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Path integral, semiclassical and stochastic propagators for Markovian open quantum systems

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Abstract. We develop the path integral theory for master equations of general Lindblad form (positive semigroups), describing Markovian open quantum systems. First the Hamiltonian path integral expression for the propagator is derived, which exhibits nicely the decoherence of pairs of phase space histories. A very appealing picture arises in the semiclassical limit where the degree of decoherence is expressible in terms of a phase space decoherence distance functional. For the important class of (effective) Hamiltonians quadratic in the momenta, we derive the Lagrangian version of the path integral propagator. We then evaluate the path integral approximately in a stationary phase approximation, leading to a Van Vleck-type propagator valid under semiclassical ($\hbar \rightarrow 0$) conditions. We also derive the propagator for the soluble damped harmonic oscillator in closed form from path integrals. Finally, connections to the active field of stochastic pure-state descriptions of open quantum systems are established, here in particular to linear quantum state diffusion.

1. Introduction

The use of path integrals to describe open quantum systems was initiated by Feynman and Vernon [1, 2], more recent developments can be found in Caldeira and Leggett [3], Grabert [4] or Weiss [5]. This approach describes open quantum systems with the help of an explicit model of the environment. The time evolution of the closed total system is governed by ordinary unitary Schrödinger dynamics, tracing over the environmental degrees of freedom leads to an effective propagator for the reduced density operator alone. Path integrals are a convenient tool in this approach, since the trace over the environment can be taken analytically due to the assumed environment of harmonic oscillators and the linear system–environment coupling.

In general, open system dynamics is non-Markovian, since the environment has a certain finite memory time. A Markovian approximation, however, is valid for many interesting systems, particularly in quantum optics. The time evolution of the reduced density operator is then given by an ordinary first-order evolution equation

$$\dot{\rho}_t = \mathcal{L}\rho_t \quad (1)$$

with a linear superoperator \mathcal{L} .

Instead of explicitly describing the environment, the time evolution of Markovian open quantum systems can be determined by an axiomatic approach. It has been shown by

Lindblad [6] that the most general Markovian master equation (1) that governs the time evolution of a density operator (positive semigroup) must be of the following form

$$\dot{\rho}_t = -\frac{i}{\hbar}[\hat{H}, \rho_t] + \frac{1}{2\hbar} \sum_{\mu} ([\hat{L}_{\mu} \rho_t, \hat{L}_{\mu}^{\dagger}] + [\hat{L}_{\mu}, \rho_t \hat{L}_{\mu}^{\dagger}]). \quad (2)$$

Here, \hat{H} is the (Hermitian) Hamiltonian of the system, while the (arbitrary) *environment operators* \hat{L}_{μ} model the effects of the environment on the system. The choice of the environment operators \hat{L}_{μ} replaces the assumptions about the microscopic interaction term of the total Hamiltonian in environment models.

This particular form of the master equation is required in order to preserve normalization and positivity of the density operator ρ . Notice that we introduced an explicit factor \hbar^{-1} in front of the environmental terms for convenience. In many applications, environment operators are annihilation operator-like, in which case this prefactor occurs naturally.

Markovian master equations are widely used in the quantum optics literature [7, 8] and solid states or chemical physics [3, 5]. Owing to various approximations in their derivation from environment models, however, the derived master equations are sometimes *not* of the physically required Lindblad form (2) [9–11]. To avoid these problems, it seems natural to *base* the path integral description of Markovian open quantum systems on the master equation (2) to ensure physically meaningful results.

The aim of this paper, therefore, is complementary to the previous use of path integrals for the description of open quantum systems. We start from the most general sensible master equation and derive the corresponding path integral expressions for the propagator. The benefit of path integral expressions for the solution of master equations is similar to the case for unitary quantum mechanics, where they serve as the starting point for efficient perturbation expansions or semiclassical methods. For relativistic generalizations, path integrals seem indispensable. This paper provides the basis for a path integral treatment of the master equation (2).

In detail, the paper is organized as follows: in section 2 we determine the propagator in the form of a Hamiltonian path integral. The result can be expressed in terms of a Feynman–Vernon-type phase space influence functional under the double path integral. In this form, the decoherent effects of the environmental terms in the Lindblad master equation (2) become very transparent, particularly in the semiclassical ($\hbar \rightarrow 0$) limit, as shown in section 3. The decoherence of pairs of phase space histories $[\alpha]$ can be measured by a *decoherence distance functional* $D[\alpha, \alpha']$.

Since Lagrangian path integrals are more common, we evaluate the momentum part of the phase space path integral for effective Hamiltonians at most quadratic in the momenta, and derive the configuration space path integral propagator in section 4. Again, we express the result in terms of a (configuration space) influence functional and also introduce the corresponding decoherence distance functional $D[\mathbf{q}, \mathbf{q}']$ between paths $[\mathbf{q}]$.

As a first benefit of a path integral expression we determine the propagator in the semiclassical ($\hbar \rightarrow 0$) limit in section 5. This procedure is similar to the derivation of the Van Vleck semiclassical propagator from path integrals in ordinary quantum mechanics [12]. In section 6 we evaluate the path integral in closed form for the soluble model of an harmonic oscillator with linear environment operators.

Recently, stochastic pure-state descriptions of open quantum systems have become an active field of research [13–18]. The master equation (2) for the density operator is replaced by stochastic Schrödinger equations governing the time evolution of individual state vectors. Taking the ensemble mean over these pure-state projectors recovers the results of the master equation. We mention the relevance of these new concepts to this paper in section 7,

particularly pointing out the connection to the stochastic path integral propagator of linear quantum state diffusion [16–18]. We close with a summary and conclusions in the final section 8.

2. Hamiltonian path integral propagator

In this section we derive the general phase space path integral expression for the propagator \mathcal{J} of the Lindblad master equation (2) which we write in the form

$$\dot{\rho} = \frac{i}{\hbar} \left(-\hat{H}_{\text{eff}}\rho + \rho\hat{H}_{\text{eff}}^\dagger - i \sum_{\mu} \hat{L}_{\mu}\rho\hat{L}_{\mu}^\dagger \right). \quad (3)$$

with the effective, non-Hermitian Hamiltonian

$$\hat{H}_{\text{eff}} = \hat{H} - \frac{i}{2} \sum_{\mu} \hat{L}_{\mu}^\dagger \hat{L}_{\mu}. \quad (4)$$

We first propagate a small timestep Δt to get

$$\begin{aligned} \langle \mathbf{q} | \rho(t + \Delta t) | \mathbf{q}' \rangle = & \int d\mathbf{q}_0 \int d\mathbf{q}'_0 \langle \mathbf{q}_0 | \rho(t) | \mathbf{q}'_0 \rangle \left(\langle \mathbf{q} | \mathbf{q}_0 \rangle \langle \mathbf{q}'_0 | \mathbf{q}' \rangle + \frac{\Delta t}{\hbar} \left\{ -i \langle \mathbf{q} | \hat{H}_{\text{eff}} | \mathbf{q}_0 \rangle \langle \mathbf{q}'_0 | \mathbf{q}' \rangle \right. \right. \\ & \left. \left. + i \langle \mathbf{q} | \mathbf{q}_0 \rangle \langle \mathbf{q}'_0 | \hat{H}_{\text{eff}}^\dagger | \mathbf{q}' \rangle + \sum_{\mu} \langle \mathbf{q} | \hat{L}_{\mu} | \mathbf{q}_0 \rangle \langle \mathbf{q}'_0 | \hat{L}_{\mu}^\dagger | \mathbf{q}' \rangle \right\} \right). \end{aligned} \quad (5)$$

Introducing the Wigner transform

$$O(\mathbf{q}, \mathbf{p}) = 2^d (2\pi\hbar)^{(d/2)} \int d\mathbf{q}' \langle \mathbf{q} - \mathbf{q}' | \hat{O} | \mathbf{q} + \mathbf{q}' \rangle \langle \mathbf{q}' | 2\mathbf{p} \rangle \quad (6)$$

of operators \hat{O} , we can replace the matrix elements $\langle \mathbf{q} | \hat{O} | \mathbf{q}' \rangle$ appearing in (5) with the help of the identity

$$\langle \mathbf{q} | \hat{O} | \mathbf{q}' \rangle = (2\pi\hbar)^{-(d/2)} \int d\mathbf{p} O\left(\frac{\mathbf{q} + \mathbf{q}'}{2}, \mathbf{p}\right) \langle \mathbf{q} - \mathbf{q}' | \mathbf{p} \rangle. \quad (7)$$

The plane waves in (6) and (7) are $\langle \mathbf{q} | \mathbf{p} \rangle = (2\pi\hbar)^{-(d/2)} \exp\{i\mathbf{q} \cdot \mathbf{p}/\hbar\}$.

With (7), we find

$$\begin{aligned} \langle \mathbf{q} | \rho(t + \Delta t) | \mathbf{q}' \rangle = & (2\pi\hbar)^{-2d} \int d\mathbf{q}_0 \int d\mathbf{q}'_0 \int d\mathbf{p} \int d\mathbf{p}' \langle \mathbf{q}_0 | \rho(t) | \mathbf{q}'_0 \rangle \\ & \times \exp \frac{i}{\hbar} \left\{ \left(\mathbf{p}(\mathbf{q} - \mathbf{q}_0) - H_{\text{eff}}\left(\frac{\mathbf{q} + \mathbf{q}_0}{2}, \mathbf{p}\right) \right) \Delta t \right. \\ & - \left(\mathbf{p}'(\mathbf{q}' - \mathbf{q}'_0) - H_{\text{eff}}^*\left(\frac{\mathbf{q}' + \mathbf{q}'_0}{2}, \mathbf{p}'\right) \right) \Delta t \\ & \left. - i \sum_{\mu} L_{\mu}\left(\frac{\mathbf{q} + \mathbf{q}_0}{2}, \mathbf{p}\right) L_{\mu}^*\left(\frac{\mathbf{q}' + \mathbf{q}'_0}{2}, \mathbf{p}'\right) \Delta t \right\} \end{aligned} \quad (8)$$

valid up to first order in Δt .

In order to determine $\rho(t)$ from $\rho(t=0)$ for a finite time t , we divide the time interval in N small timesteps $\Delta t = t/N$, and establish iteratively the relation between the final and initial density operator from N short-time propagators (8), to get

$$\langle \mathbf{q} | \rho(t) | \mathbf{q}' \rangle = \int d\mathbf{q}_0 \int d\mathbf{q}'_0 \mathcal{J}(\mathbf{q}, \mathbf{q}', t; \mathbf{q}_0, \mathbf{q}'_0, 0) \langle \mathbf{q}_0 | \rho(t=0) | \mathbf{q}'_0 \rangle \quad (9)$$

with the propagator

$$\begin{aligned} \mathcal{J}(\mathbf{q}, \mathbf{q}', t; \mathbf{q}_0, \mathbf{q}'_0, 0) &= \lim_{N \rightarrow \infty} (2\pi\hbar)^{-2Nd} \int d\mathbf{p}_1 \int d\mathbf{q}_1 \dots \int d\mathbf{q}_{N-1} \int d\mathbf{p}_N \int d\mathbf{p}'_1 \\ &\times \int d\mathbf{q}'_1 \dots \int d\mathbf{q}'_{N-1} \int d\mathbf{p}'_N \exp \frac{i}{\hbar} \sum_{k=1}^N \Delta t \left\{ (\mathbf{p}_k \dot{\mathbf{q}}_k - H_{\text{eff}}(\bar{\mathbf{q}}_k, \mathbf{p}_k)) \right. \\ &\left. - (\mathbf{p}'_k \dot{\mathbf{q}}'_k - H_{\text{eff}}^*(\bar{\mathbf{q}}'_k, \mathbf{p}'_k)) - i \sum_{\mu} L_{\mu}(\bar{\mathbf{q}}_k, \mathbf{p}_k) L_{\mu}^*(\bar{\mathbf{q}}'_k, \mathbf{p}'_k) \right\} \end{aligned} \quad (10)$$

where $\mathbf{q}_N = \mathbf{q}$ and $\mathbf{q}'_N = \mathbf{q}'$. We introduced the midpoints and velocities

$$\bar{\mathbf{q}}_k = \frac{\mathbf{q}_k + \mathbf{q}_{k-1}}{2} \quad \text{and} \quad \dot{\mathbf{q}}_k = \frac{\mathbf{q}_k - \mathbf{q}_{k-1}}{\Delta t} \quad (11)$$

determining how to evaluate the action integral in (10). This midpoint rule is a result of the use of the Wigner transform (6) as phase space functions representing the corresponding operators.

We express our main result (10) more formally as a double path integral over phase space paths $[\alpha] = [\mathbf{q}, \mathbf{p}]$,

$$\mathcal{J}(\mathbf{q}, \mathbf{q}', t; \mathbf{q}_0, \mathbf{q}'_0, 0) = \int_{(q_0,0)}^{(q,t)} \mathcal{D}[\alpha] \int_{(q'_0,0)}^{(q',t)} \mathcal{D}[\alpha'] \exp \left\{ \frac{i}{\hbar} \mathcal{S}[\alpha; \alpha'] \right\} \quad (12)$$

with the generalized double phase space action functional

$$\begin{aligned} \mathcal{S}[\alpha; \alpha'] &= \mathcal{S}[\mathbf{q}, \mathbf{p}; \mathbf{q}', \mathbf{p}'] = \int_0^t d\tau \{ \dot{\mathbf{q}}_{\tau} \mathbf{p}_{\tau} - H_{\text{eff}}(\mathbf{q}_{\tau}, \mathbf{p}_{\tau}) \} - \int_0^t d\tau \{ \dot{\mathbf{q}}'_{\tau} \mathbf{p}'_{\tau} - H_{\text{eff}}^*(\mathbf{q}'_{\tau}, \mathbf{p}'_{\tau}) \} \\ &- i \sum_{\mu} \int_0^t d\tau \{ L_{\mu}(\mathbf{q}_{\tau}, \mathbf{p}_{\tau}) L_{\mu}^*(\mathbf{q}'_{\tau}, \mathbf{p}'_{\tau}) \}. \end{aligned} \quad (13)$$

3. Hamiltonian decoherence distance functional

Expression (12) for the propagator with action functional (13) becomes more transparent if we separate the contributions originating from the true Hamiltonian $H(\mathbf{q}, \mathbf{p})$ from those of the environment functions $L_{\mu}(\mathbf{q}, \mathbf{p})$. We denote the Wigner transform of $\hat{L}_{\mu}^{\dagger} \hat{L}_{\mu}$ by $|\Lambda_{\mu}(\mathbf{q}, \mathbf{p})|^2$ which implies

$$H_{\text{eff}}(\mathbf{q}, \mathbf{p}) = H(\mathbf{q}, \mathbf{p}) - \frac{i}{2} \sum_{\mu} |\Lambda_{\mu}(\mathbf{q}, \mathbf{p})|^2. \quad (14)$$

The propagator is most conveniently written in terms of a *phase space influence functional* $\mathcal{F}[\alpha, \alpha']$ of pairs of phase space histories $[\alpha]$,

$$\mathcal{J}(\mathbf{q}, \mathbf{q}', t; \mathbf{q}_0, \mathbf{q}'_0, 0) = \int_{(q_0,0)}^{(q,t)} \mathcal{D}[\alpha] \int_{(q'_0,0)}^{(q',t)} \mathcal{D}[\alpha'] \exp \left\{ \frac{i}{\hbar} \{ S_{\text{cl}}[\alpha] - S_{\text{cl}}[\alpha'] \} \right\} \mathcal{F}[\alpha, \alpha'] \quad (15)$$

with the classical Hamiltonian action functional of the isolated system given by

$$S_{\text{cl}}[\alpha] = \int_0^t d\tau \{ \dot{\mathbf{q}}_{\tau} \mathbf{p}_{\tau} - H(\mathbf{q}_{\tau}, \mathbf{p}_{\tau}) \}. \quad (16)$$

With (14) we find

$$\mathcal{F}[\alpha, \alpha'] = \exp \left\{ -\frac{1}{2\hbar} \sum_{\mu} \int_0^t d\tau [|\Lambda_{\mu}(\mathbf{q}_{\tau}, \mathbf{p}_{\tau})|^2 + |\Lambda_{\mu}(\mathbf{q}'_{\tau}, \mathbf{p}'_{\tau})|^2 - 2 \operatorname{Re}\{L_{\mu}(\mathbf{q}_{\tau}, \mathbf{p}_{\tau})L_{\mu}^*(\mathbf{q}'_{\tau}, \mathbf{p}'_{\tau})\}] \right\} \exp \left\{ \frac{i}{\hbar} \Phi[\alpha, \alpha'] \right\} \quad (17)$$

with a phase functional

$$\Phi[\alpha, \alpha'] = \sum_{\mu} \int_0^t d\tau \operatorname{Im}\{L_{\mu}(\mathbf{q}_{\tau}, \mathbf{p}_{\tau})L_{\mu}^*(\mathbf{q}'_{\tau}, \mathbf{p}'_{\tau})\}. \quad (18)$$

Expressing the Wigner transform of $\hat{L}_{\mu}^{\dagger}\hat{L}_{\mu}$ (which we denote by $|\Lambda_{\mu}(\mathbf{q}, \mathbf{p})|^2$) in terms of the Wigner transform of \hat{L}_{μ} (which was denoted by $L_{\mu}(\mathbf{q}, \mathbf{p})$), we find a more transparent expression for the influence functional. Including only lowest orders in \hbar we find

$$|\Lambda_{\mu}(\mathbf{q}, \mathbf{p})|^2 = |L_{\mu}(\mathbf{q}, \mathbf{p})|^2 + i\hbar\{L_{\mu}(\mathbf{q}, \mathbf{p}), L_{\mu}^*(\mathbf{q}, \mathbf{p})\} + \mathcal{O}(\hbar^2) \quad (19)$$

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

Thus, neglecting higher-order terms in \hbar , the influence functional (17) takes the appealing form

$$\mathcal{F}[\alpha, \alpha'] = \exp -\frac{1}{2\hbar} \left\{ \sum_{\mu} \int_0^t d\tau |L_{\mu}(\mathbf{q}_{\tau}, \mathbf{p}_{\tau}) - L_{\mu}(\mathbf{q}'_{\tau}, \mathbf{p}'_{\tau})|^2 + \mathcal{O}(\hbar) \right\} \exp \left\{ \frac{i}{\hbar} \Phi[\alpha, \alpha'] \right\}. \quad (20)$$

While the factor involving $\Phi[\alpha, \alpha']$ is an additional phase contributing to the classical actions, the first factor is manifestly responsible for the decoherence among phase space histories. Notice that the neglected $\mathcal{O}(\hbar)$ and higher-order terms in (20) are mere constants for the important classes of linear or quadratic-Hermitian environment operators \hat{L}_{μ} . Therefore, the form (20) for the influence functional holds in these cases exactly.

We introduce a *decoherence distance functional* $D[\alpha, \alpha']$ in the space of phase space histories through

$$D[\alpha, \alpha'] = \left(\sum_{\mu} \int_0^t d\tau |L_{\mu}(\mathbf{q}_{\tau}, \mathbf{p}_{\tau}) - L_{\mu}(\mathbf{q}'_{\tau}, \mathbf{p}'_{\tau})|^2 \right)^{1/2}. \quad (21)$$

In general, in a strict mathematical sense, $D[.,.]$ is a *pseudo-metric* [19] only since the distance (21) between different histories may become zero. In terms of the decoherence distance, the propagator \mathcal{J} for the master equation (2) is given by

$$\mathcal{J}(\mathbf{q}, \mathbf{q}', t; \mathbf{q}_0, \mathbf{q}'_0, 0) = \int_{(\mathbf{q}_0, 0)}^{(\mathbf{q}, t)} \mathcal{D}[\alpha] \int_{(\mathbf{q}'_0, 0)}^{(\mathbf{q}', t)} \mathcal{D}[\alpha'] \exp \left\{ \frac{i}{\hbar} \{S_{\text{cl}}[\alpha] - S_{\text{cl}}[\alpha'] + \Phi[\alpha, \alpha']\} \right\} \times \exp \left\{ -\frac{1}{2\hbar} (D[\alpha, \alpha']^2 + \mathcal{O}(\hbar)) \right\}. \quad (22)$$

This form exhibits nicely the meaning of the environment operators in the master equation. They lead to an additional phase $\Phi[\alpha, \alpha']$ modifying the classical actions, and more importantly, they determine the distance functional (21) in the space of phase space histories. According to expression (22) this distance measures their decoherence.

We have seen how a phase space path integral approach to the master equation (2) leads to a transparent picture of dynamics and decoherence. The use of Lagrangian path integrals is very common, however, which we investigate in the next section.

4. Lagrangian path integral propagator

Here we restrict ourselves to a one degree of freedom system to keep the expressions simple.

In order to determine the Lagrangian version of the propagator, we have to evaluate the momentum path integrals in (12). This is analytically possible for Hamiltonians quadratic in the momenta,

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{q}) \quad (23)$$

and momentum-linear environment operators. For simplicity, we also assume their linear dependence on the position,

$$\hat{L}_\mu = \beta_\mu \hat{q} + \gamma_\mu \hat{p} \quad (24)$$

although this restriction is not necessary. All the results can be expressed in terms of four real parameters $|\beta|^2$, $\bar{\omega}$, Γ , $|\gamma|^2$ defined through

$$|\beta|^2 = \sum_\mu |\beta_\mu|^2 \quad \bar{\omega} - i\Gamma = \sum_\mu \beta_\mu \gamma_\mu^* \quad \text{and} \quad |\gamma|^2 = \sum_\mu |\gamma_\mu|^2. \quad (25)$$

The parameter Γ is the frictional damping rate. A set of linear environment operators like (24) therefore describes *dissipation* for $\Gamma > 0$ only.

The Wigner transform of the effective Hamiltonian (4) with (23) and (24) is

$$H_{\text{eff}}(q, p) = \frac{p^2}{2m} + V(q) - \frac{i}{2} \{ |\gamma|^2 p^2 + 2\bar{\omega} pq + |\beta|^2 q^2 \} + \frac{i\hbar}{2} \Gamma. \quad (26)$$

The Gaussian momentum integrals in (10) can now be evaluated. We find

$$\begin{aligned} \mathcal{J}(q, q', t; q_0, q'_0, 0) &= \lim_{N \rightarrow \infty} \left(\frac{m}{2\pi\hbar\Delta t} \right)^N \int dq_1 \dots \int dq_{N-1} \int dq'_1 \dots \int dq'_{N-1} \\ &\times \exp \frac{i}{\hbar} \sum_{k=1}^N \Delta t \left\{ \left(\frac{m}{2} \dot{q}_k^2 - V(\bar{q}_k) \right) - \left(\frac{m}{2} (\dot{q}'_k)^2 - V(\bar{q}'_k) \right) \right. \\ &\quad \left. + m\Gamma(\dot{q}_k \bar{q}'_k - \bar{q}_k \dot{q}'_k) - \frac{m\Gamma^2}{2} (\bar{q}_k^2 - (\bar{q}'_k)^2) \right\} \\ &\times \exp -\frac{1}{2\hbar} \sum_{k=1}^N \Delta t \{ (|\beta|^2 + m^2 |\gamma|^2 \Gamma^2 - 2m\bar{\omega}\Gamma)(\bar{q}_k - \bar{q}'_k)^2 \\ &\quad + 2m(\bar{\omega} - m|\gamma|^2 \Gamma)(\bar{q}_k - \bar{q}'_k)(\dot{q}_k - \dot{q}'_k) + m^2 |\gamma|^2 (\dot{q}_k - \dot{q}'_k)^2 \} \exp(\Gamma t) \quad (27) \end{aligned}$$

where $q_N = q$, $q'_N = q'$. Again we use the notation (11) for midpoints and velocities.

We write the resulting Lagrangian path integral propagator in a similar form to that of the phase space version (15) by introducing the *Lagrangian influence functional* $\mathcal{F}[q, q']$,

$$\mathcal{J}(q, q', t; q_0, q'_0, 0) = \int_{(q_0, 0)}^{(q, t)} \mathcal{D}[q] \int_{(q'_0, 0)}^{(q', t)} \mathcal{D}[q'] \exp \left\{ \frac{i}{\hbar} (S_{\text{cl}}[q] - S_{\text{cl}}[q']) \right\} \mathcal{F}[q, q']. \quad (28)$$

The classical action of the isolated system is expressed in its Lagrangian version

$$S_{\text{cl}}[q] = \int_0^t d\tau \left\{ \frac{1}{2} m \dot{q}_\tau^2 - V(q_\tau) \right\}. \quad (29)$$

As in the phase space description the Lagrangian influence functional $\mathcal{F}[q, q']$ consists of a phase and a decohering amplitude,

$$\mathcal{F}[q, q'] = \exp(\Gamma t) \exp \left\{ -\frac{1}{2\hbar} D[q, q']^2 \right\} \exp \left\{ \frac{i}{\hbar} \Phi[q, q'] \right\} \quad (30)$$

with the phase given by

$$\Phi[q, q'] = m\Gamma \int_0^t d\tau (\dot{q}_\tau q'_\tau - q_\tau \dot{q}'_\tau) - \frac{1}{2} m\Gamma^2 \int_0^t (q_\tau^2 - q'^2_\tau) \quad (31)$$

and the *Lagrangian decoherence distance* $D[q, q']$ turns out to be

$$D[q, q'] = \left(\sum_\mu \int_0^t |(\beta_\mu - m\Gamma\gamma_\mu)(q_\tau - q'_\tau) + m\gamma_\mu(\dot{q}_\tau - \dot{q}'_\tau)|^2 \right)^{1/2}. \quad (32)$$

The interpretation of the configuration space path integral propagator (28) with influence functional (30) is similar to that of the corresponding phase space expression (22). Again we see how contributions of configuration space paths $[q_\tau]$ with a large distance according to the metric (32) decohere. These Lagrangian results are restricted to Hamiltonians quadratic and environment operators linear in the momenta. The corresponding phase space results are valid in general.

In terms of the parameters (25) we find

$$\begin{aligned} D[q, q']^2 &= (|\beta|^2 + m^2|\gamma|^2\Gamma^2 - 2m\bar{\omega}\Gamma) \int_0^t d\tau (q_\tau - q'_\tau)^2 \\ &\quad + 2m(\bar{\omega} - m|\gamma|^2\Gamma) \int_0^t d\tau (q_\tau - q'_\tau)(\dot{q}_\tau - \dot{q}'_\tau) \\ &\quad + m^2|\gamma|^2 \int_0^t d\tau (\dot{q}_\tau - \dot{q}'_\tau)^2. \end{aligned} \quad (33)$$

A particularly simple form of the influence functional arises from $\bar{\omega} = \Gamma = 0$, resulting for instance from two environment operators

$$\hat{L}_1 = B\hat{q} \quad \text{and} \quad \hat{L}_2 = \frac{C}{m}\hat{p} \quad (34)$$

with some constants B and C . From (30), (31) and (33) we find

$$\mathcal{F}[q, q'] = \exp \left\{ -\frac{1}{2\hbar} \left(|B|^2 \int_0^t d\tau (q_\tau - q'_\tau)^2 + |C|^2 \int_0^t d\tau (\dot{q}_\tau - \dot{q}'_\tau)^2 \right) \right\}. \quad (35)$$

Keep in mind, however, that the case $\Gamma = 0$ does not describe dissipation, the decoherence in this case arises only from fluctuations.

Similar expressions for the influence functional are well known in the context of environment models like those of Feynman and Vernon in a Markovian limit (see for instance [3]).

5. Semiclassical propagator

As in ordinary quantum mechanics, the path integral propagator can be evaluated in the semiclassical ($\hbar \rightarrow 0$) limit with the help of a stationary phase evaluation of the path integral [12].

The stationary paths are determined from the generalized action (13), the variational principle

$$\delta S[q, p; q', p'] = 0 \quad (36)$$

leads to the (complex) equations of motion

$$\begin{aligned}
 \dot{\mathbf{q}} &= \frac{\partial H_{\text{eff}}(\mathbf{q}, \mathbf{p})}{\partial \mathbf{p}} + i \sum_{\mu} \frac{\partial L_{\mu}(\mathbf{q}, \mathbf{p})}{\partial \mathbf{p}} L_{\mu}^*(\mathbf{q}', \mathbf{p}') \\
 \dot{\mathbf{p}} &= -\frac{\partial H_{\text{eff}}(\mathbf{q}, \mathbf{p})}{\partial \mathbf{q}} - i \sum_{\mu} \frac{\partial L_{\mu}(\mathbf{q}, \mathbf{p})}{\partial \mathbf{q}} L_{\mu}^*(\mathbf{q}', \mathbf{p}') \\
 \dot{\mathbf{q}}' &= \frac{\partial H_{\text{eff}}^*(\mathbf{q}', \mathbf{p}')}{\partial \mathbf{p}'} - i \sum_{\mu} L_{\mu}(\mathbf{q}, \mathbf{p}) \frac{\partial L_{\mu}^*(\mathbf{q}', \mathbf{p}')}{\partial \mathbf{p}'} \\
 \dot{\mathbf{p}}' &= -\frac{\partial H_{\text{eff}}^*(\mathbf{q}', \mathbf{p}')}{\partial \mathbf{q}'} + i \sum_{\mu} L_{\mu}(\mathbf{q}, \mathbf{p}) \frac{\partial L_{\mu}^*(\mathbf{q}', \mathbf{p}')}{\partial \mathbf{q}'}
 \end{aligned} \tag{37}$$

which have to be solved with the boundary conditions

$$\mathbf{q}(0) = \mathbf{q}_0 \quad \mathbf{q}'(0) = \mathbf{q}'_0 \quad \mathbf{q}(t) = \mathbf{q} \quad \text{and} \quad \mathbf{q}'(t) = \mathbf{q}'. \tag{38}$$

As for the stationary phase approximation, we can use the semiclassical expression

$$H_{\text{eff}}(\mathbf{q}, \mathbf{p}) \approx H(\mathbf{q}, \mathbf{p}) - \frac{i}{2} \sum_{\mu} |L_{\mu}(\mathbf{q}, \mathbf{p})|^2 \tag{39}$$

for the effective Hamiltonian in (37), according to (14) and (19).

In generalizing the usual semiclassical theory [12], the propagator is given by the expression

$$\begin{aligned}
 \mathcal{J}(\mathbf{q}, \mathbf{q}', t; \mathbf{q}_0, \mathbf{q}'_0, 0) &= (2\pi i\hbar)^{-d} \det \left(\begin{array}{cc} \frac{\partial^2 \mathcal{S}}{\partial \mathbf{q} \partial \mathbf{q}_0} & \frac{\partial^2 \mathcal{S}}{\partial \mathbf{q}' \partial \mathbf{q}_0} \\ \frac{\partial^2 \mathcal{S}}{\partial \mathbf{q} \partial \mathbf{q}'_0} & \frac{\partial^2 \mathcal{S}}{\partial \mathbf{q}' \partial \mathbf{q}'_0} \end{array} \right)^{1/2} \\
 &\times \exp \left\{ \frac{i}{\hbar} \mathcal{S}_{\text{cl}}(\mathbf{q}, \mathbf{q}', t; \mathbf{q}_0, \mathbf{q}'_0, 0) \right\}
 \end{aligned} \tag{40}$$

the generalized action \mathcal{S}_{cl} (13) being evaluated along the solution of the classical equations (37).

Expression (40) together with the equations of motion (37) represents the semiclassical ($\hbar \rightarrow 0$) approximation of the propagator for the Lindblad master equation for general Hamiltonian and environment functions and serves as the starting point for a semiclassical theory of open quantum systems. Similar ideas were developed in [20], starting from the Feynman–Vernon description of the environment.

From a purely classical point of view it is remarkable that *dissipative dynamics* is derived from a variational principle (36). It is clear from (37) that this involves complex equations of motion, giving a ‘quantum foundation’ to attempts at describing classical dissipation from complex Hamiltonian dynamics (see for instance Dekker [21]).

6. Propagator for the harmonic oscillator with linear environment operators

The path integral propagator (12) can be evaluated in closed form for an harmonic oscillator

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2} m \omega^2 \hat{q}^2 \tag{41}$$

with linear environment operators

$$\hat{L}_{\mu} = \beta_{\mu} \hat{q} + \gamma_{\mu} \hat{p} \tag{42}$$

since for at most quadratic dependence of the (effective) Hamiltonian on position and momenta, the path integrals are Gaussian. Under these circumstances the semiclassical propagator (40) is exact and can be evaluated analytically. With the notations (25), equations (37) reduce to the linear equation

$$\begin{pmatrix} \dot{q} \\ \dot{p} \\ \dot{q}' \\ \dot{p}' \end{pmatrix} = \begin{pmatrix} -i\bar{\omega} & (1/m) - i|\gamma|^2 & i\bar{\omega} - \Gamma & i|\gamma|^2 \\ -m\omega^2 + i|\beta|^2 & i\bar{\omega} & -i|\beta|^2 & -i\bar{\omega} - \Gamma \\ -i\bar{\omega} - \Gamma & -i|\gamma|^2 & i\bar{\omega} & (1/m) + i|\gamma|^2 \\ i|\beta|^2 & i\bar{\omega} - \Gamma & -m\omega^2 - i|\beta|^2 & -i\bar{\omega} \end{pmatrix} \begin{pmatrix} q \\ p \\ q' \\ p' \end{pmatrix} \quad (43)$$

which has to be solved with the boundary conditions (38). We find that the action (13) evaluated along the solution of the classical equations (43) is given by

$$\mathcal{S}_{\text{cl}}(q, q', t; q_0, q'_0, 0) = \mathcal{S}_{\text{R}} + i[\mathcal{S}_{\text{I}} - \hbar\Gamma t] \quad (44)$$

where the position independent term $-i\hbar\Gamma t$ arises from the constant term of the effective Hamiltonian (26). The position dependent real and imaginary parts of the action are

$$\mathcal{S}_{\text{R}} = \frac{m\omega}{2\sin\omega t} \{ \cos\omega t [q_0^2 - (q'_0)^2 + q^2 - (q')^2] - 2\cosh\Gamma t [q_0q - q'_0q'] - 2\sinh\Gamma t [q_0q' - q'_0q] \} \quad (45)$$

and

$$\mathcal{S}_{\text{I}} = \frac{m}{8\Gamma(\omega^2 + \Gamma^2)\sin^2\omega t} \{ A(t)(q_0 - q'_0)^2 - 4B(t)(q_0 - q'_0)(q - q') - A(-t)(q - q')^2 \} \quad (46)$$

where the functions $A(t)$ and $B(t)$ are best expressed with the parameters

$$\begin{aligned} a &= \omega^2(m\omega^2|\gamma|^2 + 2m\Gamma^2|\gamma|^2 - 2\bar{\omega}\Gamma + |\beta|^2/m) \\ b &= \Gamma\omega(2\bar{\omega}\Gamma + m\omega^2|\gamma|^2 - |\beta|^2/m) \\ c &= 2\bar{\omega}\omega^2 - m\omega^2\Gamma|\gamma|^2 + \Gamma|\beta|^2/m \\ d &= (\omega^2 + \Gamma^2)(m\omega^2|\gamma|^2 + |\beta|^2/m). \end{aligned} \quad (47)$$

We find

$$\begin{aligned} A(t) &= a e^{2\Gamma t} + b \sin 2\omega t + c \cos 2\omega t - d \\ B(t) &= a \cos \omega t \sinh \Gamma t + b \sin \omega t \cosh \Gamma t. \end{aligned} \quad (48)$$

The final expression for the propagator is therefore

$$\mathcal{J}(q, q', t; q_0, q'_0, 0) = \frac{m\omega}{2\pi\hbar|\sin\omega t|} \exp(\Gamma t) \exp\left(\frac{i\mathcal{S}_{\text{R}}}{\hbar}\right) \exp\left(-\frac{\mathcal{S}_{\text{I}}}{\hbar}\right) \quad (49)$$

with \mathcal{S}_{R} and \mathcal{S}_{I} from (45) and (46). The prefactor has been determined from the second-order derivatives of the action with respect to initial and final positions according to (40).

Notice that of all the parameters only the oscillator frequency ω and damping rate Γ are directly relevant to the time dependence. The dissipationless ($\Gamma = 0$) limit is non-trivial, the relevant dynamical parameters become ω and the combination $[m\omega^2|\gamma|^2 + |\beta|^2/m]$.

Another simple observation is that the first term of the imaginary part (46) of the action together with the prefactor in (49) asymptotically ($\Gamma t \rightarrow \infty$) represents a delta function,

$$\frac{m\omega \exp(\Gamma t)}{2\pi\hbar|\sin\omega t|} \exp\left\{-\frac{mA(t)}{8\hbar\Gamma(\omega^2 + \Gamma^2)\sin^2\omega t} (q_0 - q'_0)^2\right\} \rightarrow \sqrt{\frac{2m\omega^2\Gamma(\omega^2 + \Gamma^2)}{a\pi\hbar}} \delta(q_0 - q'_0) \quad (50)$$

which implies that the asymptotic density matrix is independent of the initial condition. Since $A(t) \approx a \exp(2\Gamma t)$ for $\Gamma t \gg 1$, the delta function is approached exponentially fast.

More interesting conclusions can be drawn from the general expression (49), which simplifies considerably for special cases like the damped free particle ($\omega = 0$), no dissipation ($\Gamma = 0$) etc. We do not want to investigate the damped harmonic oscillator any further, however, and return to the general master equation (2).

7. Stochastic path integral propagators

Recently, much effort has been devoted to *unravel* the master equation (2) with the help of stochastic Schrödinger equations [13–15]. The density operator is regained by the ensemble average $\mathcal{M}[\dots]$ over stochastic pure state projectors,

$$\rho(t) = \mathcal{M}[|\psi_\xi(t)\rangle\langle\psi_\xi(t)|] \quad (51)$$

the subscript ξ for state vectors indicating the dependence on stochastic processes $\xi(t)$. In quantum measurement theories these processes are identified with an actually measured signal. The stochastic states $|\psi_\xi(t)\rangle$ model the random behaviour of individual quantum systems, their time evolution is governed by a stochastic propagator $G_\xi(t; 0)$,

$$|\psi_\xi(t)\rangle = G_\xi(t; 0)|\psi(0)\rangle. \quad (52)$$

With these propagators, property (51) translates into a *stochastic decoupling* of the density operator propagator into the product of stochastic pure state propagators,

$$\mathcal{J}(\mathbf{q}, \mathbf{q}', t; \mathbf{q}_0, \mathbf{q}'_0, 0) = \mathcal{M}[G_\xi(\mathbf{q}, t; \mathbf{q}_0, 0)G_\xi^*(\mathbf{q}', t; \mathbf{q}'_0, 0)]. \quad (53)$$

This form of stochastic decoupling must hold for any linear *unravelling* of density operator dynamics. Path integrals are very convenient tools to find such representations, since path integration and ensemble mean can be interchanged, leading to ordinary stochastic calculus under the path integrals. Even in non-Markovian cases can such a stochastic decoupling of the path integral propagator for the density operator be used to construct stochastic pure state propagators [22, 23].

It is instructive to follow this procedure in the case of the Lindblad master equation (2) with propagator (12). We use independent complex Wiener processes $\xi_\mu(t)$ with properties $\mathcal{M}[\xi_\mu(t)] = 0$ $\mathcal{M}[\xi_\mu(t)\xi_\nu(t')] = 0$ and $\mathcal{M}[\xi_\mu(t)\xi_\nu^*(t')] = \delta_{\mu\nu}\delta(t - t')$. (54)

The decoupling potential of these processes is based on the formula

$$\mathcal{M}\left[\exp\left\{\sum_\mu\int_0^t[d\xi_\mu(\tau)f_\mu(\tau) + d\xi_\mu^*(\tau)g_\mu(\tau)]\right\}\right] = \exp\left\{\sum_\mu\int_0^t d\tau f_\mu(\tau)g_\mu(\tau)\right\} \quad (55)$$

with arbitrary functions $f_\mu(t)$, $g_\mu(t)$ under the Itô-stochastic integrals on the left-hand side. The choice

$$f_\mu(t) = L_\mu(\mathbf{q}_t, \mathbf{p}_t) \quad \text{and} \quad g_\mu(t) = L_\mu^*(\mathbf{q}'_t, \mathbf{p}'_t) \quad (56)$$

leads to a decoupling of the propagator (12) of the Lindblad master equation with the stochastic phase space path integral propagator

$$G_\xi(\mathbf{q}, t; \mathbf{q}_0, 0) = \int_{(\mathbf{q}_0, 0)}^{(\mathbf{q}, t)} \mathcal{D}[\boldsymbol{\alpha}] \exp\frac{i}{\hbar} S_\xi[\boldsymbol{\alpha}]. \quad (57)$$

The complex Itô-stochastic phase space action integral is given by

$$S_\xi[\boldsymbol{\alpha}] = \int_0^t d\tau [\dot{\mathbf{q}}_\tau \mathbf{p}_\tau - H_{\text{eff}}(\mathbf{q}_\tau, \mathbf{p}_\tau)] - i \sum_\mu \int_0^t d\xi_\mu(\tau) L_\mu(\mathbf{q}_\tau, \mathbf{p}_\tau). \quad (58)$$

This is the propagator of the *linear quantum state diffusion* (LQSD) Itô-stochastic Schrödinger equation

$$|d\psi\rangle = -\frac{i}{\hbar}\hat{H}|\psi\rangle dt - \frac{1}{2}\sum_{\mu}\hat{L}_{\mu}^{\dagger}\hat{L}_{\mu}|\psi\rangle dt + \sum_{\mu}\hat{L}_{\mu}|\psi\rangle d\xi_{\mu} \quad (59)$$

which is easily shown directly to lead to the Lindblad master equation (2) in the mean. The stochastic LQSD propagator (57) was investigated in detail in [18], see also [16] and related investigations in [17].

For completeness only we mention that for numerical purposes the nonlinear *quantum state diffusion* (QSD) equation [13–15]

$$|d\psi\rangle = -\frac{i}{\hbar}\hat{H}|\psi\rangle dt - \frac{1}{2}\sum_{\mu}(\hat{L}_{\mu}^{\dagger}\hat{L}_{\mu} - 2l_{\mu}^{*}\hat{L}_{\mu} + |l_{\mu}|^2)|\psi\rangle dt + \sum_{\mu}(\hat{L}_{\mu} - l_{\mu})|\psi\rangle d\xi_{\mu} \quad (60)$$

is superior to LQSD (59) since individual realizations are normalized, while still recovering the results of the master equation (2) in the mean. QSD differs from LQSD through additional terms involving the expectation values $l_{\mu} = \langle\psi|L_{\mu}|\psi\rangle$, leading to a nonlinear stochastic Schrödinger equation.

8. Summary and conclusions

In this paper we have derived the general path integral expressions for the propagator of the most sensible Markovian master equation (2). The Hamiltonian version is valid in general, whereas for the Lagrangian version we have to restrict ourselves to standard Hamiltonian and momentum-linear environment operators.

We express both versions in terms of influence functionals, whose amplitude we were able to express with the help of decoherence distance functionals. These expressions demonstrate quantitatively how the environment operators in the master equation suppress the coherence of contributing pairs of paths under the double path integrals.

In semiclassical conditions, the propagator can be evaluated in a stationary phase approximation. We derive the relevant (complex) classical equations of motion and the final expression for the semiclassical propagator. We believe that this approach offers a useful numerical tool to solve the master equation for near-classical situations directly, a method which is complementary to Monte Carlo simulation techniques involving classical Langevin equations.

Because the semiclassical propagator is exact for at most quadratic (effective) Hamiltonians, we can use our result to determine the propagator analytically for the harmonic oscillator with general linear environment operators from path integrals.

Finally, we establish the connection to stochastic pure-state descriptions of open quantum systems, which becomes particularly transparent when using path integrals. These results have only recently been generalized to non-Markovian situations, which leaves room for further investigations.

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