + \frac{1}{2} J y, t \right) \right] \times \exp \left( \frac{i}{\hbar} (y' - y) \cdot x \right) \chi(y', t) dy' dx 
- \gamma y \cdot \frac{\partial \chi}{\partial y} (y, t) - \frac{1}{2\hbar} \left( (\mathbf{l}' \cdot y)^2 + (\mathbf{l}'' \cdot y)^2 \right) \chi(y, t).
\]  

(2.9)

The same name has been kept for the characteristic function \(\chi(y, t)\), though strictly this should be \(\chi(\xi, t) = \chi(-Jy, t)\).
The term $\mathbf{y} \cdot (\partial \chi / \partial \mathbf{y})$ can actually be included in the integral term by an integration by parts of the exponential, so

$$
\frac{\partial \chi}{\partial t}(\mathbf{y}, t) = -\frac{i}{\hbar} \mathcal{N} \int \mathbb{H}(\mathbf{x}, \mathbf{y}, t) \exp\left(\frac{i}{\hbar} (\mathbf{y}' - \mathbf{y}) \cdot \mathbf{x}\right) \chi(\mathbf{y}') d\mathbf{y}' d\mathbf{x} - \frac{1}{2\hbar} [(\mathbf{l}' \wedge \mathbf{y})^2 + (\mathbf{l}'' \wedge \mathbf{y})^2] \chi(\mathbf{y}, t),
$$

(2.10)

with

$$
\mathbb{H}(\mathbf{x}, \mathbf{y}, t) = H(\mathbf{x} - \frac{1}{2} J \mathbf{y}, t) - H(\mathbf{x} + \frac{1}{2} J \mathbf{y}, t) - \gamma \mathbf{x} \cdot \mathbf{y}
$$

$$
= H^+(\mathbf{x}, \mathbf{y}) - H^-(\mathbf{x}, \mathbf{y}) - \gamma \mathbf{x} \cdot \mathbf{y}.
$$

(2.11)

This is exactly the double Hamiltonian that generates the classical motion underlying the semiclassical approximations in [11]. Obviously, the double Hamiltonian will be time independent if it is obtained from a time-independent single Hamiltonian. Furthermore, in the absence of dissipation, both $H^+(\mathbf{x}, \mathbf{y}) = H(\mathbf{x} - \frac{1}{2} J \mathbf{y})$ and $H^-(\mathbf{x}, \mathbf{y}) = H(\mathbf{x} + \frac{1}{2} J \mathbf{y})$ will also be constants that generate independent motions for both chord tips. Indeed, the variables,

$$
\mathbf{x}^\pm = \mathbf{x} \pm \frac{1}{2} \xi = \mathbf{x} \mp \frac{1}{2} J \mathbf{y},
$$

(2.12)

are alternative coordinates for the double phase space, except for a single change of sign [15,16]. Thus, the non-dissipative double-phase-space trajectory can be identified with a pair of single-phase-space trajectories. These arise in the semiclassical limit of the path integral theory for dissipative systems created by Feynman & Vernon [28] and further developed by Caldeira & Leggett [29].

Alternatively, the definition of the complex double Hamiltonian

$$
\mathbb{H}_c(\mathbf{x}, \mathbf{y}, t) = \mathbb{H}(\mathbf{x}, \mathbf{y}, t) - \frac{i}{2} [(\mathbf{l}' \wedge \mathbf{y})^2 + (\mathbf{l}'' \wedge \mathbf{y})^2]
$$

(2.13)

leads to

$$
\frac{\partial \chi}{\partial t}(\mathbf{y}, t) = -\frac{i}{\hbar} \mathbb{H}_c \left(-\frac{\hbar}{i} \frac{\partial}{\partial \mathbf{y}} \right)^{(1)} \mathbf{y}^{(2)}, t) \chi(\mathbf{y}, t),
$$

(2.14)

where $(1)$ and $(2)$ mean that the derivatives are taken first and then the $\mathbf{y}$ terms are multiplied. Given this specific choice of ordering for the operators $\hat{\mathbf{y}} = \mathbf{y}$ and $\hat{\mathbf{x}} = -(\hbar/i)(\partial/\partial \mathbf{y})$, this is completely analogous to the Schrodinger equation, which thus allows us to extend the various forms of WKB theory, once it is recalled that variations in operator ordering have effects that are semiclassically small.

The differential term on the r.h.s. of equation (2.14) (or the integral term on the RHS of equation (2.10)) represents the unitary part of the evolution. In other words, in the chord representation, the commutator is specified by the real double Hamiltonian as

$$
[\hat{H}, \hat{\rho}] \text{chord} = \mathbb{H} \left(-\frac{\hbar}{i} \frac{\partial}{\partial \mathbf{y}} \right)^{(1)} \mathbf{y}^{(2)}, t) \chi(\mathbf{y}, t).
$$

(2.15)
3. Semiclassical approximation

We here assume that the chord representation $\chi(y,0)$ of the initial state has the usual semiclassical form. Following the real theory in [11], we start by considering its semiclassical evolution under the action of the real double Hamiltonian (2.11), which takes the form

$$\chi^0(y, t) = A(y, t) \exp \frac{i}{\hbar} S(y, t), \quad (3.1)$$

where $S(y, t)$ is a real-valued function of order $O(\hbar^0)$. This is the correct semiclassical treatment for unitary evolution, but, so far, the only effect of the Lindblad operators lies in the dissipative term of the Hamiltonian. It is important to note that we can evolve any linear combination of such states, as a consequence of the linearity of the Lindblad equation. This is necessarily the case in the presence of caustics, as will be discussed in §5.

This semiclassical form naturally induces an $\hbar$-expansion of the unitary part of the equation,

$$\mathbb{H} \left( -\frac{\hbar}{i} \frac{\partial}{\partial y} (1), y, t \right) \chi(y, t) = \left[ \mathbb{H} \left( -\frac{\partial S}{\partial y}(y, t), y, t \right) + O(\hbar) \right] \chi(y, t). \quad (3.2)$$

Hence, one obtains the Hamilton–Jacobi equation

$$\frac{\partial S}{\partial t}(y, t) = -\mathbb{H} \left( -\frac{\partial S}{\partial y}(y, t), y, t \right) + O(\hbar), \quad (3.3)$$

which leads to a double-phase-space generalization of WKB theory. The present Hamilton–Jacobi equation is defined by a Hamiltonian of unusual form: it does not separate into the familiar kinetic- and potential-energy terms. Because of this unusual feature, we work directly with the Hamiltonian formalism in the full double phase space, rather than attempting to connect the evolving action to a Lagrangian.

In general, the initial action specifies a Lagrangian surface of half the dimension of the double phase space,

$$y_0 = z \quad \text{and} \quad x_0 = -\frac{\partial S_0}{\partial y}(z). \quad (3.4)$$

To obtain the formal solution of the Hamilton–Jacobi equation, it is convenient to define a family of classical trajectories $(x_t, y_t)$ in the double phase space, with initial conditions on this initial surface and driven by the double Hamiltonian (2.11) through Hamilton’s equations

$$\dot{y}_\tau = -\frac{\partial \mathbb{H}}{\partial x}(x_\tau, y_\tau, \tau) \quad \text{and} \quad \dot{x}_\tau = \frac{\partial \mathbb{H}}{\partial y}(x_\tau, y_\tau, \tau). \quad (3.5)$$

In the present simple case of a single degree of freedom, this family is spanned by variables $z$ (two dimensions) and $\tau$ (one dimension). Hence, this forms a real submanifold $\mathcal{M}$ with three dimensions, within a phase space of four dimensions of $(x, y)$. This submanifold, which will serve as a backbone to build our solution, is completely parametrized by $(y, \tau)$ through a function $x_{\mathcal{M}}(y, \tau)$, such that $(x_{\mathcal{M}}(y, \tau), y)$ is the most general point of $\mathcal{M}$. 

*Phil. Trans. R. Soc. A* (2011)
It is well known that the solution $S(y, t)$ of the Hamilton–Jacobi equation (3.3) is the generating function of the submanifold $(x_M(y, t), y)$ for each $t$ [30]. Hence, we can define the solution

$$S(y, t) = S_0(y_i) + \int_{y_i, 0}^{y, t} \delta s,$$

(3.6)

where $y_i$ is arbitrary and the integral can be performed along any path of $\mathcal{M}$ joining $(y_i, 0)$ to $(y, t)$. A natural choice of such a path is $(\tilde{y}_t, \tau)$, such that $(\tilde{x}_t, \tilde{y}_t)$ is the classical trajectory of $\mathcal{M}$ with $\tilde{y}_t = y$, literally the history of $y$ at time $t$. We have, in particular, $x_M(\tilde{y}_t, \tau) = \tilde{x}_t$. The choice of this trajectory sets the value of $y_i = \tilde{y}_0$. Then, one can write more explicitly

$$S(y, t) = S_0(\tilde{y}_0) + \int_0^t \left[ -\tilde{x}_t \cdot \frac{\partial \tilde{y}_t}{\partial \tau} - H(\tilde{x}_t, \tilde{y}_t, \tau) \right] d\tau.$$

(3.7)

One should keep in mind that $(\tilde{x}_t, \tilde{y}_t)$ implicitly depends on $(y, t)$, and in particular $\tilde{y}_0$ and $\tilde{x}_0 = -\left( \frac{\partial S_0}{\partial y}(\tilde{y}_0) \right)$ are functions of $(y, t)$. The final expression of the solution, in terms of the double Hamiltonian, is then

$$\chi^0(y, t) = \mathcal{K} \left| \det \frac{\partial^2 S}{\partial y^2} \right|^{1/2} \exp \left( \frac{i}{\hbar} S(y, t) \right).$$

(3.8)

Here, the normalization constant, $\mathcal{K}$, may depend on the presence of caustics that will be discussed in §5.

Our final task is to include the full effect of the Lindblad operators on the WKB evolution described above. The outcome of the real semiclassical theory in [11] is that

$$\chi(y, t) = \chi^0(y, t) \exp \left[ -\frac{1}{2\hbar} D(y, t) \right],$$

(3.9)

where the decoherence functional, in the simple case where the Lindblad operators are linear functions of positions and momenta (2.6), is just

$$D(y, t) = \int_0^t \left[ (I' \wedge \tilde{y}_\tau)^2 + (I'' \wedge \tilde{y}_\tau)^2 \right] d\tau.$$

(3.10)

One should note that it is a full double-phase-space trajectory that enters this definition, as specified by equation (3.5). The final chord $y$ determines the final centre, $x(y)$, given by the evolved Lagrangian surface, and it is along the previous trajectory of this point that the integration is performed. The more satisfactory derivation of equation (3.9) in [21] is based on the full complex WKB theory, with the complex Hamiltonian (2.13), but deals with its imaginary part through classical perturbation theory. This holds, under our assumption that the effect of the environment is weak and that the initial action of the chord function is real. The latter requirement holds for initial Bohr-quantized states and for the particularly simple initial action of the propagator in §5.

No matter how full of quantum correlations the initial state might be, the exponential of the decoherence functional in equation (3.9) progressively squeezes them out. This process, by which the large chords are quenched, proceeds irreversibly, since $D(y, t)$ is a non-decreasing function of time. The only possibility for the decoherence functional not to increase arises for pairs
of classical trajectories generated by $H(x)$, lying along a level submanifold of the linear Lindblad–Weyl function, $L(x)$, i.e. the condition is that the Poisson bracket $\{L, H\} = 0$, which holds when the operators $\hat{L}$ and $\hat{H}$ commute.

The semiclassical evolution of the Wigner function for open conservative Markovian systems is obtained by the Fourier transform of expression (3.9) for the chord function. The evolving Wigner function, $W(x, t)$, is a convolution of the unitarily evolving semiclassical Wigner function with the Fourier transform of the decaying amplitude term. This diffusive window, which coarse-grains the Wigner function, will broaden with time, as its inverse Fourier transform narrows down the range of the chord function. In the case of a quadratic Hamiltonian, to be treated in the following section, the window will be Gaussian, and this description of the evolution of the Wigner function becomes exact [31].

4. The quadratic case

In the quadratic case, the solution of the semiclassical approximation, combining equation (3.9) with equation (3.8), coincides with the exact solution derived in [31]. In this respect, the situation is entirely analogous to that of ordinary WKB approximations for evolving pure states, though it may not be so obvious, in view of the extra factor depending on the decoherence functional. However, this just becomes part of the phase in the complex theory in [21] and it turns out that, for this special case, the complex and the real results are equal.

We start from a quadratic Hamiltonian

$$H(x) = x \cdot Hx,$$  \hspace{1cm} (4.1)

with some symmetric matrix $H$. The double-phase-space Hamiltonian,

$$H_h(x, y) = -2x \cdot HJy - \gamma x \cdot y,$$  \hspace{1cm} (4.2)

induces the following linear double-phase-space dynamics:

$$\dot{x}_r = (2JH - \gamma)x_r \quad \text{and} \quad \dot{y}_r = (2HJ + \gamma)y_r.$$  \hspace{1cm} (4.3)

Note that the classical evolution of centres and chords is completely decoupled in this simple case. The effect of the dissipative term in the double Hamiltonian is to produce a contraction of the space of centres, $x$, whereas the chords (both $y$ and $\xi$) expand, if the dissipation coefficient, $\gamma$, is positive. Then, the ‘history’ of $(y, t)$ is

$$\tilde{y}_t = P_t^\top y,$$  \hspace{1cm} (4.4)

in the notation of §3. Here, $P_t$ defines the classical propagation operator for the linear chord evolution in (4.3), that is

$$P_t = \exp(2JHt + \gamma I),$$  \hspace{1cm} (4.5)

$P_t^\top$ stands for its transpose and $I$ is the identity matrix. The expression of $S(y, t)$ given by equation (3.7) becomes simply

$$S(y, t) = S^0(P_t^\top y),$$  \hspace{1cm} (4.6)
whereas the decoherence functional is a quadratic form in $y$,

$$
D(y, t) = \int_{0}^{t} \left[ (l' \wedge P_{l-t}^{\top} y)^{2} + (l'' \wedge P_{l-t}^{\top} y)^{2} \right] dt'.
$$

(4.7)

Hence, the full real WKB solution can be written as

$$
\chi(y, t) = \chi^{0}(P_{t}^{\top} y) \exp \left( -\frac{1}{2\hbar} D(y, t) \right).
$$

(4.8)

Recalling our use of the same symbol, $\chi(y)$, as a shorthand for $\chi(x, t) = \chi(-Jy, t)$, it is shown in [11] and [21] that the real WKB approximation coincides exactly with the exact solution in the quadratic case.

Thus, the general picture is that of exact classical propagation of the chord function (the same as the unitary evolution generated by the quadratic Hamiltonian), multiplied by a Gaussian factor that progressively attenuates the contribution of long chords. It must be emphasized that this exact theory for the case of quadratic evolution is in no way restricted, as concerns the nature of the initial density operator to be evolved. The problem of caustics, to be addressed in the following section, does not arise, and coherent, or otherwise, localized states are also included. In particular, this exact result also governs the evolution of the reflection operator itself, in its role of propagator, because of the linearity of the Lindblad equation.

5. Semiclassical Markovian propagators

So far, we have ignored the problem of caustics in the discussion of the semiclassical evolution of a density operator that corresponds to a Lagrangian surface in double phase space. For common Bohr-quantized pure states, the corresponding Lagrangian surface has more than one branch. Mostly, this merely requires us to sum over the branches, as in [11], but these branches join along caustics, where simple WKB theory breaks down and it must, hence, be replaced by improved uniform approximations [32,33]. It turns out that, for the Bohr-quantized states studied in these references, the classical small-chord region lies in the neighbourhood of a caustic for both the chord function and the Wigner function. In other words, the region of the Lagrangian submanifold, lying close to the centre subspace $y = 0$ in double phase space, projects singularly onto both the $x$-subspace and the $y$-subspace. This is a serious problem, as in the present semiclassical picture for Markovian evolution of the density operator, the decoherence functional quickly quenches the contribution of large chords, so that only the caustic survives! Hence, the direct semiclassical theory above is only applicable to the initial stages of Markovian evolution, before the long chords are mostly quenched.

One way out of this problem is to consider alternative Lagrangian surfaces, which do not have caustics, at least initially. This is the approach adopted in Ozorio de Almeida & Brodier [20]. Instead of a surface that corresponds to $R(t)$, but has undesirable caustics, we evolve the coordinate planes themselves, $x = \text{const.}$, corresponding to a unitary reflection, $R_{x}$. The $x = \text{const.}$ plane has no caustic in its $y$-projection. Furthermore, a finite time must pass before the
evolution generated by the double Hamiltonian can bend these submanifolds sufficiently to produce caustics, until which time the chord representation of \( \hat{R}_x(t) \) will be represented in a simple semiclassical form, i.e. \( \tilde{R}_x(\xi, t) \) or \( \tilde{R}_x(y, t) \), will have a single semiclassical branch.

In this way, we obtain a semiclassical approximation to the evolution, whether unitary or Markovian, by inserting the approximate evolved operators in the exact relations [20]

\[
W(x, t) = N \int dx' W(x')2R_{xx}(x, t)
\]

or

\[
\chi(\xi, t) = N \int dx W(x)2\tilde{R}_x(\xi, t).
\]

In the first equation, we recognize that the evolving reflection operator \( \hat{R}_x \) in the Weyl representation, that is \( R_x(x', t) \), is the propagator for Wigner functions. Its semiclassical form has been studied by Dittrich et al. [14], in the case of purely unitary evolution. However, we shall see that the alternative chord representation for this same operator, \( \tilde{R}_x(\xi, t) \), i.e. the mixed Wigner-chord propagator, is simpler to treat semiclassically.

The reason for this is that the pure reflection from which this operator will evolve has the chord representation

\[
2\tilde{R}_x(\xi) = \exp \left( \frac{i}{\hbar} x \wedge \xi \right) \quad \text{or} \quad 2\tilde{R}_x(y) = \exp \left( \frac{i}{\hbar} x \cdot y \right),
\]

which is already in a convenient WKB form because the linear action, \( S_x(y) = x \cdot y \), has no caustics. In contrast, the Weyl representation of this operator is

\[
2R_x(x') = \delta(x - x'),
\]

corresponding to a plane that projects singularly onto the \( x \)-coordinate plane.

At this point, it is important to discuss the classical correspondence of the reflection operators and their evolution. Each classical reflection through a centre \( x \) defines a bundle of segments centred on this point. A nonlinear classical evolution maps the original reflection centre, \( x \rightarrow x'(t) \), while it maps the original segment lying between each pair of reflected points \( x_+ \) onto a curve containing \( x'(t) \). This is portrayed in figure 1a. The centres, \( x'(\xi', t) \), of finite chords do not generally coincide with \( x'(t) \), but we still have the same centre, if we exchange the endpoints \( x_+ \) with \( x_- \), i.e. \( x'(\xi', t) = x'(-\xi', t) \).

If this evolution is now viewed in double phase space, we thus see that the original vertical plane \( x = \text{const.} \) is bent into the Lagrangian surface \( x = x(y, t) \), which defines the evolving action \( S_x(y, t) \). In figure 1b, this is portrayed in three dimensions, as a curve that evolves from a vertical straight line. It is shown in Ozorio de Almeida & Brodier [20] that

\[
S_x(y, t) = x(t) \cdot y + O(y^3),
\]

which is still an approximate linear reflection about \( x(t) \) for small chords. All even powers in the components of \( y \) are missing in \( S_x(y, t) \) because of the involution property of the evolving reflections, that is \( R_x(t)^2 = I \), the identity. The trajectories represented in the identity plane, \( y = 0 \), correspond to
Figure 1. (a) A nonlinear classical evolution maps the original reflection centre, $x \rightarrow x'(t)$, but the linear reflection about this point is only a local linear approximation to the evolved transformation, $R_x(t)$; the centres, $x'(\xi')$, of finite chords do not generally coincide with $x'(t)$. However, for all chords, $x'(\xi') = x'(-\xi')$. (b) In double phase space, a linear reflection is represented by a vertical plane. This is curved by a nonlinear evolution, but the involution property requires that the Lagrangian surface always be symmetric about the identity plane $y = 0$ and, hence, that its tangent be vertical there. (Online version in colour.)

trajectories of single phase space, $x$ (including dissipation). Hence, the quenching of the large chords $y$, owing to decoherence, leads to a merely classical (dissipative) dynamics.

The mixed propagator for a unitary transformation has the semiclassical form defined by a single evolving classical generating function, $S_x(y, t)$,

$$\tilde{R}_x(y, t) = |\det(I - M_x(y, t))|^{-1/2} \exp[i\hbar^{-1}S_x(y, t)].$$  \hfill (5.6)

Here, the monodromy matrix $M_x$ defines the local linearization of the transformation from $x_- = x - \xi/2$ to $x_+ = x + \xi/2$ and $M_x(y, 0) = -I$. The approximation for small chords that follows from (5.5) is just$^1$

$$2\tilde{R}_x(y, t) = \exp[i\hbar^{-1}x(t) \cdot y].$$  \hfill (5.7)

The classical evolution is driven by the same double Hamiltonian (2.11) as for the density operator, and we obtain the non-unitary Markovian evolution by substituting $\chi^0(y, t)$ by this expression in (3.9), that is,

$$\tilde{R}_x(y, t) = \tilde{R}_x^0(y, t) \exp\left\{- \frac{1}{2\hbar} \int_0^t [(l' \wedge \tilde{y}_{\tau})^2 + (l'' \wedge \tilde{y}_{\tau})^2] \, d\tau \right\}. \hfill (5.8)$$

The Weyl or the chord representation of the propagator for density operators should not be mistaken for these same representations, $U_t(x)$ or $\tilde{U}_t(y)$, of the unitary evolution operator itself, $\hat{U}_t$. Nonetheless, in the unitary context,

$^1$If extrapolated to all $y$, this would lead to the classical evolution of the Wigner function, $W_x(x', t) = \delta(x(t) - x')$, which is only valid for quadratic Hamiltonians.

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the propagator for operators can be expressed exactly [13] from the Weyl symbol for $\hat{U}_t$, using the Weyl product rules [27],

$$2R_x(x', t) = \int d\mathbf{r} U_t \left( \frac{x' + x}{2} + r \right) U_t \left( \frac{x' + x}{2} - r \right)^* \exp \left( \frac{2i}{\hbar} \mathbf{r} \wedge (x' - x) \right). \quad (5.9)$$

Playing with more elaborate versions of these product rules, as presented in Ozorio de Almeida [22], we can now proceed from the definition, $\hat{R}_x(t) = \hat{U}_t \hat{R}_x \hat{U}_t^\dagger$, and equation (4.3) in [11] to derive the much simpler formula for the mixed propagator

$$2\hat{R}_x(y, t) = U_t(x^+) U_t(x^-)^* \exp \left( \frac{i}{\hbar} \mathbf{x} \cdot \mathbf{y} \right), \quad (5.10)$$

recalling that $\mathbf{x}^= = \mathbf{x} \pm \xi/2 = \mathbf{x} \mp \mathbf{J} \mathbf{y}/2$.

$\hat{U}_t$ is here given by its Weyl symbol instead of the chord representation that specifies $\hat{R}_x$. The Weyl propagator has been expressed in Ozorio de Almeida [22] as a path integral with an appealing semiclassical limit given by the centres and chords of classical trajectories. An explicit expression there is obtained in the limit of small times, for a unitary evolution driven by the Hamiltonian with the Weyl symbol, $H(\mathbf{x})$. In terms of the Hessian matrix $\mathbf{H}_x$ of second derivatives of $H(\mathbf{x})$, and the Hamiltonian velocities $\mathbf{x} = J(\partial H/\partial \mathbf{x})$, eqn (B.10) in Ozorio de Almeida [22] leads to

$$U_t(\mathbf{x}) = \left| \det \left[ I - \frac{t}{2} J \mathbf{H}_x \right] \right|^{1/4} \exp \left[ -\frac{i}{\hbar} \left( tH(\mathbf{x}) + \frac{t^3}{24} \mathbf{\dot{x}} \mathbf{H}_x \mathbf{\dot{x}}^\dagger \right) \right]. \quad (5.11)$$

Inserting this expression in equation (5.10) now determines the classical action for the mixed propagator in the short time limit, which evolves from $\mathbf{x} \cdot \mathbf{y} = \mathbf{x} \wedge \xi$, as

$$S_x(y, t) = \mathbf{x} \cdot \mathbf{y} - t[H(\mathbf{x}^+) - H(\mathbf{x}^-)] - \frac{t^3}{24} [\mathbf{x}^+ \mathbf{H}_x \mathbf{\dot{x}}^+ - \mathbf{\dot{x}}^+ \mathbf{H}_x \mathbf{x}^- \mathbf{\dot{x}}^-]. \quad (5.12)$$

To first order in time, this is just the additional action, $-t\mathbb{H}(\mathbf{x}, \mathbf{y})$, appropriate for unitary evolution ($\gamma = 0$), that would result from classical perturbation theory in double phase space. Furthermore, the first-order expansion of the action in $\mathbf{y}$ reduces to equation (5.5), with $\mathbf{x}(t) = \mathbf{x} + \mathbf{t}\dot{x}$. So, to obtain the form of the corrections to this simple approximation, we need the third-order terms in $\mathbf{y}$. The most natural is to start with the assumption that the single Hamiltonian is just

$$H(\mathbf{x}) = \frac{1}{2} \mathbf{p}^2 + V(q). \quad (5.13)$$

Then, $\dot{\mathbf{x}} = (\dot{p}, \dot{q}) = (-V_q(q), p)$ and all the third-order terms in equation (5.12) have the coefficient $V_{qqq}(q)$, leading to

$$S_x(y, t) = (\mathbf{x} - t\mathbf{\dot{x}}) \cdot \mathbf{y} + \frac{t^3}{12} \mathbf{p}^2 V_{qqq}y_p + \frac{t}{24} V_{qqq}[y_p^3 + 2t^2 y_p y_q^2] + \mathcal{O}(y^5). \quad (5.14)$$

A symplectic change of chord variables, $(y_p, y_q) \rightarrow (y_1, y_2)$, takes the cubic term to $y_1^3 + y_2^3$ [34,35]. The same transformation in the centre variables, $(p, q) \rightarrow (x_1, x_2)$, is also implemented. Because the involution symmetry prevents the presence of second-order terms, the local form of the Lagrangian surface in double phase space is $x_1 = 3y_1^2$ and $x_2 = 3y_2^2$, so that the $y$-plane is projected fourfold onto a quarter of the $x$-plane. This is one of the standard normal forms for

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the hyperbolic umbilic catastrophe, i.e. Thom’s theorem guarantees the structural stability of this projection singularity (e.g. [35]). In terms of the classical evolution of a bundle of segments, originally centred on the point \( x \), which is portrayed in (figure 1a), our result signifies that there will be a pair of semi-infinite lines meeting at the transported centre \( x' (t) \), defined as the envelopes for the centres of all the wavy segments that evolve from the original bundle. Indeed, the area between each wavy segment and the chord, \( y' (t) \), joining its tips is just the centre action \( S_x (x' (y'), t) \) that determines the phase of the semiclassical propagator of Wigner functions: \( R_x (x', t) \).

It is now easy to make contact with the semiclassical unitary propagator of Wigner functions, \( R_x (x', t) \), developed by Dittrich et al. [14], by taking the Fourier transform of our mixed propagator, \( \tilde{R}_x (y, t) \). Near the chord origin, it is not possible to employ the stationary phase approximation, so one must resort to a uniform approximation, based on the hyperbolic umbilic catastrophe integral [36,37], since the cubic term in equation (5.14) is in the normal form for this singularity for the projection \( y \to x \). Thus, because of the involution symmetry, the hyperbolic umbilic catastrophe integral is reduced to a product of Airy functions, as derived in Dittrich et al. [14].

In the presence of a diffusive Markovian environment (no dissipation), the mixed propagator \( \tilde{R}_x (y, t) \) is just multiplied by the decoherence factor, a deformed Gaussian that narrows in time. Therefore, its Fourier transform, \( R_x (x', t) \), is the convolution of a broadening window (the Fourier transform of the decoherence factor) with the unitarily evolving pair of Airy functions. In time, only the pair of caustic lines meeting at the evolved reflection centre, \( x' (t) \), survive the coarse-graining of the fine fringes characteristic of the full hyperbolic umbilic. The structural stability guaranteed by Thom’s theorem now permits us to extend this result to the weakly dissipative case, seen as a perturbation of the double Hamiltonian. Other small perturbations, such as a weak inhomogeneous magnetic field, must also preserve this overall structure.

6. Asymptotic equilibrium

It is important to consider explicitly the way that our formalism can generate asymptotic equilibrium solutions for an evolving impure state. Intuitively, we can understand this process as a balance between dissipation, which would classically contract the (single) phase-space volume occupied by the state, and the diffusive broadening of the Wigner function.

It is best to start with the exact quadratic case, for which the classical equations of motion (4.3) are decoupled. A positive dissipation coefficient, \( \gamma \), implies that the centre motion is contractive, whereas the areas in the \( y \)-plane (the chord plane) expand. In the case where the closed system is a harmonic oscillator, the open system will have inward spiralling trajectories in the centre plane (the stable plane in double phase space) and outward spirals in the chord plane (the unstable plane). This hyperbolicity in the dynamics is responsible for the limit of the decoherence functional towards the fixed value

\[
D\{y, \infty\} = \int_0^\infty \left[ (I' \wedge P^T_{t-\tau} y)^2 + (I'' \wedge P^T_{t-\tau} y)^2 \right] dt'. \tag{6.1}
\]

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This convergence only arises because the past history of the chord trajectory ending in any point \( y \) must start in the neighbourhood of the origin. However, the normalization restriction that the chord function must be unity at this point then implies that \( \chi^0(P^T_t y) \to 1 \). Thus, the asymptotic solution is just the Gaussian

\[
\chi(y, \infty) = N \exp \left( -\frac{1}{2\hbar} D\{y, \infty\} \right).
\] (6.2)

To extend this result to the general non-quadratic case, we need to consider the full trajectories in double phase space given by equation (3.5), in which the chords and the centres are now coupled. Nonetheless, the identity plane, \( y = 0 \), is easily seen to be an invariant plane \([11]\), because of the special form of the double Hamiltonian (2.11). Moreover, a positive dissipation coefficient, as defined by equation (2.8), implies that any elliptic equilibrium point of the original dynamics (generated by \( H(x) \) in the single phase space) will become a hyperbolic saddle point for the system (3.5). It follows that the identity plane is just the unstable manifold for such an equilibrium.

The difficulty now is that our approximate semiclassical theory only applies to states corresponding to Lagrangian surfaces in double phase space, i.e. we must feed in this property of the initial state. With this in mind, consider the extrapolation of the short-chord behaviour deduced in the quadratic case, so that \( \chi^0(y) = 1 \) everywhere. At first hand, it is not clear that this represents a density operator, even though it is correctly normalized. Actually, it corresponds to the Wigner function, \( W^0(x) = \delta(x) \), and hence we are dealing with representations of the operator \( \hat{R}_0 \). Thus, we are back with our now familiar propagator of Wigner functions and chord functions. Since this has negative eigenvalues \([\text{e.g.} 16]\), it is not a density operator, but its evolution under a quadratic Lindblad equation attracts it to the same asymptotic solution (6.2) as proper pure or mixed states.

The semiclassical approximation for the Markovian evolution of the reflection operators is given by equation (5.8). Since the decoherence functional cuts off the long chords, the unitary part of the evolution can be further approximated by equation (5.7). But for an equilibrium at the origin, the trajectory is simply \( x(t) = 0 \), so that we may approximate \( \hat{R}_x^0(y, \infty) = 1 \). Thus, the stationary solution, which we expect to attract all initial chord functions is again (6.2), though the infinite time decoherence functional, \( D\{y, \infty\} \), now assumes the general form (3.10) with \( t \to \infty \).

### 7. Discussions

Semiclassical Wigner functions or chord functions stand to double phase space as do semiclassical position- and momentum-wave functions to single phase space. In strict analogy to the more familiar theory, each of these conjugate representations is defined in its own subspace and contains complete information concerning the quantum state, be it pure or mixed. However, mixed systems demand a density-operator description, rather than as states in Hilbert space, which can be provided by the Wigner function or the chord function. For strictly unitary evolution, it is still possible to restrict consideration to the single phase spaces on which these functions are originally defined, but not for general quantum Markovian processes.
A qualitative picture for generalized semiclassical evolution emerges that is pleasingly intuitive: the decoherence functional quickly quenches the contribution of all large chords, just as in the exact quadratic case [31]. Hence, after a short decoherence time, we may restrict the analysis to the neighbourhood of the centre subspace \( y = 0 \) in double phase space. Given that this is just the subspace where the Wigner function is supported, one surmises that the conjugate pair of the Weyl and the chord representations constitute a privileged frame for the study of Markovian evolution for quantum systems.

The fact that the present semiclassical theory is exact in the case of a quadratic internal Hamiltonian, even in the presence of linear Lindblad operators, can be considered as an indication that it provides a useful generalization of this simple case. It will certainly be necessary to make detailed comparisons of the approximate semiclassical evolution to the direct integration of the exact equation in the case of non-quadratic Hamiltonians.

The various semiclassical representations of the density operator are derived from a single Lagrangian surface in double phase space, with its Hamiltonian evolution. A simple adaptation, resulting from the choice of a set of more favourable Lagrangian surfaces, furnishes an optimum semiclassical propagator that avoids the caustics present in the density operator. This is interpreted as an evolving reflection operator. Though resulting from a semiclassical approximation, it will transport any kind of pure or mixed Wigner function, including (squeezed) coherent states, Schrödinger cat states, as well as Bohr-quantized states. We have shown that Dittrich’s semiclassical propagator of Wigner functions is a particular representation of the evolving reflection operator and that its chord symbol has a simpler structure. Thus, the Markovian version of this propagator results immediately from the inclusion of the decoherence factor in the Fourier transform from our mixed propagator. Furthermore, the identification of this propagator with the hyperbolic umbilic catastrophe signifies that the double Airy function form derived in Dittrich et al. [14] will be structurally stable with respect to perturbations of the driving Hamiltonian. This includes the addition of an inhomogeneous magnetic field because of the enforced symmetry of the chord action.

We thank R. Vallejos for relevant comments. Partial financial support from the National Institute for Science and Technology of Quantum Information (Brazil), FAPERJ, CNPq and CAPES-COFECUB is gratefully acknowledged.

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