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Classical mechanics from quantum state diffusion—a phase-space approach

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Abstract. Quantum state diffusion (QSD) provides a natural unravelling of a mixed-state open quantum system into component pure states. We investigate the semiclassical limit of QSD in a phase-space approach using the Wigner function. As $\hbar \rightarrow 0$, QSD exhibits two very different dynamical regimes, depending on the volume of phase space covered by the quantum state. For large volumes there is a *localization regime* represented by classical nonlinear and nonlocal diffusion processes. For small volumes, comparable in size with a Planck cell, there is a *wavepacket regime*. Here, the centroid of the wavepacket follows a classical Langevin equation, obtained through the adiabatic elimination of the dynamics of the second-order moments of the wavepacket. The corresponding Fokker–Planck equation is identical to the one obtained from the classical limit of the original mixed-state dynamics. In the companion paper we present an axiomatic approach to a classical theory of quantum localization without using the underlying QSD theory.

1. Introduction

Classical behaviour of a quantum system can be related to the loss of coherence produced by interaction with the environment. This has been shown in a number of investigations based on the reduced density operator of an open quantum system (see for instance Joos and Zeh [2], Unruh and Zurek [3] or Zurek [4]). In this paper, however, we base our investigations on a stochastic pure-state description of open quantum systems, quantum state diffusion (QSD). We demonstrate how, as $\hbar \rightarrow 0$, QSD localizes quantum states to wavepackets of near-Planck cell volume. These wavepackets remain localized and their centroid follows a closed classical (dissipative and diffusive) equation of motion. The derivation of this result is subtle and surprisingly requires careful consideration of the second-order moments of the localized wavepacket.

1.1. Quantum description of open systems

The traditional ensemble description of Markovian open quantum systems is based on the quantum master equation

$$\dot{\rho} = -\frac{i}{\hbar}[H, \rho] + \frac{1}{2} \sum_{\mu} ([L_{\mu}\rho, L_{\mu}^{\dagger}] + [L_{\mu}, \rho L_{\mu}^{\dagger}]) \quad (1)$$

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here written in Lindblad form [5, 6]. In (1), ρ is the density operator of the open quantum system, H is its Hamiltonian and the Lindblad operators L_μ represent the effects of the environment on the system. Their dependence on \hbar is crucial for the results of this paper and we devote a whole section to this problem.

For the Markovian equation (1) to be valid, the memory time of the environment has to be much shorter than relevant system timescales. Usually, (1) is derived from the dynamics of the total system within the so-called Born–Markov approximation [7], which relies not only on a Markov but also on a weak-coupling assumption. In the very important class of a harmonic oscillator environment with an environment-linear coupling to the system, the derivation of a Markovian master equation can be based on the Markov assumption alone [8–10].

Instead of the mixed-state ensemble approach (1), open quantum systems can be described by means of the stochastic QSD equation for pure states,

$$|d\psi_\xi\rangle = -\frac{i}{\hbar}H|\psi_\xi\rangle dt - \frac{1}{2}\sum_\mu(L_\mu^\dagger L_\mu - 2\langle L_\mu^\dagger\rangle L_\mu + |\langle L_\mu\rangle|^2)|\psi_\xi\rangle dt + \sum_\mu(L_\mu - \langle L_\mu\rangle)|\psi_\xi\rangle d\xi_\mu \quad (2)$$

as introduced by Gisin and Percival [11–13], based on earlier work by Gisin [14, 15] and Diósi [16–18]. The density operator evolving according to (1) is recovered by the ensemble mean $M(\dots)$ over the stochastic pure state projectors obtained as solutions of the QSD unravelling (2),

$$\rho(t) = M(|\psi_\xi(t)\rangle\langle\psi_\xi(t)|). \quad (3)$$

We use the subscript ξ to indicate the dependence on the stochastic processes ξ_μ . The complex Wiener increments $d\xi_\mu$ in (2) satisfy the fundamental properties [12, 13]

$$M(d\xi_\mu) = 0 \quad M(d\xi_\mu d\xi_\nu) = 0 \quad \text{and} \quad M(d\xi_\mu d\xi_\nu^*) = \delta_{\mu\nu} dt. \quad (4)$$

The QSD equation (2) is nonlinear because of the terms which include the expectation values $\langle L_\mu\rangle_\xi$. In QSD, it is important to distinguish between quantum expectation values $\langle A\rangle_\xi = \langle\psi_\xi|A|\psi_\xi\rangle$ and the classical ensemble mean $M(\dots)$. From (3) we see the equivalence $\text{Tr}(A\rho) = M(\langle A\rangle_\xi)$.

QSD has proven to be an effective quantum trajectory method for the numerical solution of the master equation (1) [12, 21–28] which is due to the localization property of QSD: state vectors tend to localize towards wavepackets, thus reducing the computational effort tremendously. This has been shown by Diósi [17], Gisin and Percival [12], Percival [19] and Halliwell and Zoupas [20]. Many numerical investigations also show, and some exploit, the localizing property of QSD, see Gisin and Percival [13], Spiller and Ralph [21], Garraway and Knight [22], Steimle *et al* [23], Schack *et al* [24, 27], Gisin and Rigo [25, 26] or Brun *et al* [28].

From a fundamental viewpoint, QSD represents a dynamical model for quantum measurement [11–18]. As such it can be derived microscopically as the evolution equation of the state vector of a continuously measured system conditioned on the measurement outcome [7].

We focus on the classical $\hbar \rightarrow 0$ limit of QSD, which shows a rich dynamical structure ultimately leading to the classical dynamics of point particles. Classical dynamics emerges from quantum dynamics not only through Ehrenfest classical evolution equations for quantum expectation values, but also through a mechanism for localization, preventing quantum wavepackets from spreading. The localization becomes stronger as the open

quantum system becomes more classical. This paper investigates the semiclassical ($\hbar \rightarrow 0$) limit of QSD in the phase-space approach, to clarify the general mechanism for localization in QSD and the emergence of classical evolution equations. First, however, we review the classical theory of open systems.

1.2. Classical description of open systems

In classical physics, the distribution $\rho(\mathbf{q}, \mathbf{p})$ in $2d$ -dimensional phase space replaces the quantum density operator. Its time evolution is given by a diffusion equation, in the simplest case a phase-space Fokker–Planck equation [29, 30]

$$\frac{\partial \rho(\mathbf{q}, \mathbf{p}, t)}{\partial t} = - \sum_i \partial_i [\mathcal{A}_i \rho] + \frac{1}{2} \sum_{ij} \partial_i \partial_j [(\mathcal{B}\mathcal{B}^T)_{ij} \rho] \quad (5)$$

with drift vector \mathcal{A} and diffusion matrix \mathcal{B} . We use the phase-space notation for the derivatives,

$$(\partial_1, \dots, \partial_d, \partial_{d+1}, \dots, \partial_{2d}) = \left(\frac{\partial}{\partial q_1}, \dots, \frac{\partial}{\partial q_d}, \frac{\partial}{\partial p_1}, \dots, \frac{\partial}{\partial p_d} \right). \quad (6)$$

The Fokker–Planck equation (5) describes the time evolution of an ensemble of point particles whose diffusive dynamics is given by the associated classical Langevin–Itô equation [29, 30]

$$\begin{pmatrix} d\mathbf{q} \\ d\mathbf{p} \end{pmatrix} = \mathcal{A}(\mathbf{q}, \mathbf{p}) dt + \mathcal{B}(\mathbf{q}, \mathbf{p}) d\mathbf{w} \quad (7)$$

with $2d$ -dimensional Wiener increment vectors $d\mathbf{w} = (dw_1, \dots, dw_{2d})$, satisfying

$$\mathbb{M}(dw_i dw_j) = \delta_{ij} dt. \quad (8)$$

Expression (7) clarifies the use of the terms ‘drift vector’ and ‘diffusion matrix’ for \mathcal{A} and \mathcal{B} [29].

The relation between the classical Fokker–Planck equation (5) for the ensemble and the classical stochastic Langevin–Itô equation (7) for a pure state of the ensemble is analogous to the relation between the quantum master equation (1) and the QSD equation (2). See figure 1 for a visualization of this relation. As in the quantum case, for a pure-state initial distribution, we recover the solution of the Fokker–Planck equation (5) as the ensemble mean over the classical pure states (point distributions),

$$\rho(\mathbf{q}, \mathbf{p}, t) = \mathbb{M}(\delta(\mathbf{q} - \mathbf{q}_w(t))\delta(\mathbf{p} - \mathbf{p}_w(t))) \quad (9)$$

where the trajectories $(\mathbf{q}_w(t), \mathbf{p}_w(t))$ are solutions of the Langevin–Itô equation (7) and the ensemble mean is taken over the stochastic processes $\mathbf{w}(t)$ with increments (8).

1.3. The \hbar -dependence of the environmental terms

We are interested in the semiclassical $\hbar \rightarrow 0$ limit of open quantum systems whose time evolution is described by a master equation of Lindblad form (1). We keep only those contributions from Lindblad operators $L_\mu = L_\mu(\hbar)$ that actually survive the classical $\hbar \rightarrow 0$ limit.

In this respect, non-Hermitian Lindblad operators $L \neq L^\dagger$ with a contribution

$$\frac{1}{2}([L\rho, L^\dagger] + [L, \rho L^\dagger]) \quad (10)$$

to the master equation and Hermitian Lindblad operators $L = L^\dagger \equiv K$ with

$$\frac{1}{2}([K\rho, K] + [K, \rho K]) = -\frac{1}{2}[K, [K, \rho]] \quad (11)$$

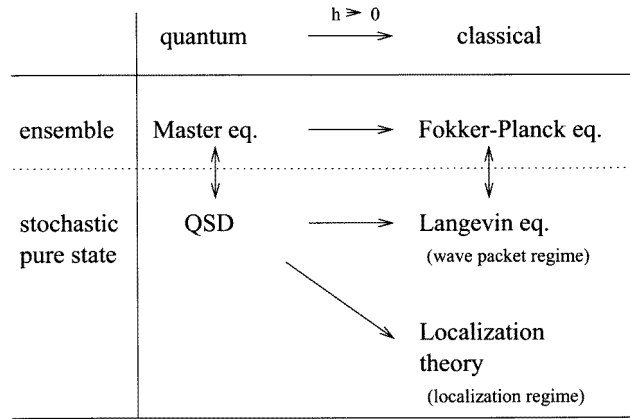


Figure 1. Relation between various descriptions of open systems.

behave quite differently as $\hbar \rightarrow 0$. As will be demonstrated in detail in section 2, we can replace—to lowest order in \hbar —commutators $[,]$ by Poisson brackets $i\hbar\{, \}$. While contributions of the form (10) gain a factor \hbar , contributions of Hermitian Lindblad operators (11) gain a factor \hbar^2 . If terms (10) and (11) are to survive the $\hbar \rightarrow 0$ limit, they have to be of the form

$$\frac{1}{2\hbar}([L\rho, L^\dagger] + [L, \rho L^\dagger]) \quad (12)$$

for the case of non-Hermitian operators L , and

$$-\frac{1}{2\hbar^2}[K, [K, \rho]] \quad (13)$$

for Hermitian Lindblad operators K , where we assume that both operators approach a finite operator as $\hbar \rightarrow 0$. These arguments for the \hbar -dependence of the environmental terms in the Lindblad master equation are supported by well known examples of open system master equations, as for instance a cavity mode coupled to a thermal reservoir [6, 7] or the quantum Brownian motion master equation [9, 10].

The L -terms (12) lead to classical *dissipation* while the K -terms (13) describe classical *diffusion*. If the master equation is to describe the coupling to heat bath, for instance, these contributions are related through the fluctuation–dissipation theorem. If the master equation describes the coupling to a zero-temperature bath, there is only dissipation and no thermal fluctuations ($K \equiv 0$) [6, 7].

If the master equation represents the effects of a measurement only, there is no dissipation ($L \equiv 0$) and the Hermitian operator K represents the measured observable [31]. We consider this situation in the companion paper [1].

We conclude that as $\hbar \rightarrow 0$, keeping relevant terms, the environmental contribution to the Lindblad master equation has to be of the form

$$\frac{1}{2\hbar} \sum_{\mu} ([L_{\mu}\rho, L_{\mu}^{\dagger}] + [L_{\mu}, \rho L_{\mu}^{\dagger}]) - \frac{1}{2\hbar^2} \sum_{\nu} [K_{\nu}, [K_{\nu}, \rho]] \quad (14)$$

with Lindblad operators $L_{\mu} \neq L_{\mu}^{\dagger}$ and $K_{\nu} = K_{\nu}^{\dagger}$ independent of \hbar . This form (14) of the environmental terms in the Lindblad master equation is the basis of our investigations. It is interesting to see the effects of the various terms when open systems are described in terms of QSD.

1.4. The semiclassical limit

In the traditional ensemble description of open systems, as $\hbar \rightarrow 0$, a classical phase-space Fokker–Planck equation can be derived from the quantum master equation (section 2) (see figure 1). However, on the pure-state level, the corresponding semiclassical limit is subtle (section 3). QSD shows two very different semiclassical limits.

If the quantum state is not yet localized in phase space, then, in the semiclassical limit, QSD works in its localization regime (section 4). This is a very interesting regime since it incorporates a classical, nonlinear and nonlocal, purely diffusive evolution equation for a phase-space density, leading to its localization in phase space. The derivation of this localization theory is one of the main results of this paper. It can be seen as the dynamical way QSD chooses random initial conditions to be propagated by a classical Langevin equation. In the traditional simulation of the Fokker–Planck equation with the classical Langevin equation, random initial conditions have to be chosen ‘by hand’. Therefore, this localization theory has no counterpart in the traditional classical dynamical theory of open systems (Fokker–Planck or Langevin equations). Nevertheless, the companion paper [1] introduces a classical theory of this localization regime.

When the localization has taken place we enter the wavepacket regime of QSD (section 5). The phase-space volume occupied by the quantum state is of the order \hbar^d . The stochastic evolution equation for the centroid of the wavepacket corresponds—to leading order in \hbar —exactly to the Fokker–Planck equation, which was originally derived directly from the quantum master equation (see figure 1). We clarify these subtle connections in detail.

This paper is organized as follows. In section 2 we review the traditional semiclassical approach in deriving the Fokker–Planck equation from the master equation and state the corresponding classical Langevin–Itô equation. We express the classical drift vector \mathcal{A} and the diffusion matrix \mathcal{B} in terms of the Wigner–Moyal transforms of the quantum operators H , L_μ and K_ν . Remarkably, we see the first hints of QSD even in this traditional approach.

The main results appear in sections 3–5. In section 3 we derive the semiclassical limit of QSD in a phase-space approach. Two dynamical regimes emerge, the localization regime investigated in section 4 and the wavepacket regime developed in section 5. In the latter regime, it is appropriate to describe the state vector in terms of the centroid and moments of the wavepacket, establishing in detail the connection to the classical Langevin equation as derived in section 2. We close with a summary and conclusions in the final section 6.

2. Traditional semiclassical limit of the master equation

The starting point is the most general quantum master equation (1) for a Markovian open quantum system

$$\dot{\rho} = -\frac{i}{\hbar}[H, \rho] + \frac{1}{2\hbar} \sum_{\mu} ([L_{\mu}\rho, L_{\mu}^{\dagger}] + [L_{\mu}, \rho L_{\mu}^{\dagger}]) - \frac{1}{2\hbar^2} \sum_{\nu} [K_{\nu}, [K_{\nu}, \rho]] \quad (15)$$

written in the form (14) to help the investigation of the $\hbar \rightarrow 0$ limit. We show that the non-Hermitian operators L_{μ} lead to dissipation and *quantum* fluctuations, while the Hermitian operators K_{ν} describe *classical* fluctuations and sometimes also contribute to dissipation.

In order to investigate the semiclassical limit of the master equation (15), we replace the density operator by its corresponding Wigner function $W(\mathbf{q}, \mathbf{p})$ [32] in $2d$ -dimensional

phase space,

$$W(\mathbf{q}, \mathbf{p}) = 2^d (2\pi\hbar)^{-(d/2)} \int d\mathbf{x} \langle \mathbf{q} - \mathbf{x} | \rho | \mathbf{q} + \mathbf{x} \rangle \langle \mathbf{x} | 2\mathbf{p} \rangle. \quad (16)$$

Likewise we replace the operators by their Wigner–Moyal transforms [33] $H(\mathbf{q}, \mathbf{p})$, $L_\mu(\mathbf{q}, \mathbf{p})$ and $K_\nu(\mathbf{q}, \mathbf{p})$. Expanding the resulting evolution equation for the Wigner function to first order in \hbar , it takes the differential form

$$\begin{aligned} \frac{\partial W}{\partial t} = & \{H, W\} + \left(\frac{i}{2}\right) \sum_{\mu} (\{L_{\mu} W, L_{\mu}^*\} + \{L_{\mu}, W L_{\mu}^*\}) + \frac{1}{2} \sum_{\nu} \{K_{\nu}, \{K_{\nu}, W\}\} \\ & - \left(\frac{\hbar}{4}\right) \sum_{\mu} (\{L_{\mu}, \{W, L_{\mu}^*\}\} + \{\{L_{\mu}, W\}, L_{\mu}^*\}) \end{aligned} \quad (17)$$

where $\{, \}$ denotes the classical Poisson bracket

$$\{f, g\} = \sum_{i=1}^d \left(\frac{\partial f}{\partial q_i} \frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i} \frac{\partial g}{\partial q_i} \right). \quad (18)$$

Notice that to zeroth order ($\hbar = 0$), the evolution equation (17) is formally just the original master equation with the canonical replacement of commutators by Poisson brackets, $[,] \rightarrow i\hbar\{, \}$.

2.1. Fokker–Planck equation

Equation (17) is in fact a phase-space Fokker–Planck equation [29, 30]. This implies that if the initial Wigner function is a classical phase space probability distribution, it remains a probability distribution for all times. After rearranging, (17) takes the Fokker–Planck form (5):

$$\begin{aligned} \frac{\partial W}{\partial t} = & - \sum_i \partial_i [A_i W] + \frac{1}{2} \sum_{\nu} \left\{ \sum_{ij} \partial_i \partial_j [(B_{\nu} B_{\nu}^T)_{ij} W] \right\} \\ & + \frac{\hbar}{2} \sum_{\mu} \left\{ \sum_{ij} \partial_i \partial_j [(C_{\mu} C_{\mu}^T)_{ij} W] \right\} \end{aligned} \quad (19)$$

with the phase-space notation (6) for the derivatives ∂_i .

The drift vector \mathbf{A} in (19) consists of the Hamiltonian contribution \mathbf{A}_H , contributions from the non-Hermitian ($\mathbf{A}_{L_{\mu}}$) and from the Hermitian ($\mathbf{A}_{K_{\nu}}$) Lindblad operators so that

$$\mathbf{A} = \mathbf{A}_H + \sum_{\mu} \mathbf{A}_{L_{\mu}} + \sum_{\nu} \mathbf{A}_{K_{\nu}}. \quad (20)$$

We find

$$\mathbf{A}_H = \begin{pmatrix} \frac{\partial H}{\partial \mathbf{p}} \\ -\frac{\partial H}{\partial \mathbf{q}} \end{pmatrix} \quad \mathbf{A}_{L_{\mu}} = \begin{pmatrix} Y_{\mu} \frac{\partial X_{\mu}}{\partial \mathbf{p}} - X_{\mu} \frac{\partial Y_{\mu}}{\partial \mathbf{p}} \\ X_{\mu} \frac{\partial Y_{\mu}}{\partial \mathbf{q}} - Y_{\mu} \frac{\partial X_{\mu}}{\partial \mathbf{q}} \end{pmatrix} \quad \mathbf{A}_{K_{\nu}} = \begin{pmatrix} \frac{1}{2} \left\{ \frac{\partial K_{\nu}}{\partial \mathbf{p}}, K_{\nu} \right\} \\ \frac{1}{2} \left\{ K_{\nu}, \frac{\partial K_{\nu}}{\partial \mathbf{q}} \right\} \end{pmatrix} \quad (21)$$

where $L_{\mu}(\mathbf{q}, \mathbf{p}) = X_{\mu}(\mathbf{q}, \mathbf{p}) + iY_{\mu}(\mathbf{q}, \mathbf{p})$.

It is apparent that the contribution $\mathbf{A}_{K_{\nu}}$ of the Hermitian Lindblad operators to the drift vanishes for linear operators $K_{\nu}(\mathbf{q}, \mathbf{p})$ as in many important applications. It also vanishes for purely position- or momentum-dependent operators $K_{\nu}(\mathbf{q})$ or $K_{\nu}(\mathbf{p})$. In these cases the phase-space divergence of the vector field \mathbf{A} is determined from the contribution of the non-Hermitian environmental terms only,

$$\text{div } \mathbf{A} = \sum_{\mu} \text{div } \mathbf{A}_{L_{\mu}} = -2 \sum_{\mu} \{X_{\mu}, Y_{\mu}\}. \quad (22)$$

We see that the Fokker–Planck equation describes classical dissipation for $\sum_{\mu} \{X_{\mu}, Y_{\mu}\} > 0$, since, according to Liouville’s theorem [34], phase-space volumes then shrink under time evolution.

The diffusion terms in the Fokker–Planck equation describe fluctuations. They are determined by the $2d \times 2d$ diffusion matrices B_v and C_{μ} in (19)

$$\begin{aligned}
 B_v &= \frac{1}{\sqrt{d}} \begin{pmatrix} -\frac{\partial K_v}{\partial p_1} & \dots & -\frac{\partial K_v}{\partial p_1} & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ -\frac{\partial K_v}{\partial p_d} & \dots & -\frac{\partial K_v}{\partial p_d} & 0 & \dots & 0 \\ \frac{\partial K_v}{\partial q_1} & \dots & \frac{\partial K_v}{\partial q_1} & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \frac{\partial K_v}{\partial q_d} & \dots & \frac{\partial K_v}{\partial q_d} & 0 & \dots & 0 \end{pmatrix} \\
 C_{\mu} &= \frac{1}{\sqrt{d}} \begin{pmatrix} -\frac{\partial X_{\mu}}{\partial p_1} & \dots & -\frac{\partial X_{\mu}}{\partial p_1} & -\frac{\partial Y_{\mu}}{\partial p_1} & \dots & -\frac{\partial Y_{\mu}}{\partial p_1} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ -\frac{\partial X_{\mu}}{\partial p_d} & \dots & -\frac{\partial X_{\mu}}{\partial p_d} & -\frac{\partial Y_{\mu}}{\partial p_d} & \dots & -\frac{\partial Y_{\mu}}{\partial p_d} \\ \frac{\partial X_{\mu}}{\partial q_1} & \dots & \frac{\partial X_{\mu}}{\partial q_1} & \frac{\partial Y_{\mu}}{\partial q_1} & \dots & \frac{\partial Y_{\mu}}{\partial q_1} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \frac{\partial X_{\mu}}{\partial q_d} & \dots & \frac{\partial X_{\mu}}{\partial q_d} & \frac{\partial Y_{\mu}}{\partial q_d} & \dots & \frac{\partial Y_{\mu}}{\partial q_d} \end{pmatrix}. \tag{23}
 \end{aligned}$$

The Hermitian K_v in the master equation describe classical fluctuations (matrices B_v). If the master equation describes the relaxation to a steady equilibrium density operator, these fluctuations and the dissipative terms are related by the fluctuation–dissipation theorem [6, 29, 30].

When there are no classical fluctuations, as for a zero-temperature bath, there are still quantum fluctuations (matrices C_{μ}) arising from the non-Hermitian L_{μ} . The reason for their appearance is that the shrinking due to the dissipative drift would eventually lead to a violation of Heisenberg’s indeterminacy principle, if it were not for these terms of order \hbar .

We conclude that the non-Hermitian Lindblad terms L_{μ} contribute to zeroth order in \hbar to the drift and to first order in \hbar to the diffusion (*quantum noise*), while the Hermitian Lindblad terms K_v contribute to zeroth order to the diffusion (*classical noise*) and for some K_v also to the drift, but they have no first-order contribution.

2.2. Classical Langevin equation

Here we show that the classical Langevin–Itô equation associated with the Fokker–Planck equation (19)

$$\begin{pmatrix} dq \\ dp \end{pmatrix} = \mathbf{A}(\mathbf{q}, \mathbf{p}) dt + \sum_v B_v(\mathbf{q}, \mathbf{p}) d\mathbf{w}_v + \sqrt{\hbar} \sum_{\mu} C_{\mu}(\mathbf{q}, \mathbf{p}) d\mathbf{w}_{\mu} \tag{24}$$

with drift vector (20), diffusion matrices (23) and $2d$ -dimensional independent Wiener increment vectors $d\mathbf{w}_v, d\mathbf{w}_{\mu}$ ($dw_{\kappa}^{(i)} dw_{\lambda}^{(j)} = \delta_{\kappa\lambda} \delta_{ij} dt$) can be conveniently described in terms of complex Wiener increments which already suggest a connection with QSD.

To zeroth order in \hbar , (24) describes a classical dynamical system with a (in general non-Hamiltonian) vector field $\mathbf{A}(\mathbf{q}, \mathbf{p})$ and diffusion matrices B_v . The first quantum effect in (24) appears as quantum noise, preventing the evolution equation (24) from approaching a stationary solution, the manifestation of Heisenberg’s indeterminacy principle.

At first sight, it appears that the Langevin equation (24) requires $2d$ independent Wiener increments $dw_v^{(i)}$ (or $dw_\mu^{(i)}$) for each of the Lindblad operators K_v (or L_μ). Due to the special form of the diffusion matrices B_v and C_μ (23) however, we can define the combined real Wiener increments

$$dw_v \equiv \frac{1}{\sqrt{d}}(dw_v^{(1)} + \dots + dw_v^{(d)}) \quad (25)$$

for the classical fluctuations and the *complex* Wiener increments

$$d\xi_\mu \equiv \frac{1}{\sqrt{2d}}((dw_\mu^{(d+1)} + \dots + dw_\mu^{(2d)}) + i(dw_\mu^{(1)} + \dots + dw_\mu^{(d)})) \quad (26)$$

for the quantum fluctuations, which satisfy the fundamental properties of complex noise (4). Rewriting the classical Langevin–Itô equation (24) in terms of these newly defined Wiener increments, we get

$$\begin{pmatrix} dq \\ dp \end{pmatrix} = A(q, p) dt + \sum_v \mathcal{J}[\nabla K_v] dw_v + 2\sqrt{\hbar} \text{Re} \left(\sum_\mu \left(-\frac{i}{\sqrt{2}} \mathcal{J}[\nabla L_\mu] \right) d\xi_\mu \right) \quad (27)$$

where $(\nabla K_v)_i = \partial_i K_v$ and \mathcal{J} is the $2d \times 2d$ symplectic unit matrix

$$\mathcal{J} = \begin{pmatrix} 0 & -E \\ E & 0 \end{pmatrix} \quad (28)$$

with the $d \times d$ unit matrix $E_{ij} = \delta_{ij}$. It is remarkable that this classical pure-state description already hints, through the complex noise in the quantum fluctuations, at an underlying quantum description in terms of QSD. The QSD equation (2) also requires complex independent increments, one for each Lindblad operator, just like the quantum fluctuations of the classical Langevin equation (27).

To summarize this traditional approach to open quantum systems, one takes the semiclassical limit at the *ensemble* level, leading from the quantum master equation to a classical Fokker–Planck equation. The associated classical pure-state description in terms of a Langevin–Itô equation (27) is then interpreted as the (semi)classical dynamics of an individual member of the original quantum ensemble.

3. Phase-space QSD and its semiclassical limit

We now investigate what happens if we take the semiclassical limit directly at the quantum pure-state level, starting from a stochastic QSD description of the open system dynamics. We see that this limit shows some new features.

The quantum pure-state description is given by the QSD equation (2) [11–13], which for the master equation (15) takes the form

$$\begin{aligned} |d\psi_\xi\rangle = & -\frac{i}{\hbar} H |\psi_\xi\rangle dt - \frac{1}{2\hbar} \sum_\mu (L_\mu^\dagger L_\mu - 2\langle L_\mu^\dagger \rangle L_\mu + |\langle L_\mu \rangle|^2) |\psi_\xi\rangle dt \\ & + \frac{1}{\sqrt{\hbar}} \sum_\mu (L_\mu - \langle L_\mu \rangle) |\psi_\xi\rangle d\xi_\mu - \frac{1}{2\hbar^2} \sum_v (K_v - \langle K_v \rangle)^2 |\psi_\xi\rangle dt \\ & + \frac{1}{\hbar} \sum_v (K_v - \langle K_v \rangle) |\psi_\xi\rangle d\xi_v \end{aligned} \quad (29)$$

where the independent complex Wiener increments $d\xi_\mu, d\xi_v$ satisfy (4).

In analogy with the derivation of the Fokker–Planck equation from the quantum master equation, we use a phase-space description to investigate the semiclassical limit of QSD. We introduce the Wigner function

$$W_\xi(\mathbf{q}, \mathbf{p}) = 2^d (2\pi\hbar)^{-(d/2)} \int d\mathbf{x} \langle \mathbf{q} - \mathbf{x} | \psi_\xi \rangle \langle \psi_\xi | \mathbf{q} + \mathbf{x} \rangle \langle \mathbf{x} | 2\mathbf{p} \rangle \quad (30)$$

to represent an individual member of the ensemble. The Wigner function $W(\mathbf{q}, \mathbf{p}, t)$ of the ensemble as introduced in the last section is recovered by the ensemble mean

$$W(\mathbf{q}, \mathbf{p}, t) = \text{M}(W_\xi(\mathbf{q}, \mathbf{p}, t)). \quad (31)$$

The QSD time evolution of these stochastic Wigner functions W_ξ is based on the stochastic evolution of the pure-state projectors $|\psi_\xi\rangle\langle\psi_\xi|$ of the QSD solutions $|\psi_\xi\rangle$ as investigated by Diósi [16, 17], Gatarek and Gisin [36] and Gisin and Rigo [25]. We find an expression of the form

$$dW_\xi = [\text{drift}] dt + 2\text{Re} \left(\sum_\mu [L\text{-diffusion}]_\mu d\xi_\mu \right) + 2\text{Re} \left(\sum_\nu [K\text{-diffusion}]_\nu d\xi_\nu \right). \quad (32)$$

The terms ‘drift’ and ‘diffusion’ here refer to the dynamics in the space of Wigner functions and must not be confused with the drift and diffusion of phase space points described by the Fokker–Planck equation. Since the diffusion terms in (32) vanish in the mean, we see from (31) that the drift in (32) is given by the ensemble evolution and thus the quantum master equation. In the semiclassical limit, keeping terms up to first order in \hbar , this is just the Fokker–Planck expression (19),

$$[\text{drift}] = [\text{Fokker–Planck}] + \mathcal{O}(\hbar^2) \quad \text{for } \hbar \rightarrow 0. \quad (33)$$

More interesting are the stochastic contributions. To be consistent, we keep terms up to order $\sqrt{\hbar}$ only and find

$$\begin{aligned} [L\text{-diffusion}]_\mu &= \frac{1}{\sqrt{\hbar}} (L_\mu(\mathbf{q}, \mathbf{p}) - \langle L_\mu \rangle) W_\xi(\mathbf{q}, \mathbf{p}) + \frac{i\sqrt{\hbar}}{2} \{L_\mu, W_\xi\} \\ [K\text{-diffusion}]_\nu &= \frac{1}{\hbar} (K_\nu(\mathbf{q}, \mathbf{p}) - \langle K_\nu \rangle) W_\xi(\mathbf{q}, \mathbf{p}) + \frac{i}{2} \{K_\nu, W_\xi\} \end{aligned} \quad (34)$$

where $\{, \}$ denotes the classical Poisson bracket (18). The quantum expectation values $\langle L_\mu \rangle$ and $\langle K_\nu \rangle$ in (34) can be expressed in terms of Wigner–Moyal transforms, e.g.

$$\langle L_\mu \rangle = \int d\mathbf{q} \int d\mathbf{p} L_\mu(\mathbf{q}, \mathbf{p}) W_\xi(\mathbf{q}, \mathbf{p}, t). \quad (35)$$

The semiclassical evolution equation for the Wigner function of a solution of the QSD equation (29) is therefore given by equation (32) with the Fokker–Planck drift term (19) and the diffusion terms (34),

$$\begin{aligned} dW_\xi &= \left[- \sum_i \partial_i [A_i W_\xi] + \frac{1}{2} \sum_\nu \left\{ \sum_{ij} \partial_i \partial_j [(B_\nu B_\nu^T)_{ij} W_\xi] \right\} \right. \\ &\quad \left. + \frac{\hbar}{2} \sum_\mu \left\{ \sum_{ij} \partial_i \partial_j [(C_\mu C_\mu^T)_{ij} W_\xi] \right\} \right] dt \\ &\quad + 2\text{Re} \left(\sum_\mu \left[\frac{1}{\sqrt{\hbar}} (L_\mu(\mathbf{q}, \mathbf{p}) - \langle L_\mu \rangle) W_\xi(\mathbf{q}, \mathbf{p}) + \frac{i\sqrt{\hbar}}{2} \{L_\mu, W_\xi\} \right] d\xi_\mu \right) \\ &\quad + \sum_\nu \frac{1}{\hbar} [(K_\nu(\mathbf{q}, \mathbf{p}) - \langle K_\nu \rangle) W_\xi(\mathbf{q}, \mathbf{p}) 2\text{Re}(d\xi_\nu)] - \{K_\nu, W_\xi\} \text{Im}(d\xi_\nu). \end{aligned} \quad (36)$$

Some algebra shows that since $dN_W = 0$, this semiclassical QSD equation preserves the norm

$$N_W = \int d\mathbf{q} \int d\mathbf{p} W_\xi(\mathbf{q}, \mathbf{p}) = 1. \quad (37)$$

Equation (36) is the semiclassical QSD evolution for the Wigner function and a main result of this paper. While a lot is known about the Fokker–Planck drift term [29, 30], the additional diffusion terms (34) arising from a QSD description are of a new type. They give rise to the classical localization theory introduced in the next section.

Finally, notice also that the semiclassical QSD equation (36) is exact for a quadratic Hamiltonian and linear Lindblad operators.

4. The localization regime

The classical limit of QSD as described by the evolution equation (36) appears to be singular because of the factors \hbar^{-1} in the K -diffusion and $\hbar^{-\frac{1}{2}}$ in the L -diffusion. The ensemble description had a regular classical ($\hbar = 0$) limit. Here, as $\hbar \rightarrow 0$, even the drift term, which includes the Hamiltonian term and is of the order \hbar^0 , becomes negligible by comparison with the dominant \hbar^{-1} K -diffusion. In this limit, the system becomes indistinguishable from a wide open system [19] and the evolution has fluctuations but no drift

$$dW_w = \frac{\sqrt{2}}{\hbar} \sum_\nu (K_\nu - \langle K_\nu \rangle) W_w dw_\nu \quad (38)$$

where we introduced the normalized real Wiener increments $dw_\nu \equiv \sqrt{2}\text{Re } d\xi_\nu$. This is an interesting nonlinear and nonlocal evolution equation for a phase-space density, which is discussed in more detail in the companion paper [1]. It is in itself norm preserving $dN_W = 0$.

In general, the evolution with (38) localizes the Wigner function W_w to a phase-space point (our analysis follows the quantum theory of wide open systems [19]): for a single Lindblad function K , the time evolution of its expectation value is

$$d\langle K \rangle = \frac{\sqrt{2}}{\hbar} (\langle K^2 \rangle - \langle K \rangle^2) dw \quad (39)$$

showing that a stationary solution has minimum uncertainty in the value of K . Thus, W_w becomes localized on a $(2d - 1)$ -dimensional hypersurface $K(\mathbf{q}, \mathbf{p}) = \text{constant}$ in phase space. This reflects the ability of QSD to model a quantum measurement situation.

For many independent Lindblad functions K_ν , the intersection of all localization hypersurfaces $K_\nu(\mathbf{q}, \mathbf{p}) = \text{constant}$ is in general a single phase-space point, the stationary phase-space distribution becomes a delta function. Due to the singular $\sqrt{2}/\hbar$ prefactor, this localization process is faster the more classical (i.e. macroscopic) the system, just as expected. The localization properties of equation (38) are discussed in greater detail in the companion paper [1].

However, caution is required. QSD has an inbuilt mechanism to regularize the semiclassical limit. If the evolution with (38) has localized the Wigner function to a phase space region that compares with the Planck volume \hbar^d , the term $(K_\nu - \langle K_\nu \rangle) W_w$ is itself of the order of \hbar in the relevant phase-space region. The whole expression (38) is now of the order of $\hbar^0 = 1$, implying that the drift and the remaining K -diffusion term is now of the same order and may no longer be neglected.

The strong localization (\hbar^{-1}) arises from K -diffusion and thus from classical fluctuations. If the fluctuations are purely quantal ($K_v \equiv 0$), there is still singular ($\hbar^{-\frac{1}{2}}$) localization arising from L -diffusion. This contribution, however, becomes negligible ($\hbar^{\frac{1}{2}}$) as the extension of the wavepacket approaches the volume of a Planck cell and complete localization might not occur.

We see that the semiclassical phase-space picture of QSD consists of two very different dynamical regimes. As long as the Wigner function is spread over a large phase-space volume, singular (\hbar^{-1}) diffusion according to (38) is the dominant process, producing fast localization of the Wigner function to a phase-space point. For a state of macroscopic extension the localization is instantaneous for all practical purposes. As soon as the spread of the Wigner function approaches the fundamental quantum volume \hbar^d , however, the remaining terms in (36) become comparable, including the drift, regularizing the $\hbar \rightarrow 0$ limit. The dynamics of this resulting wavepacket is treated in the next section. The classical limit of localization by Hermitian operators K_v is treated in detail in the companion paper [1].

5. The wavepacket regime

Once the state vector has localized to near-Planck volume \hbar^d , we enter the wavepacket regime of QSD. Here we demonstrate that the \hbar expansion has a different form in the wavepacket regime. The semiclassical QSD time evolution of the Wigner function must be described by the whole expression (36).

It is appropriate to describe a localized state in terms of its centroid and spread in phase space. Such evolution equations were derived by Salama and Gisin [35] and Halliwell and Zoupas [20]. We introduce the expectation values

$$\mathbf{Q}(t) = \langle \mathbf{q} \rangle = \int d\mathbf{q} \int d\mathbf{p} \mathbf{q} W_\xi(\mathbf{q}, \mathbf{p}, t) \quad \text{and} \quad \mathbf{P}(t) = \langle \mathbf{p} \rangle \quad (40)$$

and the phase-space deviations

$$\Delta_i = q_i - Q_i \quad \text{and} \quad \Delta_{d+i} = p_i - P_i \quad (i = 1, \dots, d) \quad (41)$$

with scaled moments

$$\sigma_{i_1 i_2 \dots i_n} = \hbar^{-\frac{n}{2}} \langle \Delta_{i_1} \Delta_{i_2} \dots \Delta_{i_n} \rangle. \quad (42)$$

In the regime of interest, the scaling ensures that all moments $\sigma_{i_1 i_2 \dots i_n}$ are of the order of $\hbar^0 = 1$.

We can now derive an approximate evolution equation for the centroid ($\mathbf{Q}(t), \mathbf{P}(t)$) and the second-order moments σ_{kl} by consistently expanding in powers of \hbar . With the full semiclassical evolution equation (36) and a lengthy calculation of the lowest orders in \hbar we find

$$\begin{aligned} \begin{pmatrix} d\mathbf{Q} \\ d\mathbf{P} \end{pmatrix} &= \mathbf{A} dt + \sum_v (2\sigma \text{Re}(d\xi_v) + \mathcal{J} \text{Im}(d\xi_v)) [\nabla K_v] \\ &+ 2\sqrt{\hbar} \text{Re} \left(\sum_\mu \left(\left(\sigma - \frac{i}{2} \mathcal{J} \right) [\nabla L_\mu] \right) d\xi_\mu \right) \end{aligned} \quad (43)$$

for the evolution of the centroid and

$$d\sigma = \frac{1}{2\hbar} (\mathcal{M} - 4\sigma \mathcal{J} \mathcal{M} \mathcal{J}^T \sigma) dt + \mathcal{O}(\hbar^0) \quad (44)$$

for the evolution of the moment matrix. We use the same notation as for the classical Langevin equation (27) and in (44) the $(2d \times 2d)$ matrix \mathcal{M} is

$$\mathcal{M} = \mathcal{M}(\mathbf{Q}, \mathbf{P}) = \sum_{\nu} B_{\nu} B_{\nu}^T = \sum_{\nu} \begin{pmatrix} \frac{\partial K_{\nu}}{\partial p_i} \frac{\partial K_{\nu}}{\partial p_j} & -\frac{\partial K_{\nu}}{\partial p_i} \frac{\partial K_{\nu}}{\partial q_j} \\ -\frac{\partial K_{\nu}}{\partial q_i} \frac{\partial K_{\nu}}{\partial p_j} & \frac{\partial K_{\nu}}{\partial q_i} \frac{\partial K_{\nu}}{\partial q_j} \end{pmatrix}. \quad (45)$$

We see from (43) that in QSD, as $\hbar \rightarrow 0$, the drift of the centroid is identical to the drift in the classical equation (27). The fluctuations in (43), however, are made up of two parts. One depends on the imaginary part $\text{Im}(d\xi_{\nu})$ of the QSD fluctuations. This term coincides with the fluctuations of the classical Langevin equation (27) apart from a factor of $\sqrt{2}$, arising from the normalization of the noise: $(\text{Im}(d\xi_{\nu}))^2 = dt/2$. Such a term describes the effect of the Hermitian environmental contributions as originating from a fluctuating Hamiltonian. The second contribution to the classical fluctuations of the centroid in (43), however, depends on σ , the second-order moments of the wavepacket, even as $\hbar \rightarrow 0$. These fluctuations originate from the localization ($\text{Re}(d\xi_{\nu})$) in QSD.

The singular prefactor $(2\hbar)^{-1}$ in (44) makes the dynamics of the moments extremely fast by comparison with the dynamics of the centroid. Consequently the moments $\sigma = \sigma(\mathbf{Q}, \mathbf{P})$ adjust almost instantaneously to the value $\bar{\sigma}(\mathbf{Q}, \mathbf{P})$ determined by putting the time dependence in (44) equal to zero (adiabatic elimination). This gives

$$\bar{\sigma} \mathcal{J} \mathcal{M} \mathcal{J}^T \bar{\sigma} = 4\mathcal{M}. \quad (46)$$

Replacing $\sigma(\mathbf{Q}, \mathbf{P})$ by $\bar{\sigma}(\mathbf{Q}, \mathbf{P})$ in (43), we get a closed evolution equation for the centroid (\mathbf{Q}, \mathbf{P}) of the QSD wavepacket. While it appears impossible to solve for $\bar{\sigma}(\mathbf{Q}, \mathbf{P})$ in (46) in the general case, it is easy to show, using Itô calculus, that the Fokker–Planck equation corresponding to the QSD-Langevin equation (43) with the ‘classical’ moments $\bar{\sigma}(\mathbf{Q}, \mathbf{P})$ determined by (46), coincides with the classical Fokker–Planck equation (19) to leading order in \hbar .

We now see that in the classical limit of the wavepacket regime the centroid of the QSD wavepackets follows a closed evolution equation which is stochastically equivalent to the classical Langevin equation (27), but the way this emerges is very subtle. The fluctuations of the centroid depend on the shape σ of the wavepacket and it is the almost instantaneous adjustment of these moments to their value $\bar{\sigma}$ given by (46) on which this equivalence is based.

6. Summary

We have presented a comprehensive theory of the semiclassical limit of QSD using the Wigner representation in phase space. We find two qualitatively very different dynamical regimes, confirming and extending earlier results on localization in QSD [19].

If the phase-space volume occupied by the quantum state is large compared with the Planck volume \hbar^d , QSD acts in its localization regime. The limit is a classical localization theory represented by a nonlinear, nonlocal, purely diffusive evolution equation for a phase-space density, reflecting the localization property of QSD. Further properties of this regime are presented in the companion paper [1].

Once localization has taken place so that the state vector covers a phase-space volume comparable with \hbar^d , QSD enters its wavepacket regime, when the localization is essentially complete. As $\hbar \rightarrow 0$, the QSD-Langevin equation for the centroid of the wavepacket is stochastically equivalent to the classical Langevin equation. This shows explicitly and generally that QSD results in classical dynamics of wavepackets in the limit as $\hbar \rightarrow 0$.

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