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Decoherence of semiclassical Wigner functions

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Abstract

The Lindblad master equation governs the general Markovian evolution of a density operator for an open quantum system. Semiclassical Wigner functions represent density operators in phase space in terms of chords on a classical manifold, so that the amplitude and phase of each chord contribution is classically defined. Inserting such a Wigner function into a phase space version of the master equation, its explicit evolution is derived in the absence of dissipation. There results a simple extension of the unitary evolution of the semiclassical Wigner function, which does not affect the phase of each chord contribution, while dampening its amplitude exponentially. Projecting the Wigner function on to an orthogonal position or momentum basis, the dampening of long chords emerges as the exponential decay of off-diagonal elements of the density matrix.

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1. Introduction

A Wigner function, $W(x)$, represents a density operator, $\hat{\rho}$, in the phase space, $x = (p, q) = (p_1, \dots, p_l, q_1, \dots, q_l)$, for a system with l degrees of freedom. Given the position representation $\langle q_+ | \hat{\rho} | q_- \rangle$, the Weyl–Wigner transformation defines [1]

$$W(x) \equiv \int dq' \left\langle q + \frac{1}{2}q' \left| \frac{\hat{\rho}}{(2\pi\hbar)^l} \right| q - \frac{1}{2}q' \right\rangle \exp\left(-\frac{i}{\hbar}p \cdot q'\right). \quad (1.1)$$

If we replace within equation (1.1) $\hat{\rho}/(2\pi\hbar)^l$ by an arbitrary operator \hat{B} , which acts on the Hilbert space of the quantum system, the resulting function $B(x)$ is then known as the Weyl representation, or the Weyl symbol, for \hat{B} .

The semiclassical approximation for pure states, $\hat{\rho} = |\psi\rangle\langle\psi|$, has the familiar WKB form

$$\langle q | \psi \rangle \approx \sum_j a_j(q) \exp\left[\frac{i}{\hbar}s_j(q)\right] \quad (1.2)$$

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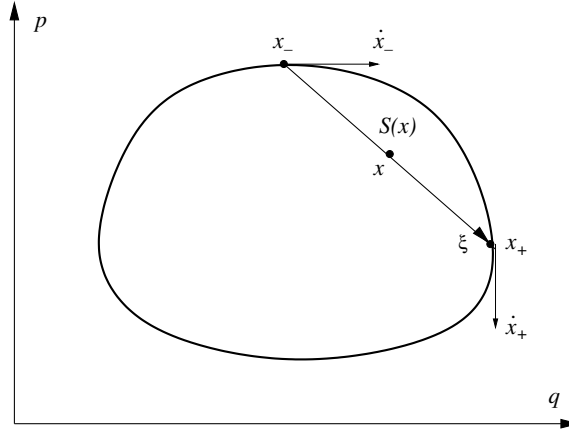


Figure 1. A single chord, ξ , is centred on x if it is close to a convex energy shell in the case of one degree of freedom. The phase of the Wigner function is proportional to the area $S(x)$ between the chord and the shell, while the amplitude, $A(x)$, depends on both phase space velocities at the tips of ξ , as described in the appendix.

where s_j are classical actions defined on a classical manifold, i.e. the integral of $p \cdot dq$ from some arbitrary position. The corresponding Wigner function, obtained by inserting equation (1.1) into equation (1.2) and evaluating the integral by stationary phase, can be decomposed into

$$W(x) \approx \sum_j \tilde{W}_k(x) \quad (1.3)$$

where each term has the form

$$\tilde{W}_k(x) = A_k(x) \cos \frac{S_k(x)}{\hbar}. \quad (1.4)$$

The sum in equation (1.3) runs over all chords centred on x that connect appropriate paths on the classical manifold, which corresponds to $|\psi\rangle$. For instance, in the case where $l = 1$, this is just the Bohr-quantized energy shell and S_k is the area between the chord and the shell (plus a semiclassically small Maslov phase) as shown in figure 1. Both semiclassical approximations (1.2) and (1.4) break down along caustics, where the amplitudes a_j , or A_k , display spurious divergences. The caustics of Wigner functions are the loci of coalescing chords. It is therefore necessary to resort to uniform approximations for the integral (1.1), resulting in Wigner functions that have large but finite values in the neighbourhood of the caustics. Detailed studies of these are given by Berry [2], for $l = 1$, and in [3] for general integrable systems. The various expressions for the semiclassical amplitudes in equation (1.4), also given by these references, are presented in the appendix. The verification that equation (1.4) is consistent with the pure state condition, $\hat{\rho}^2 = \hat{\rho}$, within the semiclassical approximation, irrespective of caustics, was carried out in [4].

In order to describe mixed states

$$\hat{\rho} = \sum_n c_n |\psi_n\rangle \langle \psi_n| \quad (1.5)$$

we merely superpose the corresponding semiclassical Wigner functions. This is simpler than in the position representation, in which we must multiply the sums for the bras and the kets. Indeed, there are cases where the semiclassical approximation to the mixed Wigner function

is approached directly, instead of relying on the pure states [5]. Such is the case of the spectral Wigner function [6]. This is defined as

$$\mathcal{W}(x; E, \epsilon) \equiv \frac{(2\pi\hbar)^l}{\sqrt{2\pi\epsilon}} \sum_n W_n(x) \exp\left[-\frac{(E - E_n)^2}{2\epsilon^2}\right] \quad (1.6)$$

where $W_n(x)$ is the pure state Wigner function for the n th eigenstate of a given Hamiltonian. If the width of the energy window, ϵ , is classically small, but contains many eigenstates, then the semiclassical limit of equation (1.6) can also be decomposed into

$$\mathcal{W}(x; E, \epsilon) \approx \sum_k \tilde{\mathcal{W}}_k(x; E, \epsilon) \quad (1.7)$$

where

$$\tilde{\mathcal{W}}_k(x; E, \epsilon) = \mathcal{A}_k \exp\left[-\frac{\epsilon^2 \tau_k^2}{2\hbar^2}\right] \cos\left[\frac{S_k(x)}{\hbar}\right]. \quad (1.8)$$

Here $S_k(x)$ is again the area closed off by a chord centred on x , but both its tips are now further constrained to lie on the same classical trajectory, within the energy shell of energy E . The time taken for the traversal of this trajectory segment is τ_k and the amplitudes \mathcal{A}_k are given in [6, 7]. If an alternative Lorentzian energy window is used, such as in [8], then the chord contributions decay exponentially, rather than with a Gaussian factor. It is important to note that equation (1.8) holds for any kind of classical motion, whether integrable, or chaotic to any degree, since it depends only on finite times of the order of \hbar/ϵ . In the case of chaotic motion, the semiclassical limit of the individual $W_n(x)$ in equation (1.6) is not known, but we can still work with the semiclassical mixture (1.8).

Even initially pure density operators evolve into a mixture if the system is open. Thus, the Wigner function of a system that attains equilibrium with a heat bath at the temperature T is given by the canonical distribution

$$W_T(x) = \frac{1}{Z(T)} \sum_n \exp\left(-\frac{E_n}{kT}\right) W_n(x) \quad (1.9)$$

where $Z(T)$ is the partition function. The semiclassical limit of $W_T(x)$, in the case of $l = 1$, was obtained by Korsch [9].

How can we take the external environment into account in the evolution of an initially pure state? The influence functional approach to this problem is to construct a specific (simplified) model of the environment and its interaction with the system, so as to subsequently trace out the external variables [10, 11]. Alternatively, the theory of semigroups starts from the mathematical restrictions that the resulting mixed density matrix must satisfy. A remarkable simplification follows from the assumption that the environment reacts to the system sufficiently fast so as to lose all memory of prior states of the system, i.e. the evolution is assumed to be Markovian. The density operator must then satisfy a linear differential master equation of the following form:

$$\frac{d\hat{\rho}}{dt} = -\frac{i}{\hbar}[\hat{H}, \hat{\rho}] + \frac{1}{\hbar} \sum_j \left(\hat{L}_j \hat{\rho} \hat{L}_j^\dagger - \frac{1}{2} \hat{L}_j^\dagger \hat{L}_j \hat{\rho} - \frac{1}{2} \hat{\rho} \hat{L}_j^\dagger \hat{L}_j \right). \quad (1.10)$$

This theorem represents a culmination of work on open systems [12–15] and is known as the Lindblad equation.

The first term accounts for the unitary evolution of the closed system under its own internal Hamiltonian operator, \hat{H} . The Lindblad operators, \hat{L}_j , are arbitrary in principle, but physically they must be related to the observables which couple the internal system to the environment. The simplest example is that of a system that is subjected to an external field,

so that the interaction depends on its position, but where there is no net exchange of energy with the environment. In this case, we can assume that $\hat{L}_j = c_j \hat{q}_j$, i.e. the Lindblad operators are proportional to the components of the position operator. The dependence of the coupling constants on \hbar is already divided out in equation (1.10) as discussed in [16]. Once the master equation has been constructed on the basis of physical assumptions about the way in which the system is affected by the external world, the dynamical variables of the environment play no further explicit role in the internal evolution. It is important to distinguish the Hamiltonian appearing in equation (1.10), which drives the internal motion, from the one that defines the pure or mixed initial states in previous equations. If these happen to coincide, then the density operator will be constant in the absence of interaction with the environment.

The purpose of this paper is to analyse the evolution of Wigner functions that initially have the semiclassical pure state form (1.3), or the spectral form (1.7), under the influence of an arbitrary Hamiltonian and a wide class of Lindblad operators. It goes without saying that discovering alternative methods, rather than the decomposition of the master equation in an orthogonal basis, is much more valuable than for the Schrödinger equation, since the number of states in the truncated basis needs to be squared for the former. This is the reason for the popularity of stochastic formalisms reviewed in [16]. However, the simple adaptation for the inclusion of Hermitian Lindblad operators in the semiclassical evolution allows us to work directly with the Wigner function and its projections. The technical restriction to Hermitian operators that is necessary for the integration of the semiclassical master equation excludes the treatment of dissipative interactions with the environment, i.e. the system loses its quantum coherence, but the average energy is preserved to zeroth order in Planck's constant.

The fact that both the Weyl–Wigner transformation (1.1) and the Lindblad equation (1.10) are linear with respect to superpositions of density operators allows us to deal separately with each chord contribution, $\tilde{W}_k(x)$, or $\tilde{\mathcal{W}}_k(x; E, \epsilon)$, as if it represented a chord density $\hat{\rho}_k$. The only added assumption is that both \hat{H} and \hat{L}_j are represented by smooth phase space functions in the Weyl representation. This is the usual case for an isolated system, where the observable \hat{H} is given in phase space by a function that is at least very close to its classical limit. Though Lindbladian dynamics are less familiar, the more commonly considered examples [16] couple the internal system to the environment through observables, represented by real phase space functions, or for instance the annihilation operator of the harmonic oscillator, which is represented by a complex (but smooth) function. Only for the former case will the semiclassical master equation be integrated.

No attempt will be made to analyse the accuracy of the approximate Markovian evolution in a concrete physical situation. This is merely an extension of the procedure followed in ordinary Hamiltonian quantum mechanics. Though no system is completely closed, it is worthwhile to build general quantum theories under the assumption of isolation, with the eventual option of later including external interactions. Likewise, we can now analyse the semiclassical limit of Lindbladian dynamics, which in some cases should be a preliminary step in the study of more complex non-Markovian interactions with the environment². Evidently, general Lindbladian dynamics (semigroups) also encompass the ordinary (unitary group) evolution of closed systems. It will be shown that the effect of the environment is easily accommodated within the semiclassical evolution in the case of Hermitian Lindblad operators. Furthermore, the generality of the semigroup evolution here derived in the semiclassical limit leads to a broad qualitative picture that bypasses the difficulty of choosing the specific Lindblad operators that should model a given open system. (Indeed all the deductions are valid for arbitrary time-dependent Hermitian Lindblad operators.) The analysis of the evolution of a

² For discussions of non-Markovian stochastic treatments, see, for example, [17] or [18].

measure of decoherence, and the linear entropy is part of the subject of a companion paper [19].

It is important to establish distinctions and connections between this paper and previous work on the semiclassical limit of open systems. Perhaps this is the first time that the theory has been developed entirely in phase space. Although Caldeira and Leggett [11] have already made some use of the Wigner function, it appears only in an auxiliary role. This is also the case of Grossmann [20] who has discussed the semiclassical limit of the influence functional approach. A remarkable paper by Strunz [21] comes much closer to the present work. A path integral is developed there but, unlike the usual influence functionals, it is constructed for Markovian Lindblad evolution. The propagator is defined in the position representation, using the Wigner function. Its semiclassical limit is derived, but this does not immediately describe the propagation of the semiclassical Wigner functions themselves. Indeed, this is a tricky problem even for pure Hamiltonian evolution, which has been fully understood only recently [22, 23]. The important point is that Strunz defines a decoherence influence functional for pairs of arbitrary paths in phase space, which is here shown to account for the dampening of the amplitude of each chord of the semiclassical Wigner function. The same decaying factor is easily seen to affect the off-diagonal elements of the semiclassical density matrix in the position representation.

Thus, in the next section we review the unitary evolution of semiclassical Wigner functions and we discuss the purity of the states. This is followed, in section 3, by the derivation of the Lindblad equation for the Wigner function without the Hamiltonian term. The equation is integrated in the case of Hermitian Lindblad operators. Section 4 combines the Hamiltonian and Lindbladian evolutions of both preceding sections to produce the semiclassical description of decoherence of an evolving Wigner function over a finite time interval. The expectation for observables and energy diffusion of a stationary Wigner function in an open system is discussed in section 5. In section 6 we show how the inverse Weyl–Wigner transformation leads to a semiclassical approximation in the position representation that is again described by the decoherence distance functional. The delicate issue of normalization is treated in the appendix.

2. Review of unitary evolution

The Moyal formula [24]

$$\frac{\partial}{\partial t} W(x) \approx \{H(x), W(x)\} + O(\hbar^2) \quad (2.1)$$

where $\{, \}$ denotes the classical Poisson bracket, suggests that the semiclassical evolution follows the classical trajectory for the argument of the Wigner function. This is indeed the exact result for quadratic Hamiltonians and also holds approximately if $W(x)$ is a smooth function within the scale of \hbar . For pure semiclassical states such as equation (1.4), or for the mixture (1.8), this is certainly not the case. However, it has been shown that the evolution then depends only on the orbits of both tips of each chord centred on x [22, 23]. Since neither of the two previous treatments of this problem relied directly on the differential equation for $\hat{\rho}_t$, i.e. the unitary part of equation (1.10), it is a useful exercise to rederive the Hamiltonian evolution in this way, preliminary to the inclusion of the new terms in the master equation.

The main ingredient is the integral form for the product of two operators \hat{B}_2 and \hat{B}_1 in the Weyl representation, due to Berezin [25],

$$B_2 B_1(x) = \left(\frac{1}{\pi\hbar}\right)^{2l} \int dx_2 dx_1 B_2(x_2) B_1(x_1) \exp\left[\frac{i}{\hbar} \Delta(x, x_1, x_2)\right] \quad (2.2)$$

which was subsequently extended to higher-order products [7, 26]. Here,

$$\Delta(x, x_1, x_2) = 2(x \wedge x_1 + x_1 \wedge x_2 + x_2 \wedge x) \quad (2.3)$$

where the skew product $a \wedge b = (\mathbf{J}a) \cdot b$, with

$$\mathbf{J} = \left(\begin{array}{c|c} 0 & -1 \\ \hline 1 & 0 \end{array} \right) \quad (2.4)$$

the matrix that exchanges positions and momenta in Hamilton's equations:

$$\frac{dx}{dt} = \mathbf{J} \frac{\partial H}{\partial x}. \quad (2.5)$$

Each term in equation (2.3) is the (symplectic) area of the parallelogram defined by the corresponding vectors (i.e. just the area itself for $l = 1$). It is much more useful to consider Δ as the symplectic area of the unique triangle that has (x, x_1, x_2) as its midpoints. This is the circumscribed triangle, rather than the usual inscribed triangle defined by its corners.

The equation that governs unitary evolution of the Wigner function is thus

$$\frac{\partial}{\partial t} W(x) = \frac{2}{\hbar} \left(\frac{1}{\pi \hbar} \right)^{2l} \int dx_2 dx_1 H(x_2) W(x_1) \sin \left[\frac{\Delta}{\hbar}(x, x_1, x_2) \right]. \quad (2.6)$$

The evolution of the semiclassical Wigner functions can be decomposed into separate chord contributions. Hence, we insert equations (1.4) or (1.8) into equation (2.6) and we evaluate the integral within the stationary phase approximation³. Expressing the sines and cosines as the sum of exponentials, there will be four integrals for each chord of the Wigner function:

$$\begin{aligned} \frac{\partial}{\partial t} \tilde{W}_k(x) &\approx -\frac{i}{2\hbar} \left(\frac{1}{\pi \hbar} \right)^{2l} \sum_{\pm} \int dx_1 dx_2 H(x_2) A_k(x_1) \\ &\times \left\{ \exp \left[\frac{i}{\hbar} [\Delta \pm S_k(x_1)] \right] - \exp \left[-\frac{i}{\hbar} [\Delta \pm S_k(x_1)] \right] \right\}. \end{aligned} \quad (2.7)$$

The stationary phase points are now obtained from the rule that the derivative, $\partial/\partial x$, of a symplectic area, bounded by a chord ξ , is just $\mathbf{J}\xi$ [7]. Hence, from

$$\begin{aligned} (\partial/\partial x_1)[\Delta \pm S_k(x_1)] &= -2\mathbf{J}(x_2 - x) \pm \mathbf{J}\xi_k(x_1) = 0 \\ (\partial/\partial x_2)[\Delta \pm S_k(x_1)] &= 2\mathbf{J}(x_1 - x) = 0 \end{aligned} \quad (2.8)$$

it follows that the circumscribed triangle, Δ , collapses at the stationary configuration for which $x_1 = x$ and $\xi_k(x_1) = \pm 2(x_2 - x)$, i.e. the Hamiltonian must be evaluated at the stationary points, which coincide with the tips of the chord centred on x . At these points, the Hessian determinant of the phase is just

$$\det \begin{bmatrix} \frac{\partial^2 S}{\partial x_1 \partial x_2} & -2\mathbf{J} \\ 2\mathbf{J} & 0 \end{bmatrix} = 2^{4l} \quad (2.9)$$

and the signature of the Hessian matrix (the number of positive eigenvalues minus the number of negative eigenvalues) is zero. To obtain this result, note that it obviously holds for $S = 0$ and we can always connect the eigenvalues of equation (2.9) continuously with this particular case (avoiding caustics). Since the eigenvalues remain finite along any path and their product is unity, the signature remains zero.

³ The following development will be made for the pure Wigner function (1.4). This holds also for the spectral Wigner function (1.8), by including the exponential factor in the amplitude.

Combining all these ingredients, we obtain the stationary phase evaluation of equation (2.7) as

$$\frac{\partial}{\partial t} \tilde{W}_k(x) \approx \frac{1}{\hbar} \left[H \left(x + \frac{\xi_k}{2} \right) - H \left(x - \frac{\xi_k}{2} \right) \right] A_k(x) \sin \frac{S_k(x)}{\hbar} \quad (2.10)$$

which can be immediately compared with the straightforward differentiation of equation (1.4). The dominant term is

$$\frac{\partial}{\partial t} W(x) \approx -\frac{1}{\hbar} \sum_k \frac{\partial S_k}{\partial t} A_k(x) \sin \frac{S_k(x)}{\hbar} \quad (2.11)$$

which agrees with equation (2.10), provided that

$$-\frac{\partial S_k}{\partial t} = H \left(x + \frac{\xi_k}{2} \right) - H \left(x - \frac{\xi_k}{2} \right). \quad (2.12)$$

But this form of the Hamilton–Jacobi equation, derived explicitly in [23], is just the derivative of the action in [22]. It differs from Marinov’s Hamilton–Jacobi equation, which depends on just a single tip of the chord [27].

Thus, we find that the stationary phase evaluation captures the dominant term of the unitary evolution of the Wigner function, while neglecting the variation in the amplitude $A_k(x)$. This propagation depends on the classical flow, through the orbits of both tips of each chord, $\xi_k(x)$. (Only if $H(x)$ is quadratic, will the difference of the Hamiltonian vector fields at the chord tips in equation (2.10) be proportional to $\mathbf{J} \partial H / \partial x$ at the centre.) Of course, we can also evolve the entire classical manifold and then reconstruct the Wigner function at the centre of the evolving chords as described by Berry and Balazs [28], resulting in a relatively slow change of amplitude [22, 23] that is not captured by equation (2.10).

To conclude this section, we note that both pure and mixed states can undergo unitary evolution but that, in the former case, the purity of an initial state is not destroyed, i.e. we must have $\hat{\rho}^2 = \hat{\rho}$ for the whole time if this is true initially. In the Weyl representation, the product rule (2.2) leads to

$$W(x) = \left(\frac{2}{\pi \hbar} \right)^l \int dx_1 dx_2 W(x_1) W(x_2) \exp \left[\frac{i}{\hbar} \Delta(x, x_1, x_2) \right] \quad (2.13)$$

which has been shown to hold for general integrable systems within the stationary phase approximation [4]. It is quite remarkable that this result is entirely impervious to the multiplicity of chords or their coalescence at caustics, which are washed out by the integration.

An important consequence of the fact that pure state Wigner functions satisfy the pure state condition is that we can take the trace of both sides to obtain

$$\text{tr } \hat{\rho} = \int dx W(x) = (2\pi\hbar)^l \int dx [W(x)]^2. \quad (2.14)$$

It happens that the integral involving the square of the Wigner function does indeed equal unity, within the stationary phase approximation, while the first integral does not, though its semiclassical value is independent of Planck’s constant. These results were first obtained by Berry [2], for $l = 1$, and are extended to general integrable systems in the appendix. It may be said that the pure state Wigner functions are indirectly normalized.

3. Pure Lindbladian evolution

The Weyl representation of the remaining terms of the master equation (1.10) requires the integral form for the product of three operators \hat{B}_3 , \hat{B}_2 and \hat{B}_1 . Sometimes, as in [22], it is

necessary to use the full generalization of equation (2.2), integrating over three phase space variables with a phase that is a circumscribed quadrilateral [7]. However, in this case it is possible to use the following shortcut also provided by [7]:

$$B_3 B_2 B_1(x) = \left(\frac{1}{\pi\hbar}\right)^{2l} \int dx_2 dx_1 B_3(x_2 - x_1 + x) B_2(x_2) B_1(x_1) \exp\left[\frac{i}{\hbar} \Delta(x, x_1, x_2)\right]. \quad (3.1)$$

Thus, the Lindbladian evolution for a single chord of the semiclassical Wigner function (1.4) becomes

$$\begin{aligned} \frac{\partial}{\partial t} \tilde{W}_k(x) &\approx \frac{1}{2\hbar} \left(\frac{1}{\pi\hbar}\right)^{2l} \sum_{j,\pm} \left\{ \int dx_2 dx_1 L_j(x_2 - x_1 + x) A_k(x_2) L_j(x_1)^* \right. \\ &\quad \times \exp\left[\frac{i}{\hbar} (\Delta(x, x_1, x_2) \pm S_k(x_2))\right] - \text{Re} \int dx_2 dx_1 L_j(x_2 - x_1 + x)^* L_j(x_2) A_k(x_1) \\ &\quad \left. \times \exp\left[\frac{i}{\hbar} (\Delta(x, x_1, x_2) \pm S_k(x_1))\right] \right\} \end{aligned} \quad (3.2)$$

if we neglect the effect of the Hamiltonian. Here, Re stands for the real part and we note that an adjoint operator \hat{B}^\dagger is represented by the complex conjugate function $B(x)^*$. Presuming that the Lindblad operators are represented by smooth phase space functions, the stationary phase evaluation of equation (3.2) proceeds essentially as in the previous section. Collecting the terms, we obtain

$$\begin{aligned} \frac{\partial}{\partial t} \tilde{W}_k(x) &\approx \frac{1}{\hbar} A_k(x) \sum_j \left\{ \text{Re} \left[L_j\left(x + \frac{\xi_k}{2}\right) L_j\left(x - \frac{\xi_k}{2}\right)^* \exp\left(\frac{i}{\hbar} S_k(x)\right) \right] \right. \\ &\quad \left. - \frac{1}{2} \left[\left| L_j\left(x + \frac{\xi_k}{2}\right) \right|^2 + \left| L_j\left(x - \frac{\xi_k}{2}\right) \right|^2 \right] \cos \frac{S_k(x)}{\hbar} \right\}. \end{aligned} \quad (3.3)$$

From here on, the discussion focuses on the case of Hermitian Lindblad operators, i.e. it is assumed that the system is only coupled to the environment by observables. Then the master equation for $\tilde{W}_k(x)$ simplifies to

$$\frac{\partial}{\partial t} \tilde{W}_k(x) \approx -\frac{1}{2\hbar} A_k(x) \cos \frac{S_k(x)}{\hbar} \sum_j \left| L_j\left(x + \frac{\xi_k}{2}\right) - L_j\left(x - \frac{\xi_k}{2}\right) \right|^2. \quad (3.4)$$

In contrast to the case of Hamiltonian evolution, we see that Hermitian Lindblad operators do not affect the phase of the semiclassical Wigner function, but only its smooth amplitude function. Indeed, if we assume that the chords, $\xi_k(x)$, and the actions, $S_k(x)$, remain constant at each point, x , we can integrate the equations for the amplitudes,

$$\frac{\partial}{\partial t} A_k(x) = -\frac{1}{2\hbar} \sum_j \left| L_j\left(x + \frac{\xi_k}{2}\right) - L_j\left(x - \frac{\xi_k}{2}\right) \right|^2 A_k(x) \quad (3.5)$$

to obtain

$$A_k(x, t) = \exp \left[-\frac{t}{2\hbar} \sum_j \left| L_j\left(x + \frac{\xi_k}{2}\right) - L_j\left(x - \frac{\xi_k}{2}\right) \right|^2 \right] A_k(x, 0). \quad (3.6)$$

Thus, it is easily verified that the semiclassical Wigner function (1.4), now taken with the time-dependent amplitude (3.6), i.e.

$$\tilde{W}_k(x, t) = A_k(x, t) \cos[S_k(x)/\hbar] \quad (3.7)$$

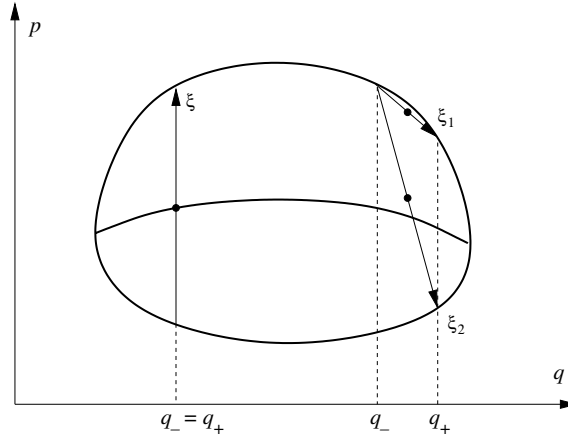


Figure 2. The chords of the energy shell between nearly equal q_{\pm} can be short, ξ_1 , or long, ξ_2 . Both will be equally damped by the Lindblad operator $\hat{L} = cq$. After a long time, the Wigner function condenses on to the energy shell and the line of midpoints of the vertical chords.

satisfies the evolution equation (3.4) and, of course, an equivalent result holds for each chord of the spectral Wigner function, $\tilde{\mathcal{W}}_k(x; E, \epsilon)$.

Evidently the extreme case of pure Lindbladian evolution will be relevant only if the coupling constants implicit in \hat{L}_j are large enough for the internal motion of the system to be effectively frozen within the decay time for the amplitudes. The Lindblad operator with the largest difference between the tips of a chord dominates the decay and the corresponding time is inversely proportional to the square of the coupling constant.

The simplest case is that of a single operator \hat{L} . Clearly the Wigner function remains constant if the state is initially an eigenstate of \hat{L} , since the tips of all chords then lie on the same manifold $L(x) = \text{constant}$. This result holds for all the cases discussed in the introduction. For $l = 1$, this manifold is just a phase space curve. For a general integrable state, the chord tips lie on an l -dimensional torus, within the $(2l - 1)$ -dimensional surface, on which $L(x) = \text{constant}$ [3]. The chords of a spectral Wigner function (1.8) also lie on the single surface $H(x) = \text{constant}$. Hence, if $H(x) = L(x)$, the Wigner function is also invariant.

Generally, for $H(x) \neq L(x)$, it must be that $L(x_+) \neq L(x_-)$ for most chords, $\xi = x_+ - x_-$. Evidently, short chords are more stable against decay due to arbitrary Lindblad operators but, for specific operators, there are long chords that will also be selected for survival. For instance, suppose that $l = 1$ and $L(x) = cq$, the position. Consider a given centre, x , with a vertical chord, $\xi(x)$, as in figure 2, then the amplitude does not decay. In this case, the full Wigner function condenses on to the classical curve and on to the line of midpoints of the vertical chords that bisects the classical curve. However, we see in the following section that this strange effect only arises in the complete absence of the Hamiltonian term in the evolution equation. No matter how strong the coupling to the environment, the Hamiltonian will eventually rotate the chords that are then erased by the Lindblad operator. For a general position coupling to the environment, with $l > 1$, i.e. $\hat{L} = (c_1q_1, \dots, c_lq_l)$, the decay rate will depend on the distance: $[c_1(q_{1+} - q_{1-})^2 + \dots + c_l(q_{l+} - q_{l-})^2]^{1/2}$.

Evidently, the above picture is entirely consistent with previous results on decoherence [11, 16, 29]. The general initial pure state may be considered as a superposition of the eigenstates of the Lindblad operator. The effect of ‘continuous measurement’ of this observable is to erode non-diagonal elements of the density matrix in this representation [16]. If we merely

place a pair of coherent states at both tips of a given chord, we obtain a Wigner function that is a Gaussian at $x_{\pm} = x \pm \xi/2$ with a width of $O(\sqrt{\hbar})$. The interference between these two states is represented by another Gaussian centred on x itself but this is modulated by narrow fringes, of wavelength $O(\hbar)$. This central Gaussian decays exponentially just as the general semiclassical Wigner function that we have been studying when a Lindblad operator is ‘turned on’, unless $L(x_+) = L(x_-)$.

An initial semiclassical Wigner function of the type (1.4), with the amplitudes specified by equation (A.7), becomes mixed due the Lindbladian decay of the amplitude (3.6). In section 5, we discuss the way that this decoherence is connected with energy diffusion, within the framework of the spectral Wigner function. An important issue is the normalization of the mixed Wigner function that results from Lindbladian evolution. It is shown in the appendix that the pure state itself is only indirectly normalized through $\text{tr } \hat{\rho}^2$, but this is now a measure of the decoherence of the mixed state and should not equal $\text{tr } \hat{\rho}$, once the environment is switched on. However, we find that the semiclassical evaluation of $\text{tr } \hat{\rho}$, though it is not unity, is stable with respect to the Lindbladian decay of amplitude, as well as with \hbar , taken as a small parameter. Therefore, we can safely attribute the semiclassical change in $\text{tr } \hat{\rho}^2$ as entirely due to decoherence.

4. General evolution

We are now in a position to combine the unitary evolution of a closed quantum system with the decoherence that results from its coupling to the environment, as modelled by Lindblad operators. Again we treat each chord contribution independently, just as in the two previous sections. The differential equation corresponding to the master equation (1.10) is just the combination of equation (2.10) with equation (3.4) in the case of Hermitian Lindblad operators, but it is hard to integrate this directly. Instead, the evolution can be taken as the result of alternate sequences of unitary and pure Lindbladian evolutions in the limit of arbitrarily small time steps. This approach has been used for the coupling of two different unitary maps by Berry *et al* [30]. The recent study of a unitary map alternating with a finite step Lindbladian evolution by Bianucci *et al* [31] is even more to the point. The important issue is that the exponential damping factor in the amplitude remains constant during the unitary evolution described in section 2 through the classical motion of each chord and its centre. Alternatively, the chord is then frozen during the interval in which the system is governed only by the Lindblad operators.

Let us define $V_k(x, t)$ as the semiclassical contribution of each chord to the Wigner function in the absence of the Lindblad operators, i.e. $V_k(x, t)$ describes purely unitary evolution. Splitting the period of evolution, t , into N half-steps of Hamiltonian evolution and N half-steps of Lindbladian evolution, we obtain

$$\tilde{W}_k(x, t) = V_k(x, t) \prod_{n=1}^N \exp \left[-\frac{t}{2\hbar N} \sum_j \left| L_j \left(x_n + \frac{\xi_k(x_n)}{2} \right) - L_j \left(x_n - \frac{\xi_k(x_n)}{2} \right) \right|^2 \right]. \quad (4.1)$$

Naturally, it has been necessary to multiply the Hamiltonian by a factor of two in this formula, since it only acts during half of each interval, and the coupling constants in the Lindblad operators are likewise increased by a factor of $\sqrt{2}$. The final dampening of the amplitude at $x = x_N$ depends on both the history of the centres, x_n , and that of their chords, $\xi_k(x_n)$. In other words, the total decay depends on the classical trajectories that arrive at $x_{k,N\pm} = x_N \pm \xi_k(x_N)$. Each factor in the product is then calculated at the centres, $x_{k,n} = (x_{k,n+} + x_{k,n-})/2$, with the

chords, $\xi_{k,n} = x_{k,n+} - x_{k,n-}$, during the half-intervals in which the Hamiltonian is switched off. (Note that the sequence of $x_{k,n}$ depends on the final chord ξ_k , as well as on x .)

Taking the limit $N \rightarrow \infty$, we obtain the continuous evolution

$$\tilde{W}_k(x, t) = V_k(x, t) \exp \left[-\frac{1}{2\hbar} \sum_j \int_0^t dt' |L_j(x_{k+}(t')) - L_j(x_{k-}(t'))|^2 \right]. \quad (4.2)$$

Therefore, the full evolution of the Wigner function in an open system combines the unitary evolution for each chord, obtained by the classical motion of the chord tips, $x_{k+}(t)$ and $x_{k-}(t)$, with the exponential decay of the amplitude, characteristic of pure Lindbladian decoherence. But now this dampening depends on the chord history. If there is more than one chord centred on x , each contribution to the evolution of the Wigner function depends on the particular motion of both tips of each respective chord. Generally, the classical motion of the centre of a chord does not coincide with the midpoint of the motions of the tips, unless the motion is linear (i.e. the internal Hamiltonian is quadratic). Even though the development has focused on the Wigner function of integrable systems, exactly the same form of general Lindbladian evolution also holds for each chord contribution, \tilde{W}_k , to the spectral Wigner function (1.8). The normalization of equation (4.2) is discussed in the appendix.

It is now feasible to make a partial connection to the path integral developed by Strunz. Indeed, the phase space influence functional in [21] has exactly the same form as the exponential in equation (4.2) in the case of Hermitian Lindblad operators, but there this is taken over all possible pairs of paths, which are not restricted to being classical trajectories. Even so, working within quite diverse frameworks, both treatments conclude that the effect of Hermitian Lindblad operators is encapsulated by the decoherence distance functional:

$$D_t[x_+(t'), x_-(t')] \equiv \left[\sum_j \int_0^{t'} dt' |L_j(x_+(t')) - L_j(x_-(t'))|^2 \right]^{\frac{1}{2}}. \quad (4.3)$$

Though Strunz also discusses the semiclassical limit, this is treated within the context of an effective Hamiltonian, $H(p, q) - \frac{i}{2} \sum |L_j|^2$, leading in general to complex trajectories. However, in the specific example of the harmonic oscillator with the Lindblad operator $\hat{L} = c\hat{q}$, the classical paths in [21], which contribute to the propagator in the position representation, turn out to be real.

The motion of the chords is important even for the Wigner function corresponding to an eigenstate of the internal Hamiltonian, i.e. even if $V_k(x, t)$ is stationary. The tips of each chord then evolve simultaneously along trajectories constrained to the invariant manifold (just the energy curve if $l = 1$) that defines the semiclassical Wigner function. Thus, the dampening of the amplitude is only small for short chords, so that the line of midpoints of vertical chords in figure 2 is erased if the internal Hamiltonian is taken into account. The same is true for spectral Wigner functions of the internal Hamiltonian. Thus, unless all $\{L_j, H\} = 0$, only the classical region of the Wigner function close to the energy shell survives the decoherence due to the external environment. This general result is compatible with a previous specific deduction for the harmonic oscillator [32].

It is important to point out that the present results are also valid for time-dependent Lindblad operators and Hamiltonians. Of course, we must restrict $\hat{L}_j(t) = \hat{L}_j^\dagger(t)$ at each instant, but the way that equation (4.2) is deduced is unaffected. The only difference is that then the time dependence of the Lindblad functions is not only due to the movement of the chord tips. Thus, the general semiclassical picture of chord amplitudes that decay in time holds for the entire sub-semigroup generated by Hermitian Lindblad operators.

5. Averages and energy diffusion

The expectation of an observable \hat{H} is $\langle \hat{H} \rangle = \text{tr} \hat{H} \hat{\rho}$. Since the Weyl representation of \hat{H} is the smooth function $H(x)$ that equals the classical variable, to zero order in Planck's constant, we should intuitively obtain its expectation by integrating $H(x)$ along the classical manifold that supports the semiclassical Wigner function [33]. This result can also be derived for a torus by approximating the Wigner function by a delta function. Alternatively, a simple generalization of the calculation of $\text{tr} \hat{\rho}$ in the appendix leads to the same result after dividing out the constant normalization factor. The classical averages of \hat{H} or \hat{H}^2 are unaffected by the action of Hermitian Lindblad operators, but will evolve unitarily if this observable does not commute with the internal Hamiltonian. The effect of classically chaotic internal motion on the growth of the variance of observables, i.e. $\langle \hat{H}^2 \rangle - \langle \hat{H} \rangle^2$, is one of the subjects treated in [19].

If \hat{H} is just the Hamiltonian of the internal system, then $\langle \hat{H} \rangle$ is a constant to zeroth order in \hbar , throughout the entire semigroup evolution. Thus, in a first approximation there is no energy dissipation or, in other words, the Hermitian Lindblad operators produce no energy drift. Likewise, $\langle \hat{H}^2 \rangle$ is also constant, i.e. there is also no energy diffusion to lowest order. Certainly, this semiclassical result does not preclude small alterations of the average energy. Indeed, it is easy to verify directly from the Lindblad equation (1.10) that, if $\hat{H} = \hat{p}^2/2 + V(\hat{q})$ and $\hat{L} = \hat{q}$, then $(d/dt)\langle \hat{H}^2 \rangle$ is a constant proportional to \hbar . It is not feasible to extend the present semiclassical treatment so as to calculate these higher corrections explicitly, but we present below an indirect method to estimate the energy diffusion around the semiclassically constant energy average. It turns out that the growth of the energy width is of order $\hbar^{1/2}$, which is classically small, but large in relation to any change of $\langle \hat{H} \rangle$.

The focus will be on an initially mixed state within a narrow energy window, corresponding to a spectral Wigner function of the internal Hamiltonian. Of course, this also includes a pure state, in the limit where the window width tends to zero, for the simplest case where $l = 1$. The amplitudes of the various chord contributions to $\mathcal{W}(x; E, \epsilon)$ in equation (1.7) decay exponentially with $(D_t[x_+(t'), x_-(t')])^2$ and the trajectories $x_{\pm}(t')$ are constrained to the stationary energy shell. Hence, only short chords with centres very close to the shell will give appreciable contributions to this Wigner function after a finite interval of time.

There are only two possibilities concerning the trajectories that connect the tips of a very small chord, ξ_k . Either this is a unique short trajectory that takes a small time, τ_k , between the two tips, or else the trajectory winds near a periodic orbit [6, 7]. For $l = 1$, the energy shell is itself a single periodic orbit, so that the difference between both types of contributions concerns only the number of repetitions around the periodic orbit (which is zero for the short orbit). Both types of contribution will arise for all centres close to the shell in this simple case. For $l > 1$, the long orbits that contribute to the Wigner function with a small $\xi_k(x)$ will be associated with neighbouring periodic orbits with varying actions, as x is moved along the $(2l - 1)$ -dimensional shell. Thus, for any number of degrees of freedom, we can separate

$$\mathcal{W}(x, t; E, \epsilon) \xrightarrow[t \rightarrow \infty]{} \tilde{\mathcal{W}}_{\tau}(x, t; E, \epsilon) + \tilde{\mathcal{W}}_{p.o.}(x, t; E, \epsilon) \quad (5.1)$$

where we lump all the periodic orbit contributions into the second term. It is important to distinguish here the duration, t , of the evolution of the open system, from the time, τ , that the classical trajectory takes to travel between the tips of the short chord. Thus, τ is a function of x , for a fixed energy surface and is independent of t .

It is easy to estimate the short orbit contribution, because

$$\xi_\tau(x) \approx \dot{x}\tau = \tau \mathbf{J} \partial H / \partial x \quad (5.2)$$

to first order in τ [7]. Hence, we can approximate the difference of the Lindblad functions in terms of a Poisson bracket:

$$|L_j(x + \xi_\tau/2) - L_j(x - \xi_\tau/2)|^2 \approx \tau^2 |\{H, L_j\}|^2. \quad (5.3)$$

Let us now assume that the closed classical system is ergodic. Then the time average of $|\{H, L_j\}|^2$ for a trajectory on the energy shell exists and generally equals the average over the shell. But, for a short chord, the classical trajectory of the midpoint $x(t) \approx [x_+(t) + x_-(t)]/2$, so that, considering now that τ is an average time for the traversal from $x_-(t)$ to $x_+(t)$, we can approximate the decoherence distance functional (4.3) so as to obtain

$$\tilde{\mathcal{W}}_\tau(x, t; E, \epsilon) \approx \mathcal{V}_\tau(x; E, \epsilon) \exp \left[-\frac{t}{2\hbar} \sum_j \overline{|\{H, L_j\}|^2} \tau^2 \right] \quad (5.4)$$

where we recall that in this case \mathcal{V}_τ , the Wigner function for the closed system, is stationary. Thus, the short orbit contribution to the spectral Wigner function, after a time t of contact with the environment, has the same form as the initial spectral Wigner function (1.8). However, the width of the energy window grows as

$$[\epsilon(t)]^2 = \epsilon^2 + \frac{\hbar t}{2} \sum_j \overline{|\{H, L_j\}|^2} \quad (5.5)$$

i.e. the internal energy of the system spreads diffusively. This will also be the case for an initially pure state if $l = 1$. It should be emphasized that the average spacing between energy levels is of order \hbar^l , so that semiclassically there is scope for the broadening of the energy window by many levels before its width becomes classically significant, in which case the Wigner function can no longer be described by the chords in a single energy shell.

If $l > 1$ a pure initial state will surely also mix with neighbouring eigenstates of the other variables that together define its invariant torus, but this effect is harder to retrieve. If the initial spectral Wigner function is defined for a different observable, \mathcal{H} , than the one that drives the internal motion of the system, the surface $\mathcal{H}(x) = \text{constant}$, which is the locus of the tips of all chords, will no longer be stationary. In this case, we can no longer invoke ergodicity to estimate the growth of the \mathcal{H}_t -energy window, though a similar argument can be used if the movement of the energy shell is adiabatically slow as compared with the time that the orbits inside the shell require to cover it. Of course, this approximately adiabatic scenario is more likely to arise for $l = 1$. In any case the decay of the amplitude of the very short chords that survive the decoherence after a finite time can still be ascribed to a net growth of the energy window.

If $\tilde{\mathcal{W}}_\tau$ were the only term in the decomposition (5.1) of the spectral Wigner function, the effect of the Lindblad operators in the semiclassical evolution would be reduced to merely mixing the state in a widening energy window. That is, the density matrix would be diagonal in the eigenbasis of the operator used in the definition of the initial state. The periodic orbit terms in equation (5.1) modify this picture in a way that requires further analysis. In other words, scars of periodic orbits may play a significant role in the semiclassical theory of decoherence, since their contribution to the evolved Wigner function is not merely the same as in a spectral Wigner function that has a very narrow energy window. Rather than being dampened by their period, the scars only decay as a function of the length of the chord, as measured by the decoherence distance functional.

6. Position representation

Instead of the basis of eigenstates of the internal Hamiltonian, let us consider another orthogonal basis, such as the position representation. Then even the density matrix for an initially pure state is viewed as a (coherent) superposition of a large number of basis states. In the case of Lindblad operators that were just functions of the positions, \hat{q} , it could have been easier to obtain the evolution of the semiclassical density matrix directly from the position representation of the Lindblad equation (1.10). For general Hermitian functions of \hat{p} and \hat{q} it is better to proceed from the inverse Fourier transform to (1.1):

$$\langle q_+ | \hat{\rho} | q_- \rangle = \int dp W \left(p, \frac{q_+ + q_-}{2} \right) \exp \left[\frac{i}{\hbar} p \cdot (q_+ - q_-) \right]. \quad (6.1)$$

Sufficiently far from diagonality, i.e. for $q_+ \neq q_-$, we need only be concerned with the stationary phase evaluation in the oscillatory interior of the Wigner function, so that the stationary phase condition is fulfilled where the chord centred at $x = (q_+ + q_-)/2$ has the component $\xi_q(x) = q_+ - q_-$. The Lindbladian dampening of the stationary chord can be factored out of the integral, so that the density matrix of the evolved system is expressed in terms of the decoherence distance functional (4.3) as

$$\begin{aligned} \langle q_+ | \hat{\rho} | q_- \rangle &\approx \sum_{j_+, j_-} a_{j_+}(q_+) a_{j_-}^*(q_-) \exp \left[\frac{i}{\hbar} (s_{j_+}(q_+) - s_{j_-}(q_-)) \right] \\ &\times \exp \left\{ -\frac{1}{2\hbar} \{ D_t[(q_+, p_{j_+})(t'), (q_-, p_{j_-})(t')] \}^2 \right\}. \end{aligned} \quad (6.2)$$

Here the label j_{\pm} specifies the different momenta, $p_{j_{\pm}}$, of the torus for the positions (q_{\pm}) and the actions $s_{j_{\pm}}$ are the usual actions in equation (1.2), measuring areas from the q -axes.

In the limit as $q_+ \rightarrow q_-$, we also obtain a short chord contribution from the classical region where the semiclassical approximation breaks down. However, the extrapolation of equation (6.2) for short chords gives the same result as follows from the simpler approximation for the Wigner function [2], $W(x) = (2\pi)^{-l} \delta(I(x) - \mathcal{I})$ for the eigenstate of an integrable Hamiltonian corresponding to the action variables $I(x) = \mathcal{I}$. Indeed, the correlation function given in [34] follows from the short chord limit of equation (6.2) by taking $(s_{j_+} - s_{j_-}) \rightarrow p_j \cdot (q_+ - q_-)$ as $q_+ \rightarrow q_-$. Of course, the decoherence distance functional vanishes in this limit, so that this contribution becomes insensitive to the Lindblad operators. We should note that there will generally also be long vertical chords, such as shown in figure 2, contributing to the density matrix. The projection of the semiclassical Wigner function on to position space is a good example of the good behaviour of this approximation within integrals, despite the presence of caustics.

The contribution of long chords to the density matrix of a mixture of energy eigenstates in a classically narrow energy window, corresponding to the spectral Wigner function, has exactly the same form as equation (6.2). The decoherence distance functional dampens the contributions from the various trajectories that satisfy the variational principle for fixed energy between q_- and q_+ , so that, if we label these by their initial and final momenta, $p_{j_{\pm}}$, the stationary action is just $s_{j_+} - s_{j_-}$. The geometry of the orbits and the semiclassical amplitudes of their contributions have been thoroughly discussed by Toscano and Lewenkopf in a recent paper [8]. They also provide the limit for the contribution of short chords as $q_+ \rightarrow q_-$, which tends to Berry's result [34] for $l > 1$

$$\mathcal{W}(x) \propto \frac{J_{l/2-1}[p(q)|q_+ - q_-|/\hbar]}{[p(q)|q_+ - q_-|/\hbar]^{l/2-1}} \quad (6.3)$$

where J_ν is a Bessel function. This result follows from the approximation of the Wigner function as a delta function over the energy shell. Of course, there is no decoherence dampening for the null chord contribution.

The semiclassical contributions from long chords to $\langle p_+ | \hat{\rho} | p_- \rangle$ are obtained by evaluating a similar integral to equation (6.1) (see, for example, [7]) by stationary phase, with analogous results to equation (6.2). However, the limiting form for the contributions of small chords to the projection of the spectral Wigner function does not generally have the same form as equation (6.3), because this was obtained under the assumption of a simple p^2 dependence of the Hamiltonian.

The same general picture holds for any basis resulting from a linear canonical transformation, $x \rightarrow x'$, of the classical phase space, because of the well-known symplectic invariance of the Weyl–Wigner formalism; see, for example, [7]. The density matrix in the q' representation follows from the transformation (6.1), after performing the classical change of variables. For each of these representations the decay of the off-diagonal elements of the density matrix $\langle q'_+ | \hat{\rho} | q'_- \rangle$ is determined by the decoherence distance functional (4.3) evaluated at the tips of the chords that project down precisely on to q'_+ and q'_- . This delicate quantum effect quickly drives the density towards a diagonal mixture of the same initial set of basis states which were superposed coherently to form the initial state, if this was an eigenstate of the internal Hamiltonian, because of the absence of drift for Hermitian Lindblad operators. The ultimate effect of the classical-like energy diffusion considered in the previous section will be manifest only on a larger timescale. Again, it should be pointed out that this qualitative scenario is well known (see, for example, [11, 16, 29]), the novelty being the complete model independence in which these general semiclassical results are here obtained.

7. Conclusion

The evolution of quantum systems that are weakly affected by the external environment can be studied within the framework of the Lindblad master equation (1.10). If the Lindblad operators are all Hermitian, the classical motion that supports semiclassical evolution is unaltered by the external environment, the only effect being to dampen the amplitude of each chord contribution to the semiclassical Wigner function. In the present context, this result embodies the known fact that Hermitian Lindblad operators produce no net drift [16]. This broad semiclassical scenario also holds for the full sub-semigroup of transformations generated by time-dependent Hermitian Lindblad operators and Hamiltonians. The decay of the semiclassical amplitudes was interpreted in section 5 as a small-scale diffusion of the energy of the initial (nearly pure) state, which is a more obvious effect of opening the system than the delicate loss of quantum coherence that immediately manifests itself as a loss of amplitude in the highly oscillatory region of the Wigner function. An intuitive explanation for this decay was recently put forward by Zurek [35] in the restricted framework of interference fringes in the Wigner function for a superposition of coherent states. These narrow oscillations arise near the centre of the chord separating a pair of Gaussians in phase space that would represent each single coherent state. Averaging over the juggling of the coherent states, effected by the external environment, destroys the interference pattern. This same intuitive interpretation can now be generalized to the slight motion of the whole classical manifold that supports extended semiclassical quantum states.

General Lindblad operators also account for energy loss. This is in principle contained in the differential equation (3.3) for the Wigner function, though no immediate separation of phase and amplitude is then possible. The path integral of Strunz [21] does lead to a semiclassical approximation in terms of complex trajectories. However, this is derived in the

position representation and, even if its Wigner–Weyl transformation (1.1) were obtained, it would still not be a clear route to the semiclassical evolution of Wigner functions. The reason is that, even for unitary evolution, the propagation of the Wigner function depends on the initial chord, through the orbit of both its tips. Thus, the semiclassical propagator of Wigner functions is paradoxically irrelevant to their motion, as discussed in [22]. In short, the general semiclassical description of the evolution of Wigner functions is undoubtedly more involved than the present restriction to Hermitian Lindblad operators, i.e. observables.

It is only in this case that the decoherence distance functional (4.3), defined by Strunz for arbitrary phase space paths, localizes on the real classical trajectories with end points at the tips of each chord of the Wigner function. The simplicity of the Weyl representation of observables as real smooth phase space functions then leads, by direct integration, to simple expressions for the density matrix in the position, or the momentum representation, in terms of the same decay factor that accounts for the decoherence of Wigner functions. The decay of large chords then appears as the dampening of off-diagonal elements in any representation.

Of course, we should be wary of the extrapolations that are required to synthesize such a simple picture. The description of a spectral Wigner function corresponding to a mixture of states in an energy window is only supported semiclassically by a single energy shell if the width of the window is classically small. Eventually, energy diffusion will widen the window beyond the limit of validity of this assumption. But, anyhow, the basic hypothesis in deriving the whole semiclassical theory, that only the oscillatory complex exponential terms in the integrals (2.7) and (3.2) were rapidly varying in phase space, eventually breaks down. Indeed, for large evolution times the amplitude functions were found to become sharply peaked along the classical manifold that supports the semiclassical state. Finally, we can add the further criticism that the simple semiclassical approximation, based on independent chords, breaks down in the neighbourhood of the classical manifold on to which the Lindblad operators concentrate the Wigner function. There, the pure states have been shown to be described by uniform approximations [2, 3] and ultimately their decoherent evolution should be ascertained.

Even so, the simplicity of a broad unified view over a wide range of diverse phenomena is a rare enough asset to be thrown away easily. For instance, we are familiar with the many uses of the Gutzwiller trace formula [36] within various branches of ‘semiclassics’, in spite of the many conceptual problems with its implementation. In the case of quantum spectra, it is also possible to find improved approximations that smooth over spurious singularities (see, for example, [37]), but at a cost. The indirect normalization of the square of the pure state Wigner function carried out in the appendix illustrates the uncanny self-consistency of the simple semiclassical approximation, which previously passed the more stringent test of the full pure state condition [4]. The difficulties with chord multiplicities and caustics simply vanish within such integrals. A companion paper [19] shows, among other things, how the simple semiclassical Wigner function developed here can be used to calculate the growth of linear entropy, an important measure of decoherence. Indeed, the stability of the direct normalization integral (also in the appendix) throughout the action of the Lindblad operators, allows us to single out the decay of the Wigner function amplitudes as a pure decoherence effect resulting from the contact of the internal system with the external environment.

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Appendix. Normalization

The normalization of pure state semiclassical Wigner functions is a delicate matter. Even though Berry [2] treated the case of one degree of freedom, it is worthwhile to rederive the integrals in a manner that is also valid for tori of higher dimensions. The main idea, already employed in [4], is to transform the integration variables from centre coordinates, x , to the canonical angles (θ_-, θ_+) at the tip of each chord on the quantized torus that is specified by its constant action variables, $I_{\pm} = \mathcal{I}$.

Let the points near each chord tip, x_{\pm} , take on local coordinates X_{\pm} , i.e., phase space points are given locally by $x = x_{\pm} + X_{\pm}$. Then we can also define local action and angle variables as $I_{\pm}(X_{\pm}) \equiv I(x)$ and $\theta_{\pm}(X_{\pm}) \equiv \theta(x)$, so that near each chord tip,

$$\delta X_{\pm} = \frac{\partial X_{\pm}}{\partial \theta_{\pm}} \delta \theta_{\pm} + \frac{\partial X_{\pm}}{\partial I_{\pm}} \delta I_{\pm}. \quad (\text{A.1})$$

Hence, for chord tips constrained to $I_{\pm} = \mathcal{I}$, the Jacobian for the change of variables, $(\theta_-, \theta_+) \rightarrow \delta x = (X_+ + X_-)/2$, is obtained from

$$\delta x = \frac{1}{2} \left. \frac{\partial X_+}{\partial \theta_+} \right|_{I_+=\mathcal{I}} \delta \theta_+ + \frac{1}{2} \left. \frac{\partial X_-}{\partial \theta_-} \right|_{I_-=\mathcal{I}} \delta \theta_- \quad (\text{A.2})$$

so that

$$\det \frac{\partial(p, q)}{\partial(\theta_-, \theta_+)} = \det \begin{bmatrix} \frac{1}{2} \frac{\partial p_+}{\partial \theta_+} & \frac{1}{2} \frac{\partial p_-}{\partial \theta_-} \\ \frac{1}{2} \frac{\partial q_+}{\partial \theta_+} & \frac{1}{2} \frac{\partial q_-}{\partial \theta_-} \end{bmatrix}. \quad (\text{A.3})$$

Each element in equation (A.3) represents an $(l \times l)$ -dimensional block matrix and each of its elements may be interpreted as a component, p_1, \dots, p_l , or q_1, \dots, q_l , of the velocity vector \dot{x}_{\pm} for the various choices of actions $I_1(x), \dots, I_l(x)$ as the Hamiltonian. In the case that $l = 1$, these are proportional to the Hamiltonian velocity vectors shown in figure 1. Thus, the Jacobian can be rewritten in the form

$$\left| \det \frac{\partial(p, q)}{\partial(\theta_-, \theta_+)} \right| = \left(\frac{1}{2} \right)^{2l} |\det \dot{x}_+ \wedge \dot{x}_-| = \left(\frac{1}{2} \right)^{2l} |\det\{I_-, I_+\}| \quad (\text{A.4})$$

which is obvious in the case that $l = 1$. In the general case, this is obtained by the same manipulations used in [3] to prove the complementary relation:

$$|\det\{I_-, I_+\}| = \left| \det \frac{\partial(I_-, I_+)}{\partial(p_-, q_-)} \right|. \quad (\text{A.5})$$

It is important to note that the matrix of Poisson brackets, $\{I_-, I_+\}$, is only $l \times l$, whereas the Jacobians in both equations (A.4) and (A.5) have $(2l) \times (2l)$ dimensions.

There is just one chord for each pair (θ_-, θ_+) , but the same chord results from the interchange of θ_- with θ_+ , so that the overall transformation of the integration variables is

$$\int \cdot dx = 2^{-(2l+1)} \int_0^{2\pi} \cdot |\det\{I_-, I_+\}| d\theta_- d\theta_+. \quad (\text{A.6})$$

In passing from integrals over centres to integrals over pairs of angles, all problems with chord multiplicities and even caustics disappear. The chord densities really take on an independent existence, so that from this new point of view, they may merely happen to share the same centre. Whereas in the original semiclassical Wigner function a pair of chords with the same

centre coalesce as the centre moves on to a caustic, here the amplitude for the single chord determined by θ_- and θ_+ becomes singular but the integral is regularized by the determinant in equation (A.6).

It is easier to deal first with the integral over the square of the Wigner function in equation (2.14). Introducing in equation (1.4) the amplitude of a chord contribution to the semiclassical pure state Wigner function as [3]

$$A(x) = \frac{2}{(\pi\sqrt{2\pi\hbar})^l} |\det\{I_-, I_+\}|^{-\frac{1}{2}} \quad (\text{A.7})$$

and averaging over oscillations, i.e. taking $\cos^2 = \frac{1}{2}$, we immediately obtain

$$\text{tr } \hat{\rho}^2 = \int \frac{d\theta_-}{(2\pi)^l} \frac{d\theta_+}{(2\pi)^l} = 1. \quad (\text{A.8})$$

Given that the pure state condition is verified semiclassically, equation (A.8) indirectly should imply that also $\text{tr } \hat{\rho} = 1$. However, this is not the result of the direct calculation of

$$\text{tr } \hat{\rho} = \int dx W(x) \approx \frac{1}{(4\pi\sqrt{2\pi\hbar})^l} \int d\theta_- d\theta_+ |\det\{I_-, I_+\}|^{\frac{1}{2}} \cos \left[\frac{S(\theta_-, \theta_+)}{\hbar} \right]. \quad (\text{A.9})$$

This integral is dominated by the region where θ_+ is near θ_- , even though the determinant on the right-hand side of equation (A.9) cancels for $\theta_+ = \theta_-$, because there the Hessian determinant of $S(\theta_-, \theta_+)$ also tends to zero. It is first necessary to estimate the area, S , for small chords. Let us return to the interpretation of a given angle, θ_v , as the time along a trajectory on the torus, generated by choosing the respective action variable, I_v , as the Hamiltonian. If we transfer the origin to the torus, at θ_- , so that $p_- = q_- = 0$, the action for the chord to θ_+ is just

$$S(\theta_-, \theta_+) = \int_{\theta_-}^{\theta_+} p(t)\dot{q}(t) dt - \frac{1}{2} p_+ \cdot q_+. \quad (\text{A.10})$$

Hence, the second derivative of the chord action is simply

$$\frac{\partial^2 S}{\partial \theta_+^2} = \frac{1}{2} (p_+ \cdot \ddot{q}_+ - q_+ \cdot \ddot{p}_+) \quad (\text{A.11})$$

so that, as $\theta_+ \rightarrow \theta_-$, we obtain

$$\frac{\partial^2 S}{\partial \theta_+^2} \longrightarrow \frac{1}{2} \dot{x}_+ \wedge \dot{x}_-. \quad (\text{A.12})$$

Therefore, the Hessian determinant for the stationary phase along $\theta_+ = \theta_-$ is just

$$\left| \det \frac{\partial^2 S}{\partial \theta_+^2} \right| = \left(\frac{1}{2} \right)^l |\det\{I_-, I_+\}|. \quad (\text{A.13})$$

As noted previously, the Poisson bracket matrix has $l \times l$ dimensions, but the power of its preceding factor in equation (A.13) is not the same as in equation (A.4), so that finally,

$$\text{tr } \hat{\rho} \approx \left(\frac{\sqrt{2}}{2} \right)^l. \quad (\text{A.14})$$

The factor previously obtained using non-canonical coordinates on the torus, in [2] for $l = 1$, was $\sqrt{2/3}$, instead of equation (A.14). The important point is not the precise factor, but the fact that this depends neither on Planck's constant, nor on the classical system, except for the number of degrees of freedom. There is no point in trying to divide the semiclassical Wigner function by the normalization factor (A.14), because this will be inaccurate locally, inside the torus, as well as destroying the indirect normalization (A.8). The failure of the

normalization of the simple semiclassical Wigner function is a consequence of its (integrable) singularity precisely in the neighbourhood of the classical manifold, which is the region that dominates the normalization integral (A.9). In contrast, the integral for $\text{tr } \hat{\rho}^2$ depends on the entire oscillatory domain of the Wigner function, so that indirect semiclassical normalization is exact.

What is the effect of evolution on the normalization? Evidently, both equations (A.8) and (A.14) are stable with respect to unitary evolution. Because the normalization integral is dominated by the region of small chords, the decoherence distance functional (4.3) cancels for the stationary phase condition, $\theta_+ = \theta_-$, in equation (A.9), so that there is no effect of decoherence on the direct normalization. The evolving semiclassical Wigner function is given correctly by equation (4.2) while the semiclassical approximation remains valid, i.e. until the amplitude becomes so concentrated on the classical manifold that the assumption of its smoothness is no longer valid. It follows that the remarkably simple expression

$$\text{tr } \hat{\rho}^2 \approx \int \frac{d\theta_-}{(2\pi)^l} \frac{d\theta_+}{(2\pi)^l} \exp -\{D_I[\theta_+, \theta_-]\}^2 \quad (\text{A.15})$$

in terms of the decoherence distance functional (4.3) over the pair of orbits that end up on θ_+ and θ_- , is valid within the present semiclassical theory.

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