Stochastic pure states for quantum Brownian motion

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Abstract. We give a new description of quantum Brownian motion in terms of stochastic pure states. The corresponding path integral propagator allows us to establish a direct connection to the classical Langevin equation, in the Schrödinger picture. We show that in the quantum domain, one is naturally led to consider two stochastic processes driving the Brownian dynamics, one of them representing thermal fluctuations, as in the classical case. The second process reflects growing entanglement between the Brownian particle and its environment, and is therefore a truly quantum noise process. Technically, our result rests on the representation of the full propagator of the Brownian particle and its environment in a coherent state basis. For open system dynamics that may be described by a master equation, such stochastic schemes have already been proven to be efficient Monte Carlo methods. Here, we give a new stochastic scheme that covers low temperatures and strong friction, the latter limit being the case Einstein originally investigated.
1. Einstein’s and Langevin’s description of Brownian motion

In his seminal work on Brownian motion [1], Einstein derived the diffusion coefficient $D$ of a Brownian particle of radius $a$ in a fluid with coefficient of viscosity $\eta$,

$$D = \frac{k_B T}{6\pi \eta a}, \quad (1)$$

where $T$ is the temperature and $k_B$ Boltzmann’s constant. Crucially, Einstein’s relation (1) allowed Perrin [2] to measure $k_B$ and therefore Avogadro’s number $N$. These investigations showed the applicability of the principles of statistical mechanics to the phenomenon of Brownian motion and were thus a crucial contribution to confirm the reality of atoms and molecules, as suggested by a statistical treatment. Einstein based his analysis on the particle density and its diffusive dynamics, combining dynamical concepts with results from equilibrium statistical physics.

Later, Langevin, in his own words [3], provided an ‘infinitely more simple’ derivation of the same result (1). His approach was truly dynamical. Langevin based his analysis on the equation of motion of an individual Brownian particle,

$$M\ddot{q}(t) + M\gamma \dot{q}(t) = X(t), \quad (2)$$

including the random force $X(t)$ exerted on the particle by the fluid, where $\gamma = 6\pi \eta a/M$ is the friction rate according to Stokes’ law. Such a Langevin equation (2) is the archetype of a stochastic differential equation and their applications in statistical physics have since been enormously fruitful, not least with an eye on computer simulations.

In the quantum domain, things are different and significantly more difficult. Clearly, one may derive the Heisenberg equations of motion for a quantum Brownian particle in analogy to the classical case (2). The corresponding stochastic Langevin force $X(t)$ becomes an operator force, highlighting the fact that it is the position and momenta of the environmental degrees of freedom that constitute the ‘random force’ acting upon the Brownian particle. Thus, the Heisenberg equation of motion of a Brownian particle is, in fact, an equation of motion in the full Hilbert space of the particle and its environment. Unless the forces are linear, these equations...
are impossible to solve. Moreover, as the Hilbert space dimension is huge, any attempt to solve these equations of motion on a computer must fail.

To overcome the problem with quantum operator-Langevin equations of motions, one therefore, very often, stays in the Schrödinger picture, and tries to evaluate the dynamics of the reduced density operator of the Brownian particle. While a formal evolution equation may be derived [4, 5], in practice its solution amounts to being able to solve the full problem which is almost always an impossible aim to achieve. However, starting with this general framework, weak coupling expansions are possible and indeed lead to effective evolution (‘master’) equations for the reduced density operator, see [6, 7]. Beyond weak coupling, a path integral description has proven most useful [8]–[12], as it allows one to investigate the dynamics under very general conditions. In order to arrive at these results, one determines the full propagator for the Brownian particle and its environment and then traces (averages) over the environmental degrees of freedom.

A description of the dynamics of a quantum Brownian particle in terms of the reduced density operator may be seen as a description in the spirit of Einstein’s seminal paper [1]. The density operator describes a mixed ensemble of states; it corresponds to Einstein’s particle density. Langevin’s dynamical description, however, explicitly takes into account the fluctuations. In his formulation, the fluctuating force \( X(t) \) depends on the environmental degrees of freedom, interacting with the Brownian particle. While in a density description, these degrees of freedom are integrated out, in the Langevin approach the environmental degrees of freedom remain an explicit part of the description through \( X(t) \). The stochasticity emerges from the uncertainty of the initial conditions of the environmental positions and momenta. As we will stress later on, in the quantum case, there is an additional, truly quantum origin of noise: entanglement between the Brownian particle and its environment.

We aim to develop a dynamical description of quantum Brownian motion in the spirit of Langevin, in the Schrödinger picture. Just as in the classical case, where the density may be obtained by simulating stochastic trajectories and averaging, we will develop a quantum theory for the stochastic pure states of a Brownian particle, such that upon taking the ensemble mean over all pure states, one recovers the reduced density operator. We said earlier that such a description will necessarily have to contain explicitly the environmental degrees of freedom. In the Heisenberg equation of motion approach, this implies that the stochastic force is an operator force. In our approach, however, we will be able, in a certain sense, to replace the operator force by a \( c \)-number stochastic force. Thus, the stochastic pure states we will determine are indeed pure states in the Hilbert space of the Brownian particle only. The influence of the quantum environment may entirely be described in terms of classical stochastic processes, also including the ‘quantum noise’. The key to such a result are coherent states. As will become clear soon, expressing the environmental degrees of freedom in a coherent state basis allows us to determine the exact stochastic pure states in analogy to the dynamics of an individual Brownian particle as in Langevin’s approach (2).

We would like to extend Langevin’s claim that a description in terms of stochastic pure states is ‘infinitely more simple’ to the quantum domain. At this stage, however, it is too early to make such a blunt statement. It is true that, through a stochastic description, a significant reduction of the dimension of the problem may arise, which was one of the original motivations to establish stochastic pure state methods [13]. The question of the general applicability of stochastic propagators of the type to be derived in this paper, however, is still open. We will further explore these issues in the near future.
This paper is organized as follows: in the next section, we present the standard model of a Brownian particle interacting with a ‘bath’ of harmonic oscillators. For completeness, we repeat the classical considerations and turn our attention to the quantum case. Next, we introduce conditioned propagators that will determine our stochastic pure states. We are able to make the connection to the classical Langevin description, here in the Schrödinger picture. Finally, we show the equivalence of our approach to the usual Feynman–Vernon theory, once we integrate over the fluctuating forces.

It should be noted that in the past years there have been many attempts to unravel the dynamics of a reduced density operator in terms of stochastic pure states, with the aim to find efficient Monte Carlo methods for the description of open quantum system dynamics. First and foremost, such stochastic pure-state descriptions have been formulated for dissipative quantum dynamics of the Lindblad class [14]. In particular in quantum optics, where a Lindblad description is valid, such stochastic Schrödinger equations were investigated in the context of continuous measurement theories [15]–[17]. It is only more recently that similar ideas have been extended to more general open system dynamics [18]–[28]. The theory we develop here has the nice feature of offering a clear physical interpretation of both the states and the stochastic processes. In fact, we will be able to establish the connection to the classical Langevin approach, starting from quantum dynamics in the useful Schrödinger picture.

2. Quantum Brownian motion model

A fundamental description of the dynamics of a quantum Brownian particle rests on a description in terms of a total Hamiltonian including both, the degrees of freedom of the Brownian particle and of the environment. The quantum dynamics of the Brownian particle is then determined as subdynamics of the unitary evolution of the total system including the environment [4]–[12]. Together, the Brownian particle and the environment constitute a closed system to which Schrödinger’s equation applies. The total Hamiltonian for system and environment may be written in the form

$$H_{\text{tot}} = H(q, p) + H_{\text{int}}(q, \{Q_\lambda, P_\lambda\}) + H_{\text{bath}}(\{Q_\lambda, P_\lambda\}),$$

where $H$ is a (renormalized) Hamiltonian of the Brownian particle, $H_{\text{bath}}$ is the Hamiltonian of the environment or ‘heat bath’, and $H_{\text{int}}$ describes the interaction between particle and environment. The environment, in order to deserve its name, consists of (infinitely) many degrees of freedom.

Classical Brownian motion as described by the Langevin equation (2) may be obtained in the appropriate limit from the Hamiltonian

$$H_{\text{tot}} = \frac{p^2}{2M} + V(q, t) + \sum_\lambda \left[ \frac{p^2_\lambda}{2m_\lambda} + \frac{1}{2}m_\lambda \omega_\lambda^2 \left( Q_\lambda - \frac{g_\lambda}{m_\lambda \omega_\lambda^2} q \right)^2 \right].$$

Here $q$ and $p$ are position and momentum of the Brownian particle, coupled to an environment of harmonic oscillators (degrees of freedom $(Q_\lambda, P_\lambda)$) through its position $q$. Note that, we include the usual potential renormalization such that $V(q, t)$ turns out to be the bare potential felt by the Brownian particle. Sometimes, we work temporarily with the ‘system’ Hamiltonian $H(q, p) = \frac{p^2}{2M} + V_*(q)$ in the form (3), which then includes the ‘counterterm’ arising from the system–environment coupling,

$$V_*(q) = V(q, t) + \sum_\lambda \frac{g_\lambda^2}{2m_\lambda \omega_\lambda^2} q^2.$$
Solving Hamilton’s equations of motion for (4), we find that the evolution of the open system is determined by the equation

\[ M \ddot{q}(t) + M \int_0^t ds \Gamma(t - s) \dot{q}(s) + V'(q(t), t) = X(t) \] (6)

with the classical damping kernel

\[ \Gamma(t - s) = \frac{1}{M} \sum_{\lambda} \frac{g_\lambda^2}{m_\lambda \omega_\lambda^2} \cos \omega_\lambda (t - s). \] (7)

The ‘stochastic force’ \( X(t) \) on the right-hand side of equation (6) is given by the expression

\[ X(t) = \sum_{\lambda} g_\lambda \left[ Q_\lambda(0) \cos \omega_\lambda t + \frac{P_\lambda(0)}{m_\lambda \omega_\lambda} \sin \omega_\lambda t \right]. \] (8)

where, we assumed that enough time has elapsed such that we may neglect an initial slip term \( M \Gamma(t) q_0 \) (see the discussion in [29]).

2.1. Initial state and correlation functions

The stochasticity of \( X(t) \) arises from the distribution of environmental initial conditions \((Q_\lambda(0), P_\lambda(0))\). For a thermal distribution \( \sim \exp(-H_{\text{bath}}/k_B T) \), \( X(t) \) is just a Gaussian fluctuating force with zero mean and correlations

\[ \langle \langle X(t)X(s) \rangle \rangle_{\text{classical}} = Mk_B T \Gamma(t - s), \] (9)

where \( \Gamma(t - s) \) is again the classical damping kernel (7). Clearly, standard Brownian motion (2) is obtained from (6) for zero external potential and an environment that may be described by delta-correlated noise \( \Gamma(t - s) = 2\gamma \delta(t - s) \). In this limit, Einstein’s result for the diffusion of a Brownian particle emerges for strong friction, when we can neglect inertia and find the usual \( q(t) - q(0) = \frac{1}{M \gamma} \int_0^t ds X(s) \). For the mean displacement we find \( \langle \langle (q(t) - q(0))^2 \rangle \rangle_{\text{classical}} = 2D t \) with \( D = k_B T/\gamma M \), confirming Einstein’s expression (1).

Having a closed system–environment model (4) at hand, quantization is straightforward [8]–[12]. In the next section, we will determine the relevant propagators for the Hamiltonian (4) in the Schrödinger picture, exploiting the fact that the propagator for the environmental harmonic degrees of freedom can be evaluated in closed form.

The correlation function (9) was obtained from the assumption of a thermal equilibrium state for the (uncoupled) environmental degrees of freedom. Such a choice may be questioned under conditions at very low temperatures and strong coupling, see for instance [29, 30]. In our attempt to formulate a Schrödinger picture analogue of a stochastic description of Brownian motion, however, we will restrict ourselves to the simple uncorrelated form \( \rho_{\text{tot}}(0) = \rho_0 \otimes \rho_{\text{bath}} \) for the total initial state. In fact, without any loss of generality we may assume an initial pure state for the Brownian particle, \( \rho_0 = |\psi_0 \rangle \langle \psi_0| \) since the general \( \rho_0 \) will always be a linear mixture of pure states. For the bath, in analogy to the classical case that led to (9), we chose the thermal equilibrium state such that

\[ \rho_{\text{tot}}(0) = |\psi_0 \rangle \langle \psi_0| \otimes e^{-H_{\text{bath}}/k_B T} / Z, \] (10)

where \( Z = \text{tr}[e^{-H_{\text{bath}}/k_B T}] \).
For completeness, we mention that the fundamental model (4), allows us to obtain Heisenberg’s equations of motion for the operator \( q(t) \) in the very same fashion as for the classical case (6), for further elaboration see for instance [12]. The ‘random force’ \( X(t) \) turns into an operator force \( \hat{X}(t) \) with zero mean and the quantum bath correlation function

\[
\alpha(t-s) \equiv \langle \langle \hat{X}(t) \hat{X}(s) \rangle \rangle_{\text{quantum}} = \sum_\lambda \frac{\hbar g^2_\lambda}{2m_\lambda \omega_\lambda} \left[ \coth \left( \frac{\hbar \omega_\lambda}{2k_B T} \right) \cos \omega_\lambda (t-s) - i \sin \omega_\lambda (t-s) \right]
\]  

(11)

at temperature \( T \).

In the following, it turns out meaningful to separate the zero temperature part from \( \alpha(t-s) \). We write

\[
\coth \left( \frac{\hbar \omega_\lambda}{2k_B T} \right) = \frac{2}{\bar{n}_\lambda} + 1 \quad \text{with the thermal occupation number}
\]

\[
\bar{n}_\lambda = \left( e^{\frac{\hbar \omega_\lambda}{k_B T}} - 1 \right)^{-1}
\]

(12)

Accordingly, we may write

\[
\alpha(t-s) = \alpha_\bar{n}(t-s) + \alpha_0(t-s),
\]

(13)

with \( \alpha_\bar{n}(t-s) \equiv 0 \) if all \( \bar{n}_\lambda = 0 \), i.e. at zero temperature. From (11), we see that the zero-temperature contribution to the bath correlation function reads

\[
\alpha_0(t-s) = \sum_\lambda \frac{\hbar g^2_\lambda}{2m_\lambda \omega_\lambda} e^{-i \omega_\lambda (t-s)}.
\]

(14)

In the high-temperature limit, when \( \coth(\hbar \omega_\lambda/2k_B T) \approx 2\bar{n}_\lambda \approx 2k_B T/\hbar \omega_\lambda \), the real part of the quantum correlation function agrees with the classical expression (9),

\[
\alpha_R(t-s) \equiv \text{Re} \alpha(t-s) \approx \alpha_\bar{n}(t-s) \approx M k_B T \Gamma(t-s).
\]

(15)

Irrespective of temperature, the imaginary part of the quantum correlation function is connected to the classical damping kernel (7) through

\[
\alpha_I(t-s) \equiv \text{Im} \alpha(t-s) = \text{Im} \alpha_0(t-s) = -\frac{\hbar M}{2} \frac{\partial}{\partial s} \Gamma(t-s).
\]

(16)

2.2. Coherent states

In the following sections, we are going to exploit the linear nature of the environmental degrees of freedom by working with the overcomplete basis of coherent states [31, 32]. We introduce creation and annihilation operators in the usual way through

\[
ad_\lambda = \left( \frac{\sqrt{m_\lambda \omega_\lambda}}{\hbar} Q_\lambda + i \frac{1}{\sqrt{2 m_\lambda \omega_\lambda}} P_\lambda \right)
\]

such that \([a_\lambda, a^\dagger_\lambda] = \delta_\lambda \lambda’\) and \( H_{\text{bath}} = \sum_\lambda \hbar \omega_\lambda (a^\dagger_\lambda a_\lambda + \frac{1}{2}) \). A coherent state \( |\xi_\lambda\rangle \) of mode \( \lambda \) is an eigenstate of the annihilation operator \( a_\lambda \), and may be given explicitly through

\[
|\xi_\lambda\rangle = e^{-\frac{1}{2} |\xi_\lambda|^2} e^{\xi_\lambda a^\dagger_\lambda} |0_\lambda\rangle.
\]

(17)

Crucially, these states form an overcomplete set, \( \mathbb{I} = \int \frac{d^2 \xi}{\pi} |\xi\rangle \langle \xi| \) with \( d^2 \xi = d(\text{Re} \xi) d(\text{Im} \xi) \) and \( \langle \xi | \xi’\rangle = e^{-\frac{1}{2} (|\xi|^2 + |\xi’|^2)} e^{\xi^* \xi’} \).
The thermal initial state of the bath of harmonic oscillators as assumed in (10) may be expressed as a Gaussian mixture of coherent states [32] according to

\[
\frac{1}{\text{tr}[e^{-\frac{H_{\text{bath}}}{\hbar}T}]} e^{-\frac{H_{\text{bath}}}{\hbar}T} = \int \frac{d^2\xi}{\pi} \frac{e^{-|\xi|^2/\bar{n}}}{\bar{n}} |\xi\rangle \langle \xi|.
\]  

(18)

Here we use the symbolic notation \(d^2\xi = d^2\xi_1 d^2\xi_2 \cdots\), and \(\frac{1}{\bar{n}} e^{-|\xi|^2/\bar{n}} = \Pi_\lambda \frac{1}{\bar{n}_\lambda} e^{-|\xi_\lambda|^2/\bar{n}_\lambda}\), where \(\bar{n}_\lambda\) is the thermal occupation number (12) of mode \(\lambda\). Furthermore, we write

\[
|\xi\rangle = |\xi_1\rangle |\xi_2\rangle \cdots |\xi_\lambda\rangle \cdots
\]

(19)

for a product of environmental coherent states.

### 3. Reduced dynamics and stochastic pure states

We are going to determine the time evolution of a system and environment given the total Hamiltonian (4) for the Brownian particle and its environment with initial state (10). It turns out that matters clarify once we change to an interaction representation with respect to the free bath Hamiltonian, such that the propagator of interest is

\[
U(t) = e^{\frac{i}{\hbar} H_{\text{bath}} t} e^{-\frac{i}{\hbar} (H + H_{\text{int}} + H_{\text{bath}}) t}.
\]

(20)

Crucially, the reduced density operator of the Brownian particle is unaffected by this transformation. The corresponding von-Neumann equation is the usual \(\dot{\rho}_{\text{tot}}(t) = \frac{1}{i\hbar} [H_{\text{tot}}(t), \rho_{\text{tot}}(t)]\) with a time-dependent total Hamiltonian

\[
H_{\text{tot}}(t) = H + e^{iH_{\text{bath}}t/\hbar} H_{\text{int}} e^{-iH_{\text{bath}}t/\hbar}.
\]

(21)

We may express the solution in the form \(\rho_{\text{tot}}(t) = U(t)\rho_{\text{tot}}(0) U^\dagger(t)\). In order to get an appealing expression for the reduced density operator, we take the trace over the environmental degrees of freedom in a coherent state basis, i.e. \(\text{tr}_{\text{bath}}[\cdots] = \int \frac{d^2z}{\pi} (z|\cdots|z)\), where a state \(|z\rangle\) is a product, according to the notation introduced in (19). Finally, we express the thermal initial state for the environment as the mixture of coherent states (18), and find for the reduced density operator

\[
\rho(t) \equiv \text{tr}_{\text{bath}}[\rho_{\text{tot}}(t)]
\]

\[
\begin{align*}
&= \int \frac{d^2z}{\pi} \int \frac{d^2\xi}{\pi} \frac{e^{-|\xi|^2/\bar{n}}}{\bar{n}} (z|U(t)|\xi\rangle \langle \psi_0|\langle \xi|U^\dagger(t)|z\rangle \\
&= \int \frac{d^2z}{\pi} e^{-|z|^2} \int \frac{d^2\xi}{\pi} e^{-|\xi|^2} G_{QBM}(t)|\psi_0\rangle \langle \psi_0|G_{QBM}^\dagger(t).
\end{align*}
\]

(22)

Here, we introduced the quantum Brownian motion propagator

\[
G_{QBM}(t) = \frac{\langle z + \sqrt{\bar{n}}\xi|U(t)|\sqrt{\bar{n}}\xi\rangle}{\langle z + \sqrt{\bar{n}}\xi|\sqrt{\bar{n}}\xi\rangle}
\]

(23)
in the Hilbert space of the Brownian particle, which may be interpreted as a conditional propagator, given the environmental initial and final coherent states involved; it clearly depends on all coherent state labels $z = (z_1, z_2, \ldots, z_\lambda, \ldots)$, and $\xi$ accordingly. We point out that the symbolic notation $z + \sqrt{n}\xi$ should be seen as being meant for each environmental oscillator with index $\lambda$. Note also that the definition is such that at $t = 0$ the quantum Brownian motion propagator is unity, irrespective of the values of $z$ and $\xi$, 

$$G_{QBM}(0) = \mathbb{1}.$$  

(24)

In the next two sections, we are going to determine the path integral expression of $G_{QBM}(t)$ to further clarify its meaning.

Here, we first show that the propagator $G_{QBM}(t)$ serves to define a stochastic pure-state description of quantum Brownian motion similar to Langevin’s description (6) in the classical case. It is clear from (22) that it is meaningful to determine time-dependent pure states of the Brownian particle through

$$|\psi(z, \xi, t)\rangle = G_{QBM}(t)|\psi_0\rangle,$$  

(25)

where our notation emphasizes that the states depend on the particular choice of environmental states $|z\rangle$ and $|\xi\rangle$ in (23); they are conditioned on these particular environmental states. The appearance of the labels $\xi$, representing the initial environmental coherent state is very similar to the appearance of the initial conditions $Q_\lambda(0)$ and $P_\lambda(0)$ in the stochastic force $X(t)$ (8) of the classical Langevin equation. Due to entanglement, however, not only is the initial state of the environment a stochastic variable (represented by $\xi$), but also the final state: in general, the final state will be a superposition involving many different possible environmental coherent states $|z\rangle$.

This is why the propagator is also conditioned on the final coherent state, represented by the labels $z$.

With definition (25), the reduced density operator is naturally expressed as a mixture of pure states at all times. According to (22) and using the definition (25) we may write

$$\rho(t) = \int \frac{d^2z}{\pi} e^{-|z|^2} \int \frac{d^2\xi}{\pi} e^{-|\xi|^2} \langle|\psi(z, \xi, t)\rangle \langle\psi(z, \xi, t)|\rangle$$

$$\langle\langle|\psi(z, \xi, t)\rangle \langle\psi(z, \xi, t)|\rangle\rangle_{z, \xi},$$  

(26)

where the last equality serves to define the classical ensemble average $\langle\langle | \rangle \rangle_{z, \xi}$ over the coherent states labels with the standard Gaussian distribution $e^{-(|z|^2+|\xi|^2)}$. We will later see that this average amounts to regarding certain time-dependent functions as classical stochastic processes. While the term involving $\xi$ is very closely related to Langevin’s random force $X(t)$ in (2) and (6), the noise arising from the dependence on $z$ should be seen as quantum noise, reflecting the growing entanglement between the Brownian particle and its environment. Before being able to further elaborate this connection, however, we need to determine the path integral expression of the propagator (23).

4. Coherent state propagator for quantum Brownian motion

In the usual path integral treatment of the Brownian motion model (4), one evaluates its propagator $U(t)$ in position representation and traces over the environmental degrees of freedom in order
to get a closed expression for the propagator of the reduced density operator \([8, 11, 12]\). Path integrals are widely used as they may also be applied for strong coupling or at low temperatures, when the Markov approximation and master equation approaches usually break down. With appropriate techniques and computer power, one may even try to evaluate the path integral propagator for the reduced density operator numerically [33]. Here, we want to determine the mixed position–coherent state representation of the full propagator

\[
\langle q|G(z, \xi, t)|q_0\rangle \equiv \langle q|\langle z|U(t)|\xi\rangle|q_0\rangle,
\]

(27)

where \(|q\rangle, |q_0\rangle\) are position eigenstates in the Hilbert space of the Brownian particle and \(|z\rangle, |\xi\rangle\) coherent states in the Hilbert space of the environment according to (19). We divide by the overlap \(\langle z|\xi\rangle\) in (27) to ensure that initially \(G(z, \xi, 0) = 1\) as before in (24). Note however, that our definition of \(G(z, \xi, t)\) is such that the previous Brownian motion propagator of (23) is

\[
G_{\text{QBM}}(t) = G(z + \sqrt{n}\xi, \sqrt{n}\xi, t)
\]

(28)

as is apparent from their respective definitions (23) and (27).

The determination of the path integral expression of the propagator \(G(z, \xi, t)\) is tedious but straightforward. We use standard results for the propagator of harmonic oscillators,

\[
\langle Q|e^{\frac{i}{\hbar}H_{\text{bath}}t}|Q_0\rangle = \prod_\lambda \left(\frac{m_\lambda\omega_\lambda}{-2\pi i\hbar \sin \omega_\lambda t}\right)^\frac{1}{2} \times \exp \left\{ -i \sum_\lambda \frac{m_\lambda\omega_\lambda}{2\hbar \sin \omega_\lambda t} ((Q^2_\lambda + Q^2_0) \cos \omega_\lambda t - 2Q_\lambda Q_0) \right\},
\]

(29)

and also for the path integral propagator of the total system [34]–[36],

\[
\langle q, Q|e^{\frac{-i}{\hbar}H_{\text{total}}t}|q_0, Q_0\rangle = \int D[q] \exp \left\{ \frac{i}{\hbar} S_+[q] - \frac{i}{\hbar} \sum_\lambda \frac{g_\lambda}{\sin \omega_\lambda t} \times \left[ Q_\lambda \int_0^t d\tau q(\tau) \sin \omega_\lambda \tau + Q_{\lambda,0} \int_0^t d\tau q(\tau) \sin \omega_\lambda (t - \tau) + \frac{g_\lambda}{m_\lambda\omega_\lambda} \int_0^t d\tau \int_0^\tau d\sigma q(\tau)q(\sigma) \times \sin \omega_\lambda (t - \tau) \sin \omega_\lambda \sigma \right] \right\} \times \langle Q|e^{\frac{-i}{\hbar}H_{\text{bath}}t}|Q_0\rangle.
\]

(30)

In (29) and (30) \(Q = (Q_1, Q_2, \ldots, Q_\lambda, \ldots)\) denotes the environmental positions and

\[
S_+[q] = \int_0^t d\tau \left\{ \frac{1}{2} Mq^2(\tau) - V_+[q(\tau)] \right\}
\]

(31)

is the classical action along a path \(q(\tau)\) of the isolated system (including the counterterm according to (5)). As usual, the path integral \(\int D[q]\) has to be extended over all paths \(q(\tau)\) of the system with \(q(0) = q_0, q(t) = q\).

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The path integral representation of the propagator \( U(t) \) in interaction representation with respect to the bath is now easily evaluated. From (20), using expressions (29) and (30), we find

\[
\langle q, Q | U(t) | q_0, Q_0 \rangle = \int D[q] \exp \left\{ \frac{i}{\hbar} S_*[q] - \frac{1}{\hbar} \sum_{\lambda} g_{\lambda} \left[ Q_{\lambda,0} \int_0^t d\tau q(\tau) \cos \omega_{\lambda} \tau \right. \right.
\]
\[
\left. \left. + \frac{g_{\lambda}}{m_{\lambda}\omega_{\lambda}} \int_0^t d\tau \int_0^\tau d\sigma q(\tau)q(\sigma) \cos \omega_{\lambda} \tau \sin \omega_{\lambda} \sigma \right\} \right\}
\]
\[
\times \prod_{\lambda} \delta \left( Q_{\lambda,0} + \frac{g_{\lambda}}{m_{\lambda}\omega_{\lambda}} \int_0^t d\tau q(\tau) \sin \omega_{\lambda} \tau - Q_{\lambda} \right). \tag{32}
\]

Next we use the Gaussian position representation of coherent states,

\[
\langle Q_{\lambda} | \xi_{\lambda} \rangle = \left( \frac{m_{\lambda}\omega_{\lambda}}{\pi \hbar} \right)^{\frac{1}{4}} e^{-\frac{\xi_{\lambda}^2}{2}} \exp \left( -\frac{m_{\lambda}\omega_{\lambda}}{2\hbar} Q_{\lambda}^2 - \frac{1}{2} \xi_{\lambda}^2 + \sqrt{\frac{2m_{\lambda}\omega_{\lambda}}{\hbar}} Q_{\lambda} \xi_{\lambda} \right), \tag{33}
\]

and perform the usual Gaussian integrations to find the propagator (27) in position representation. We arrive at

\[
\langle q | G(z, \xi, t) | q_0 \rangle = \int D[q] \exp \left\{ \frac{i}{\hbar} S_*[q] + \frac{1}{\hbar} \int_0^t d\tau q(\tau)(z^*(\tau) - \xi(\tau)) \right. \right.
\]
\[
\left. \left. - \frac{1}{\hbar^2} \int_0^t d\tau \int_0^\tau d\sigma \alpha_0(\tau - \sigma)q(\tau)q(\sigma) \right\} \right\} \tag{34}
\]

with the classical action \( S_*\left[ q \right] \) (31) of the isolated system (including the counterterm). The influence of the environment is reflected through the additional contributions

\[
\frac{1}{\hbar} \int_0^t d\tau q(\tau)(z^*(\tau) - \xi(\tau)) - \frac{1}{\hbar^2} \int_0^t d\tau \int_0^\tau d\sigma \alpha_0(\tau - \sigma)q(\tau)q(\sigma) \tag{35}
\]

to the action of the propagator. These extra terms involve the zero temperature bath correlation function \( \alpha_0(\tau - \sigma) \) from (14). The dependence of the propagator on the initial and final environmental coherent states \( | \xi \rangle \) and \( | z \rangle \) is captured entirely by the two complex, time-dependent functions

\[
\begin{align*}
\xi(\tau) &\equiv i \sum_{\lambda} \xi_{\lambda} e^{-i\omega_{\lambda} \tau} \\
z^*(\tau) &\equiv -i \sum_{\lambda} z_{\lambda} e^{i\omega_{\lambda} \tau}
\end{align*} \tag{36}
\]

Obviously, these functions are multiplied by the position of the Brownian particle in the action functional (35) and may therefore be interpreted as external (complex) forces. It will become clear in the next section that they will play the role of the stochastic process \( X(t) \) in the classical Langevin equation (6).

The non-Markovian nature of the open system dynamics, as already visible in the classical case (6) is again visible in the propagator \( \langle q | G(z, \xi, t) | q_0 \rangle \), where a path \( q(\tau) \) contributes non-locally in time \( \tau \) due to the appearance of the combination \( q(\tau)q(\sigma) \) with times \( \sigma < \tau \) in the full action of the propagator (34).
5. Quantum Brownian motion propagator

The path integral expression for the relevant quantum Brownian motion propagator $G_{QBM}(t)$ from (23) follows directly from (34) and the relation (28). According to the latter relation, we simply have to replace $z_{\lambda}$ by $z_{\lambda} + \sqrt{n_{\lambda}}\xi_{\lambda}$ and $\xi_{\lambda}$ by $\sqrt{n_{\lambda}}\xi_{\lambda}$ in (34). Therefore, the part of the action functional involving these external (complex) forces takes the form

\[
\frac{1}{\hbar} \int_{0}^{t} d\tau \left[ q(\tau)z^{*}(\tau) + \frac{1}{\hbar} \int_{0}^{t} d\sigma \Re \alpha_{0}(\tau - \sigma)q(\tau)q(\sigma) - \int_{0}^{t} d\sigma \Gamma(\tau - \sigma)q(\sigma) \right].
\]

(38)

Apparently, the imaginary part consists of three contributions. While the term involving $\Gamma(0)$ is just what is needed to cancel the counterterm (5) in the potential $V(q)$, the term $\Gamma(q)q_{0}$ corresponds to an initial slip term that was also appearing in the derivation of the classical Langevin equation (6), and there neglected. To be consistent, we will neglect it here, too. Finally, the non-local contribution to the imaginary part is due to damping as in the classical Langevin equation (6). This latter relation is, in fact, a bit more subtle and will be discussed in due course.

Let us summarize the findings and state one of the main results of this paper, namely the quantum Brownian motion propagator for pure states,

\[
\langle q | G_{QBM}(t) | q_{0} \rangle = \int D[q] \exp \left[ \frac{i}{\hbar} S_{QBM}[q] + \frac{1}{\hbar} \int_{0}^{t} d\tau q(\tau)z^{*}(\tau) - \frac{1}{\hbar} \int_{0}^{t} d\tau \Re \alpha_{0}(\tau - \sigma)q(\tau)q(\sigma) \right],
\]

(39)

where the full (real) action functional $S_{QBM}[q]$ for quantum Brownian motion reads

\[
S_{QBM}[q] = \int_{0}^{t} d\tau \left[ \frac{1}{2} M\dot{q}^{2}(\tau) - V(q(\tau), \tau) + q(\tau)\Xi(\tau) - \frac{1}{2} Mq(\tau) \int_{0}^{t} d\sigma \Gamma(\tau - \sigma)\dot{q}(\sigma) \right].
\]

(40)

with $V(q, \tau)$ the bare potential as in (6).

We cannot expect to derive the dissipative classical Langevin equation (6) straight from an action like (40) using standard variational principles. We will, however, be able to clarify crucial connections.

Neglecting the term involving the damping kernel for a moment, it is obvious that (40) corresponds to the equation of motion $M\ddot{q} + V'(q, \tau) = \Xi(\tau)$ such that $\Xi(\tau)$ should be identified with the random force $X(t)$ in the classical Langevin equation (6). Indeed, in order to obtain the correct reduced density operator, the coherent state labels $\xi_{\lambda}$ that determine $\Xi(t)$ (see (37)), may
be seen as Gaussian stochastic variables according to expression (26). As in the classical case, with $X(t)$ given by (8), in this way the function $\Xi(t)$ turns into a stochastic process with zero mean and correlation function
\[
\langle \Xi(t) \Xi(s) \rangle_{z,\xi} = \sum_{\lambda} \frac{\hbar^2 \gamma^2_{\lambda} \cos \omega_{\lambda}(t-s)}{m_{\lambda} \omega_{\lambda}} = \alpha_{\gamma}(t-s),
\]
where the real $\alpha_{\gamma}(t-s)$ is the thermal part of the quantum correlation function (11), see (13). As already mentioned, in the classical limit $\alpha_{\gamma}(t-s) \approx M k_B T \Gamma(t-s)$, so that indeed, $X(t)$ may be seen as the classical limit of $\Xi(t)$. This connection is further underlined by the fact that the stochasticity of $\Xi(t)$ emerges from the assumed initial distribution of coherent states $|\xi\rangle$ for a thermal environment (18), very much in the same way as the stochasticity of $X(t)$ arises from the Boltzmann distribution of the environmental initial positions and momenta in expression (8).

Not only may the fluctuations be identified, but also the dissipative term. While it appears rather obvious that the term involving the non-local damping kernel $\Gamma(t)\alpha$ is related to dissipation, it is quite subtle to establish this connection formally. For simplicity, we set $V(q, t) \equiv 0$ and also $\Xi(t) \equiv 0$ and furthermore assume a delta-correlated bath with $\Gamma(t) = 2\gamma(t - \alpha)$. Then, the quantum Brownian motion action reads $S_{QBM}[q] = \int_0^t d\tau \left\{ \frac{1}{2} M \dot{q}^2(\tau) - \frac{1}{2} M \gamma q(\tau) \dot{q}(\tau) \right\}$ which may be integrated to give $S_{QBM}[q] = \frac{1}{2}M \left\{ \int_0^t d\tau \dot{q}^2(\tau) - \frac{\gamma}{2}(q^2(t) - q^2(0)) \right\}$. In order to clarify the effect of this action on a quantum state, $|\psi\rangle$, we look at an infinitesimal time step $(q_0, t) \rightarrow (q, t + \Delta t)$, determined by the corresponding infinitesimal propagator
\[
\sqrt{\frac{iM}{2\pi \hbar \Delta t}} \exp \left\{ \frac{iM}{2\hbar} \left[ \frac{(q - q_0)^2}{\Delta t} - \gamma \frac{(q^2 - q_0^2)}{2} \right] \right\}. \tag{42}
\]
Apart from an irrelevant phase, the infinitesimal time step amounts to an evolution
\[
\frac{i\hbar}{\Delta t} \hat{\partial} |\psi(t)\rangle = \left( \frac{p^2}{2M} + \frac{\gamma}{2} qp \right) |\psi(t)\rangle, \tag{43}
\]
which displays the correct contribution to the well-known friction term $\frac{\gamma}{2} [q, \{ p, \rho(t) \}]$ in the evolution equation for the reduced density operator [9, 22]. Therefore, the action functional (40) does indeed contribute in the correct way to the expected dissipative time evolution. It should be stressed, however, that a full identification of the damping term in (6) in the classical limit will have to take into account the two additional terms appearing in the exponent of the full propagator (39). Clearly, the non-local term involving the real part of the zero temperature correlation function acts as a Gaussian ‘filter’ for the paths, restricting the set of all Feynman paths to be summed over. Such a restriction describes the loss of coherence, here the zero temperature contribution to decoherence.

More direct is the interpretation of the complex ‘force’ $z(t)$. In the very same way as we interpreted $\Xi(t)$ as a stochastic process due to the representation of the reduced density operator as an integral over the labels $\xi, \xi$, we may see $z(t)$ as a complex stochastic force with zero mean and complex correlation functions
\[
\langle z(t) \bar{z}(s) \rangle_{z,\xi} = \alpha_{\gamma}(t-s); \quad \langle z(t)z(s) \rangle_{z,\xi} = 0, \tag{44}
\]
where $\alpha_{\gamma}(t-s)$ is the zero temperature bath correlation (14). While we made it clear that the stochastic real force $\Xi(t)$ of (37) originates from the thermal distribution of initial states $|\xi\rangle \langle \xi|$, 

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the complex force \( z(t) \) contributes even at zero temperature, and has therefore no classical analogue. The process \( z(t) \) ensures that a pure initial state \(|\psi_0\rangle\) of the system will evolve into a mixed state \( \rho(t) \), even at zero temperature, when \( Z(t) = 0 \). It therefore reflects the growing entanglement between system and environment. Despite being a \( c \)-number stochastic process, it is truly quantum noise.

It may appear a bit pedantic to treat the processes \( /Xi_1(t) \) and \( z(t) \) separately. Since the evolution of the states depends on \( z^*(t) + iZ(t) \) only, it would be entirely justified to simply define this sum as a single complex Gaussian process with the appropriate correlation functions. We stick to two processes, however, to clearly emphasize the different physical origins and meanings (‘classical’ uncertainty versus ‘quantum’ uncertainty) of the two processes.

We close by noting that a path integral propagator somewhat similar to (39) was established some time ago in [18], without a clear physical interpretation at finite temperature. That result required only a single complex force similar to \( z(t) \), while \( Z(t) \) was missing. The crucial difference to the current result is that the propagator in [18] corresponds in fact to a zero-temperature expression of an artificial environment containing negative frequency oscillators. The new stochastic propagator \( G_{QBM}(t) \) has a clear physical interpretation as visible in (22) and (23). Furthermore, it allows us to make the direct connection to the Langevin equation (6) as accomplished in this section.

6. Relation to the Feynman–Vernon propagator

Feynman and Vernon [8] start from the Brownian motion model (4) and derive the path integral expression for the propagator \( J(q, q', t; q_0, q'_0, 0) \) of the reduced density matrix

\[
\langle q | \rho(t) | q' \rangle = \int dq_0 \int dq'_0 \ J(q, q', t; q_0, q'_0, 0) \langle q_0 | \rho_0 | q'_0 \rangle . \tag{45}
\]

In our approach, we may start from the stochastic path integral propagator (39) to determine the propagator of the reduced density operator. According to our construction, we have \( \rho(t) = \langle \langle |\psi(z, \xi, t) \rangle \langle \psi(z, \xi, t) \rangle \rangle_{z, \xi} \). Therefore, the propagators satisfy

\[
J(q, q', t; q_0, q'_0, 0) = \langle \langle q | G_{QBM}(t) | q_0 \rangle \langle q'_0 | G_{QBM}^\dagger(t) | q' \rangle \rangle_{z, \xi} . \tag{46}
\]

The ensemble mean \( \langle \langle . . . \rangle \rangle_{z, \xi} \) over the stochastic propagators amounts to taking the Gaussian integral over the processes \( Z(t) \) and \( z^*(t) \) in the path integral expressions (39). This may be done analytically, resulting in the usual double path integral expression

\[
J(q, q', t; q_0, q'_0, 0) = \int D[q] \int D[q'] \exp \left\{ \frac{i}{\hbar} (S[q] - S[q']) \right\} F[q, q'] \tag{47}
\]

with the influence functional

\[
F[q, q'] = \exp \left\{ -\frac{1}{\hbar^2} \int_0^t d\tau \int_0^\tau d\sigma (q(\tau) - q'(\tau)) [a(\tau - \sigma) q(\sigma) - a^*(\tau - \sigma) q'(\sigma)] \right\} , \tag{48}
\]

where \( a(\tau - \sigma) \) is the quantum bath correlation function (11). Clearly, we arrive at the well-known Feynman–Vernon result [8] for the propagator of the reduced density matrix.
7. Conclusions

Einstein formulated his theory of Brownian motion in terms of densities. Later, Langevin developed a direct, stochastic dynamical description for a single Brownian particle in terms of a stochastic differential equation. In his own words, the stochastic approach is ‘infinitely more simple’ [3]. For quantum Brownian motion, a similar stochastic description is available. While this has been known for some time, we here give a new description in terms of a stochastic pure state path integral propagator that has a simple and clear physical meaning. Most noteworthy, despite being formulated in the Schrödinger picture, it allows us to make a direct connection to the classical Langevin equation. It is an open question at this moment whether such a stochastic approach will in general be as fruitful in the quantum domain as it has proven indispensable in classical Monte Carlo simulations. So far, a general implementation of the stochastic approach utilizing the full path integral expression (39) for the propagator $G_{QBМ}(t)$ is missing. This will be an urgent project to be addressed in future work.

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References

[1] Einstein A 1905 Ann. Phys. (Lpz) 17 549
[2] Perrin J 1920 Atoms translated by Hammick D Ll (London: Constable)
[3] Langevin P 1908 Comptes Rendus 146 530
[4] Nakajima S 1958 Prog. Theor. Phys. 20 948
[5] Zwanzig R 1960 J. Chem. Phys. 33 1338
[6] Redfield A G 1957 IBM J. Res. Dev. 1 19
[7] Redfield A G 1965 Adv. Magn. Reson. 1 1
[8] Feynman R P and Vernon F L 1963 Ann. Phys. (NY) 24 118
[9] Caldeira A O and Leggett A J 1983 Physica A 121 587
[10] Caldeira A O and Leggett A J 1985 Phys. Rev. A 31 1059
[11] Grabert H, Schramm P and Ingold G-L 1988 Phys. Rep. 168 115
[12] Weiss U 2000 Quantum Dissipative Systems 2nd edn (Singapore: World Scientific)
[13] Dalibard J, Castin Y and Molmer K 1992 Phys. Rev. Lett. 68 580
[14] Lindblad G 1976 Commun. Math. Phys. 48 119
[15] Gardiner C W, Parkins A S and Zoller P 1992 Phys. Rev. A 46 4363
[16] Carmichael H 1994 An Open System Approach to Quantum Optics (Berlin: Springer)
[17] Plenio M B and Knight P L 1998 Rev. Mod. Phys. 70 101
[18] Strunz W T 1996 Phys. Lett. A 224 25
[19] Ðiösí L and Strunz W T 1997 Phys. Lett. A 235 569
[20] Ðiösí L, Gisin N and Strunz W T 1998 Phys. Rev. A 58 1699
[21] Strunz W T, Ðiösí L and Gisin N 1999 Phys. Rev. Lett. 82 1801
[22] Strunz W T, Ðiösí L, Gisin N and Yu T 1999 Phys. Rev. Lett. 83 4909
[23] Strunz W T 2001 Chem. Phys. 268 237
[24] Gaspard P and Nagaoka M 1999 J. Chem. Phys. 111 5668
[25] Breuer H-P, Kappler B and Petruccione F 1999 Phys. Rev. A 59 1633
[26] Stockburger J T and Grabert H 2001 *Chem. Phys.* **268** 249
[27] Gambetta J and Wiseman H M 2002 *Phys. Rev.* A **66** 012108
[28] Shao J 2004 *J. Chem. Phys.* **120** 5053
[29] Hänggi P and Ingold G L 2005 *Chaos* **15** submitted (Preprint quant-ph/0412052)
[30] Ankerhold J, Grabert H and Pechuckas P 2005 *Chaos* **15** submitted (Preprint cond-mat/0412352)
[31] Glauber R J 1963 *Phys. Rev.* **131** 2766
[32] Walls D F and Milburn G J 1995 *Quantum Optics* 2nd edn (Berlin: Springer)
[33] Thorwart M, Reimann P and Hänggi P 2000 *Phys. Rev.* E **62** 5808
[34] Feynman R P 1948 *Rev. Mod. Phys.* **20** 367
[35] Feynman R P and Hibbs A R 1965 *Quantum Mechanics and Path Integrals* (New York: McGraw-Hill)
[36] Schulman L S 1981 *Techniques and Applications of Path Integration* (New York: Wiley)