Convolutionless Non-Markovian master equations and quantum trajectories: Brownian motion revisited

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Stochastic Schrödinger equations for quantum trajectories offer an alternative and sometimes superior approach to the study of open quantum system dynamics. Here we show that recently established convolutionless non-Markovian stochastic Schrödinger equations may serve as a powerful tool for the derivation of convolutionless master equations for non-Markovian open quantum systems. The most interesting example is quantum Brownian motion (QBM) of a harmonic oscillator coupled to a heat bath of oscillators, one of the most-employed exactly soluble models of open system dynamics. We show explicitly how to establish the direct connection between the exact convolutionless master equation of QBM and the corresponding convolutionless exact stochastic Schrödinger equation.

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I. INTRODUCTION

Current attempts to push quantum coherent dynamics further towards the macroscopic or towards systems residing on more and more particles have to overcome decohering influences of the environment. Typically, the system in question becomes entangled with environmental degrees of freedom and thus coherence is lost. Even if seemingly weak, couplings to an environment may have dramatic consequences for coherences. Thus, any theoretical modeling of such quantum dynamics should take into account environmental effects.

Traditionally, open quantum systems are described in terms of their reduced density operator and the dynamics thereof. Ideally, maps, propagators or even evolution equations are derived that account for environmental effects.

The last decade has seen tremendous progress in the development of stochastic Schrödinger equations to describe open quantum system dynamics. In this framework, the reduced density operator is obtained from an ensemble mean over the pure state solutions – “quantum trajectories” – of a stochastic Schrödinger equation. While known to exist in the case of Markovian open system dynamics (when the ensemble dynamics is governed by a Lindblad master equation), it is only fairly recently that quantum trajectories were extended to cover more general non-Markovian open systems. Interestingly, in our approach the non-Markovian stochastic Schrödinger equation is derived directly from an underlying microscopic system-plus-environment model without referring to the corresponding evolution of the reduced density operator. This turns out to be an efficient way to tackle non-Markovian quantum dynamics, shedding new light on the difficulties encountered when dealing with memory effects.

Non-Markovian dynamics usually means past contributions to the current time evolution: memory effects typically enter through integrals over the past. Nevertheless, under certain circumstances, non-Markovian dynamics may be cast into a time-local, convolutionless form where the dynamics of the open system state is determined by the state at the current time only. Then, non-Markovian effects are taken into account by certain time dependent coefficients that may replace the memory integrals usually encountered.

Examples of this class are models of open quantum system dynamics that may be treated without any approximation. The famous damped harmonic oscillator bilinearly coupled to a bath of harmonic oscillators allows for a convolutionless treatment without any approximation. Such model

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systems allow us to test approximation schemes and, very oft en, they enable us to pin down important qualitative features of the dynamics of more realistic open quantum systems clearly.

The purpose of this paper is to show that our non-Markovian quantum trajectory approach, besides its powerful use in numerical simulations, provides an elegant way to derive non-Markovian convolutionless master equations for open quantum systems. We exemplify this idea by deriving the exact convolutionless non-Markovian master equation for the famous quantum Brownian motion model of a harmonic oscillator \[34, 37\]. This QBM master equation has been extensively studied in different contexts \[28, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43\]. Our approach is different from all the previous work. We show in this paper how to establish the direct link between our convolutionless stochastic Schrödinger equation and the known convolutionless master equation. The key ingredient for the derivation is a Heisenberg operator approach to our non-Markovian stochastic Schrödinger equation \[24\].

Our paper is organized as follows: in Section II we review the “non-Markovian quantum state diffusion” stochastic Schrödinger equation, sketch its derivation and display different approaches to a convolutionless formulation. Next we show how to derive master equations from the stochastic Schrödinger equation and give some simple examples. The main part of the paper follows in Sections IV and V where we discuss both the stochastic approach to the soluble QBM-model and the derivation of the convolutionless master equation based on the stochastic approach. Unavoidable technical details are left for two appendices.

II. STOCHASTIC SCHRODINGER EQUATION

Here we review the Markov and, more importantly, our non-Markovian stochastic approach to open quantum system dynamics \[18, 19\]. The dynamics of the reduced density operator $\rho_t$ is obtained from a stochastic evolution equation for pure states $\psi_t$, such that upon taking the ensemble mean $\mathcal{M}\{\ldots\}$ over the pure states, the reduced density operator is recovered:

$$\rho_t = \mathcal{M}\{|\psi_t\rangle\langle\psi_t|\}. \quad (1)$$

A. Usual Markov limit: Lindblad theory

In the standard Markov case, often encountered in quantum optical applications, the evolution equation for the reduced density operator of the open system takes the Lindblad form \[14, 17\]

$$\partial_t \rho_t = -\frac{i}{\hbar}[H, \rho_t] + \frac{1}{2} \left([L, \rho_t L^\dagger] + [L^\dagger \rho_t, L]\right). \quad (2)$$

We here restrict ourselves to the simplest case of a single non-unitary contribution involving a single operator $L$ (the Lindbladian). In general, a sum or integral over such Lindbladians may appear. Here and throughout the paper, we denote with $H$ the Hamiltonian that generates the otherwise isolated, unitary evolution of the system.

A stochastic Schrödinger equation “unraveling” Lindblad evolution \[2\] is provided by the linear quantum state diffusion \[10, 29\] equation

$$\partial_t \psi_t = \left(-\frac{i}{\hbar} H + L z_t^* - \frac{1}{2} L^\dagger L\right) \psi_t \quad (3)$$

for unnormalized stochastic states $\psi_t$. The stochastic process $z_t^*$ is complex white noise with zero mean $\mathcal{M}\{z_t^*\} = 0$ and correlations

$$\mathcal{M}\{z_t z_s^*\} = \delta(t-s) \quad \text{and} \quad \mathcal{M}\{z_t z_s\} = 0. \quad (4)$$

Equation (3) is here understood as a stochastic equation in its Stratonovich sense, though differences to the Ito case only appear in their respective nonlinear versions, which are not relevant for this paper, see \[10\]. As one may easily confirm, provided the quantum trajectories follow equation (3), the ensemble mean \[11\] indeed evolves according to Lindblad’s equation (2).

B. Non-Markovian stochastic Schrödinger equation

In order to extend the Markov theory we use a standard model for open quantum systems in the system-plus-reservoir framework: a system with Hamiltonian $H$, coupled linearly to a large number of harmonic oscillators with
distributed eigenfrequencies $\omega_\lambda$ and creation and annihilation operators $b_\lambda^\dagger, b_\lambda$. This total Hamiltonian can be written as

$$H_{\text{tot}} = H + H_{\text{int}} + H_{\text{bath}} = H + \hbar \sum_\lambda (g_\lambda^* L b_\lambda^\dagger + g_\lambda L^\dagger b_\lambda) + \hbar \sum_\lambda \omega_\lambda b_\lambda^\dagger b_\lambda,$$

where $L$ is the system operator providing the coupling to the environment, and $g_\lambda$ are coupling constants.

The interaction between system and environment may be written in the more appealing form

$$H_{\text{int}} = \hbar (LB^\dagger + L^\dagger B)$$

with a bath operator $B$ consisting of contributions of all environmental oscillators, $B = \sum_\lambda g_\lambda b_\lambda$. It turns out to be convenient to change to an interaction representation with respect to the free bath evolution, such that instead of (5) we use

$$H_{\text{tot}}(t) \equiv e^{\hat{H}_{\text{bath}} t}(H + H_{\text{int}})e^{-\hat{H}_{\text{bath}} t} = H + \hbar \left( LB^\dagger(t) + L^\dagger B(t) \right)$$

for the total Hamiltonian with

$$B(t) = e^{\hat{H}_{\text{bath}} t} B e^{-\hat{H}_{\text{bath}} t} = \sum_\lambda g_\lambda b_\lambda e^{-i\omega_\lambda t}.$$

The dynamics of the open system is thus influenced by the bath operator $B(t)$, whose statistical properties are captured in its correlation function

$$\alpha(t - s) = \langle B(t)B^\dagger(s) \rangle_{\text{env}} = \sum_\lambda |g_\lambda|^2 e^{-i\omega_\lambda(t-s)} = \hbar \int_0^\infty d\omega J(\omega) e^{-i\omega(t-s)},$$

here for a zero temperature bath (for finite temperature see below). The last equality in (9) defines the spectral density $J(\omega)$ of bath oscillators.

If the dynamics of system and environment is such that the bath correlation function in (9) may be replaced by a delta function, the reduced dynamics is Markovian and $\rho_t$ evolves according to the Lindblad master equation (2). For a general correlation function $\alpha(t - s)$, however, memory effects of the environment may be important and matters become exceedingly more difficult. Such non-Markovian effects are known to be relevant in many situations, in particular at low temperatures and as soon as narrow energy splittings occur, as in tunneling processes. They are also relevant for structured environments, as for instance the electro-magnetic vacuum in the presence of a photonic band gap material. Moreover, non-Markovian effects play a role in output coupling dynamics of atoms from a Bose Einstein condensate with the aim to build an atom laser.

Also, it may happen that the dynamics appears to be Markovian, yet the evolution equation is not of the standard Lindblad class. This is the case, for instance, in the high-temperature limit of the standard quantum Brownian motion model to be discussed in Sect. IV. In such cases, transient effects (initial slips, see also [46, 47]) are important and violate the semigroup property required for Lindblad-class evolution.

The open quantum system described by the system-bath model, allows to derive the linear non-Markovian generalization of (3), henceforth referred to as the “Non-Markovian quantum state diffusion” (NMQSD)- equation. The starting point is the formal solution $|\Psi_t\rangle$ of the Schrödinger equation for the total system

$$i\hbar \partial_t |\Psi_t\rangle = H_{\text{tot}}(t)|\Psi_t\rangle,$$

in a special representation. For simplicity, in this section we assume a zero temperature bath: the initial pure state of system and environment is

$$|\Psi_0\rangle = |\psi_0\rangle \otimes |0_1\rangle \otimes |0_2\rangle \cdots \otimes |0_\lambda\rangle \otimes \cdots .$$

The system state $|\psi_0\rangle$ is arbitrary and all environmental oscillators start in their respective ground state $|0_\lambda\rangle$. By using a Bargmann coherent state basis for the environmental degrees of freedom: $|z_\lambda\rangle = \exp\{z_\lambda a_\lambda^\dagger\}|0_\lambda\rangle$, and the resolution of the identity

$$I_\lambda = \int \frac{d^2 z_\lambda}{\pi} e^{-|z_\lambda|^2} |z_\lambda\rangle \langle z_\lambda|,$$

(12)
the total state $|\Psi_t\rangle$ in (10) can be expanded as
\[
|\Psi_t\rangle = \int \frac{d^2z}{\pi} e^{-|z|^2} |\psi_t(z^*)\rangle \otimes |z\rangle,
\]
where $|z\rangle = |z_1\rangle \otimes |z_2\rangle \otimes \cdots \otimes |z_\lambda\rangle \cdots$, $d^2z = d^2z_1d^2z_2 \cdots d^2z_\lambda \cdots$ and $|z|^2 = \sum_\lambda |z_\lambda|^2$. It follows from (13) that the reduced density operator of the open system may be obtained by an ensemble mean over the system states $|\psi_t(z^*)\rangle$,
\[
\rho_t = \text{Tr}_{\text{bath}}[|\Psi_t\rangle \langle \Psi_t|] = \int \frac{d^2z}{\pi} e^{-|z|^2} |\psi_t(z^*)\rangle \langle \psi_t(z^*)| \equiv \mathcal{M}\{ |\psi_t\rangle \langle \psi_t| \}.
\]

The last equality defines the ensemble mean $\mathcal{M}\{ \ldots \}$ as the Gaussian integral $\int \frac{d^2z}{\pi} e^{-|z|^2} \{ \ldots \}$ over all coherent state labels $z_\lambda$. Using the Schrödinger equation (10), the pure states $|\psi_t(z^*)\rangle$ of the system in (10) were shown to satisfy the non-Markovian QSD equation (15), involving the bath correlation function and a functional derivative of the current state.

\[
\frac{\delta \psi_t(z^*)}{\delta z^*_s} = O(t, s, z^*) \psi_t(z^*),
\]
acting in the Hilbert space of the open system on the current state $\psi_t(z^*)$ (18). We indicate that $O$ may depend on the times $t$ and $s$, and possibly on the (entire history of the) stochastic process $z^*_s$. Relevant examples of this replacement will be given shortly. One way to determine the operator $O(t, s, z^*)$ in actual applications (18) is to insert Ansatz (16) in (15) and use the “consistency condition”

\[
\partial_t \frac{\delta \psi_t(z^*)}{\delta z^*_s} = \frac{\delta}{\delta z^*_s} \partial_t \psi_t(z^*)
\]

(17) together with the initial condition:

\[
O(t = s, s, z^*) = L
\]

for all $s$.

One finds the formal evolution equation

\[
\partial_t O(t, s, z^*) = \left[ -\frac{i}{\hbar} H + L z^*_t - L^1 \bar{O}(t, z^*), O(t, s, z^*) \right] - L^1 \frac{\delta \bar{O}(t, z^*)}{\delta z^*_s}
\]

(19) with the time-integrated operator $\bar{O}(t, z^*)$:

\[
\bar{O}(t, z^*) = \int_0^t \alpha(t - s) O(t, s, z^*) ds.
\]

Equation (19) has to be solved with initial condition (18) for all $s$. As has been shown in previous publications (18), one can determine the $O$-operator in (16) for many interesting and relevant physical models. Moreover, approximate $O$-operators can always be found systematically and be easily implemented in numerical simulations (22, 23, 52).

C. Convolutionless stochastic Schrödinger equation

Memory effects of non-Markovian evolution clearly make themselves felt through the integral over the past in equation (15), involving the bath correlation function and a functional derivative of the current state $\psi_t(z^*)$ with respect to earlier noise $z^*_t$. In many relevant cases, it is possible to replace that functional derivative by some time dependent operator $O$,

\[
O(t, s, z^*) \psi_t(z^*) = O(t, s, z^*) \psi_t(z^*)
\]

acting in the Hilbert space of the open system on the current state $\psi_t(z^*)$ (18).
Once the replacement (10) of the functional derivative by an operator is known – sometimes only approximately – the NMQSD equation (15) takes the more useful convolutionless form

$$\partial_t \psi_t(z^*) = \left( -\frac{i}{\hbar}H + Lz_t^* - L^1\bar{O}(t, z^*) \right) \psi_t(z^*),$$

(21)

where we used the notation $\bar{O}(t, z^*)$ from (20), see also (20). The determination of $\psi_t(z^*)$ is now reduced to solving the simple time-local stochastic Schrödinger equation (21). For a memory-less bath with $\alpha(t-s) = \gamma \delta(t-s)$, we see from (18) and (20) that $\bar{O}(t, z^*) = \frac{\gamma}{2}L$ holds. Then equation (21) reduces indeed to the Markov linear quantum state diffusion equation (4).

We recall that (21) does not preserve the norm of the states $\psi_t(z^*)$. Thus, if only a numerical linear solution of (21) is possible, it is most often more advisable to use its nonlinear, norm-preserving version (18).

D. Heisenberg approach

There is an alternative approach to the convolutionless NMQSD stochastic Schrödinger equation (21), see (24). We find it most appropriate to work in terms of a stochastic propagator $G_t(z^*)$ for the states $\psi_t(z^*)$. By definition, we have

$$|\psi_t(z^*)\rangle = G_t(z^*)|\psi_0\rangle.$$  

(22)

We use the unitary propagator $U_t$ for the total state (13), satisfying

$$i\hbar \partial_t U_t = H_{tot}(t)U_t \quad \text{and} \quad U_0 = I,$$  

(23)

with $H_{tot}(t)$ from (7). Since $|\Psi_t\rangle = U_t|\Psi_0\rangle$ and $|\psi_t(z^*)\rangle = \langle z|\Psi_t\rangle$ according to (13), the stochastic propagator $G_t(z^*)$ may be expressed as

$$G_t(z^*) = \langle z|U_t|0\rangle.$$  

(24)

We take the time derivative of the propagator in (24) and obtain from the Schrödinger equation (28) $i\hbar \partial_t G_t(z^*) = \langle z|H_{tot}(t)U_t|0\rangle$. With Hamiltonian (5), we arrive at

$$\partial_t G_t(z^*) = -\frac{i}{\hbar}HG_t(z^*) + Lz_t^*G_t(z^*) - iL^1\sum_{\lambda} g_\lambda e^{-i\omega_\lambda t}\langle z|b_\lambda U_t|0\rangle,$$  

(25)

with $z_t^* = -i\sum_\lambda g_\lambda^* z_\lambda^* e^{i\omega_\lambda t}$ as before.

As in (24), we write $\langle z|b_\lambda U_t|0\rangle = \langle z|U_t b_\lambda(t)|0\rangle$ with the Heisenberg operator $b_\lambda(t) = U_t^{-1}b_\lambda U_t$. From the corresponding Heisenberg equation of motion,

$$i\hbar \partial_t b_\lambda(t) = U_t^{-1}[b_\lambda, H_{tot}(t)]U_t = \hbar g_\lambda^* e^{i\omega_\lambda t} L(t)$$  

(26)

with the Heisenberg operator $L(t) \equiv U_t^{-1}L U_t$, we find upon integration

$$b_\lambda(t) = b_\lambda - ig_\lambda^* \int_0^t ds L(s)e^{i\omega_\lambda s}.$$  

(27)

We may conclude that

$$\langle z|b_\lambda U_t|0\rangle = \langle z|U_t b_\lambda(t)|0\rangle = -ig_\lambda^* \int_0^t ds e^{i\omega_\lambda s}\langle z|U_t L(s)|0\rangle,$$  

(28)

where we have used $b_\lambda|0\rangle = 0$.

Replacing the last term in (25) by expression (28), the evolution equation for the stochastic propagator becomes

$$\partial_t G_t(z^*) = -\frac{i}{\hbar}HG_t(z^*) + Lz_t^*G_t(z^*) - L^1\int_0^t ds \alpha(t-s)\langle z|U_t L(s)|0\rangle,$$  

(29)

with the expected correlation function $\alpha(t-s) = \sum_\lambda |g_\lambda|^2 e^{-i\omega_\lambda (t-s)}$, at zero temperature.
Next it turns out appropriate to introduce the operator
\[ O(t, s) = U_t L(s) U_t^{-1} = U_t U_s^{-1} L U_s U_t^{-1} \]
in the Hilbert space of system and environment. It allows us to express the term under the memory integral in (29) in the form
\[ \langle z | U_t L(s) | 0 \rangle = \langle z | O(t, s) U_t | 0 \rangle. \] (31)
Comparing equation (29) with the NMQSD equation (16) with replacement (10) and recalling equation (24), we see that we aim to find an operator \( O(t, s, z^*) \) satisfying
\[ \langle z | O(t, s) U_t | 0 \rangle = O(t, s, z^*) \langle z | U_t | 0 \rangle = O(t, s, z^*) G_t(z^*). \] (32)
Relation (32) is crucial for finding an evolution equation for \( O(t, s, z^*) \) with respect to \( s \), as to be shown in Section IV. With expression (32) it is clear that equation (24) is the linear convolutionless non-Markovian stochastic Schrödinger equation (21).

Thus, the operator \( O(t, s, z^*) \) in (32) (or (16)) may be found by investigating the equation of motion for the Heisenberg coupling operator \( O(t, s) = U_t U_s^{-1} L U_s U_t^{-1} \) in the Hilbert space of system and environment. Depending on the application, this approach may offer a more transparent way to establish an expression for the \( O(t, s, z^*) \)-operator of a convolutionless formulation than the evolution equation (19). In particular, it allows us to derive evolution equations for \( O(t, s, z^*) \) with respect to \( s \), rather than \( t \).

### III. MASTER EQUATION

Our stochastic approach to open quantum systems will be employed to derive the master equation for the ensemble evolution (22, 24). A particularly simple and straightforward route to the master equation is possible as soon as the operator \( O(t, s, z^*) \) in (16) (or (22)) and thus the integrated operator \( \bar{O}(t, z^*) \) from (24) turns out to be independent of the noise \( z^* \). This happens to be true for many interesting cases, as shown below. We stress, however, that for the main part of this paper, the Brownian motion model of Section IV, \( \bar{O}(t, z^*) \) does depend on the noise process \( z_t^* \) and matters are more difficult.

#### A. Density operator evolution

According to our construction, the reduced density operator \( \rho_t \) is given by the ensemble mean over the solutions of the stochastic Schrödinger equation (21). We write \( \rho_t = \mathcal{M}\{P_t\} \) with \( P_t = |\psi_t(z^*)\rangle \langle \psi_t(z^*)| \). Upon taking the time derivative in (1) and employing (24), we get
\[ \dot{\rho}_t = -\frac{i}{\hbar}[H, \rho_t] + L \mathcal{M}\{z_t^* P_t\} - L^\dagger \mathcal{M}\{\bar{O}(t, z^*) P_t\} + \mathcal{M}\{P_t z_t\} L^\dagger - \mathcal{M}\{P_t \bar{O}^\dagger(t, z^*)\} L. \] (33)

Apparently, this is still far from being a closed evolution equation for \( \rho_t \). Using a version of Novikov’s theorem (51),
\[ \mathcal{M}\{P_t z_t\} = \mathcal{M}\left\{ \int_0^t ds \alpha(t-s) \frac{\delta}{\delta z_s^*} P_t \right\}, \] (34)

which amounts to a partial integration under the Gaussian probability distribution in (14), we may use the replacement of the functional derivative by the operator \( \mathcal{O} \) in (16) and find \( \mathcal{M}\{P_t z_t\} = \mathcal{M}\{\bar{O}(t, z^*) P_t\} \). Then equation (33) takes the form
\[ \dot{\rho}_t = -\frac{i}{\hbar}[H, \rho_t] + [L, \mathcal{M}\{P_t \bar{O}^\dagger(t, z^*)\}] + [\mathcal{M}\{\bar{O}(t, z^*) P_t\}, L^\dagger]. \] (35)

A convolutionless evolution equation for the non-Markovian dynamics of the reduced density operator may be derived from the knowledge of the operator \( \bar{O}(t, s, z^*) \) in (16). For instance, as soon as the exact \( \bar{O}(t, s, z^*) \) is independent of the noise \( z^*_s \) or as soon as a noise-dependent \( \bar{O}(t, s, z^*) \) can be approximated well by a noise-independent operator \( \bar{O}(t, s) \), we find \( \bar{O}(t, s, z^*) = \bar{O}(t, s) \) and therefore \( \bar{O}(t, z^*) = \bar{O}(t) \). In these cases, equation (35) is a convolutionless closed master equation for \( \rho_t \) due to \( \mathcal{M}\{\bar{O}(t) P_t\} = \bar{O}(t) \mathcal{M}\{P_t\} = \bar{O}(t) \rho_t \), we find
\[ \dot{\rho}_t = -\frac{i}{\hbar}[H, \rho_t] + [L, \rho_t \bar{O}^\dagger(t)] + [\bar{O}(t) \rho_t, L^\dagger]. \] (36)
Let us emphasize that equation (36) is not of Lindblad form in general, not even in the long-time limit due to its non-Markovian nature. Nevertheless, as long as we deal with exact master equations – as for most of this paper – positivity issues do not appear. By construction, despite their apparent non-Lindblad form, these exact non-Markovian convolutionless master equations represent (completely) positive maps. However, as soon as the master equation follows from an approximate replacement of the operator $O(t, s, z^*)$, positivity is a difficult and delicate subject well beyond the scope of this paper. For such investigations on positivity (importance of initial slips etc.) the interested reader is referred to the literature [24, 22, 40, 17, 51].

Clearly, the convolutionless master equation (36) covers a much wider class of open system dynamics than the Lindblad equation (14). The non-Markovian properties are encoded in a finite width correlation function $a(t-s)$, and so in time-dependent coefficients appearing in the master equation. By construction, we already know the corresponding stochastic Schrödinger equation (21). Remarkably, here we derive the master equation from the stochastic Schrödinger equation.

We stress that the master eqn. (36) holds for a noise independent operator $O(t, s, z^*)$ only. Whenever $O(t, s, z^*)$ does depend on the noise $z^*$, eqn. (35) is still valid yet the step to eqn. (36) fails and matters are considerably more difficult. In this case, no general closed evolution equation for $\rho_0$ is known. However, starting from (35), one may still be able to derive an evolution equation for specific cases, as shown in this paper: an important example of this class is provided in Section IV on Brownian motion, where $O(t, s, z^*)$ depends linearly on the stochastic process $z^*_s$.

**B. Convolutionless master equations: simple examples**

As noted before, the operator $O(t, s, z^*)$ appearing in (14) is generally dependent on the noise $z^*$, so there is no general recipe how to derive the corresponding master equation (see our approach in Sec. IV). Before proceeding to our main task, in what follows, we review a few examples where either the operator $O(t, s, z^*)$ according to (14) may be approximated by a noise-independent operator $\hat{O}(t)$ or the exact $O(t, s, z^*)$ does not contain the noise $z^*_s$. In both these cases, the corresponding convolutionless master equation (36) is valid.

1. **Weak coupling**

In many interesting cases, the assumption that the interaction between system and environment is weak is a good approximation. The action of the functional derivative in (16) may be systematically expanded in powers of the interaction $H_{\text{int}}$ [22, 24, 52, 53],

$$O(t, s, z^*) = \sum_{n=0}^{\infty} g^n O_n(t, s, z^*)$$

where $g$ represents the coupling strength. To lowest order, one finds

$$\delta \psi_t(z^*)/\delta z^*_s = \left[ e^{-iH(t-s)/\hbar} L e^{iH(t-s)/\hbar} + \ldots \right] \psi_t(z^*)$$

and thus in this lowest order the operator

$$O(t, s, z^*) \approx O_0(t, s, z^*) = O_0(t, s) = e^{-iH(t-s)/\hbar} L e^{iH(t-s)/\hbar},$$

independent of the noise. The relevant time-integrated expression reads

$$\tilde{O}(t) \approx \tilde{O}_0(t) = \int_0^t ds \ a(s) e^{-iHs/\hbar} L e^{iHs/\hbar},$$

and enters the master equation (36) for the ensemble evolution. Indeed, the resulting equation is nothing but the weak coupling so-called “Redfield” master equation [17, 52], including an “initial slip” captured by the initial time dependence of $\tilde{O}(t)$. A weak coupling stochastic Schrödinger equation equivalent to (21) (with replacement (40)) was derived in [52] in a formulation that kept the memory integral over the bath correlation function. The convolutionless formulation (21) is easier to handle, as there is no need to store the state vector $\psi_s(z^*)$ at earlier times $s < t$. 

2. Near Markov

If the bath correlation function \( \alpha(t-s) \) falls off rapidly under the memory integral in (45), an expansion of the functional derivative in terms of the time delay \( (t-s) \) is sensible \[22, 23, 50\]. With \( A_n(t) = \int_0^t ds \ s^n \alpha(s) \) and \( n = 0, 1, 2, \ldots \), we find for the relevant integrated operator \[20\] to first order,

\[
\hat{O}(t) \approx A_0(t) L + A_1(t) \left( \frac{-i}{\hbar} [H, L] + A_0(t) [L, L^\dagger] L \right),
\]

(41)

neglecting contributions \( A_n(t) \) with \( n \geq 2 \). Once again, to the order accepted, we see the operator \( O(t, s, z^*) \) turns out to be independent of the noise \( z^* \) and the master equation \[36\] immediately applies (see also \[50\]).

Of particular interest is the standard Markov limit: the correlation function may be replaced by a delta function, \( \alpha(t-s) = \gamma \delta(t-s) \), with some constant \( \gamma \). The only relevant term in \[41\] is the \( A_0 \)-term which may be replaced by the constant \( \hat{O} = \frac{\gamma}{2} L \). As noted earlier, the stochastic Schrödinger equation \[21\] (and thus, \[15\]) reduces to the linear version of the Markov quantum state diffusion equation \[8\]. Correspondingly, the master equation \[36\] is nothing but Lindblad’s equation \[2\]. The next order \( A_1 \)-term in expansion \[41\] turns out to be relevant for the high temperature limit of the quantum Brownian motion model \[23\] and quite generally leads to a theory of “post-Markov” evolution \[50\].

We remark that very often, Markov and weak coupling approximation are only meaningful in combination, referred to as \textit{Born-Markov} approximation.

3. Soluble models

For some choices of system Hamiltonian \( H \) and coupling operator \( L \) in the interaction Hamiltonian \[6\], the functional derivative may be replaced by an operator \( O(t, s, z^*) \) without any approximation \[18\]. Two examples are mentioned, where the \( O \)-operator turns out independent of the noise \( z^* \). The third, more complicated case of Brownian motion of a harmonic oscillator will be the subject of the following Sections.

The first simple example is an harmonic oscillator with \( H = \Omega \sigma_z a \), coupled to the environment through a rotating-wave-type coupling, \( L = a \) in the total Hamiltonian \[5\]. It turns out \[18\] that the functional derivative in \[10\] may be replaced by an operator \( O(t, s) \) being proportional to the annihilation operator without any approximation,

\[
O(t, s) = \frac{c(s)}{c(t)} a.
\]

(42)

Here, \( c(t) \) is a complex function satisfying the equation of motion

\[
\dot{c}(t) + i \Omega c(t) + \int_0^t ds \ \alpha(t-s) c(s) = 0,
\]

(43)

involving the bath correlation function. We recognize the damped motion of the amplitude of the oscillator. The integrated operator \( \hat{O}(t) \) thus becomes

\[
\hat{O}(t) = C(t) a
\]

(44)

without any approximation, where \( C(t) = \int_0^t ds \ c(s) \alpha(t-s)/c(t) \). The resulting exact convolutionless master equation \[54\] thus follows from the general expression \[36\]:

\[
\dot{\rho}_t = -i [\Omega^\dagger a, \rho_t] + C^*(t) [a, \rho_t a^\dagger] + C(t) [a \rho_t, a^\dagger]
= -i [\Omega + \text{Im} \{C(t)\}] a^\dagger a, \rho_t] + \text{Re} \{C(t)\} \ ( [a, \rho_t a^\dagger] + [a \rho_t, a^\dagger])
\]

(45)

A similar result may be derived for a damped two-level system with Hamiltonian \( H = \Omega \sigma_z /2 \) and the rotating-wave type coupling \( L = \sigma_- \) \[18\]. Similar to the case of the damped (rotating-wave) harmonic oscillator above, one finds

\[
O(t, s) = \frac{c(s)}{c(t)} \sigma_-
\]

(46)

with the very same function \( c(t) \) from \[43\]. Thus, an exact convolutionless master equation \[36\] of a form similar to \[45\] follows, with \( a \) replaced by \( \sigma_- \) in the non-unitary part of the evolution equation.
To summarize, in all the cases presented in this subsection it is possible to replace the functional derivative in (10) by an operator $O(t, s)$ that is independent of the noise $z^*_t$. In such cases, the ensemble mean follows the convolutionless master equation (36). In the weak coupling case with $O(t)$ from (39), for instance, we recover the so-called Redfield master equation (42) or (46), equation (36) is the exact convolutionless master equation. In these latter cases, asymptotically for large $t$, when the time dependent function $C(t)$ approaches a constant, the exact master equation turns into one of the Lindblad class (2). In the following Sections we discuss yet another exactly soluble case, where the convolutionless master equation is more involved due to the dependence of the operator $O(t, s, z^*)$ in (10) on the noise $z^*_t$.

IV. QUANTUM BROWNIAN MOTION

A. Brownian motion model

Brownian motion of a harmonically bound particle may be obtained from the Hamiltonian

$$H_{\text{tot}} = \left(\frac{p^2}{2M} + \frac{1}{2} M \Omega^2 q^2\right) + q \sum_{\lambda} G_\lambda q_\lambda + \sum_{\lambda} \left\{ \frac{p^2_{\lambda}}{2m_\lambda} + \frac{1}{2} m_\lambda \omega_\lambda^2 q^2_{\lambda} \right\}$$

(47)

of an oscillator with mass $M$ and frequency $\Omega$, coupled to an environment of harmonic oscillators through its position $q$ (28, 31, 32, 33). In this form, the usual “counterterm” arising from the coupling should be understood to be included in the harmonic potential, see (6) for more details.

The Brownian motion Hamiltonian (47) is of the form (15) and thus may be treated with our stochastic approach to open quantum systems. With $q_\lambda = \sqrt{\frac{\hbar}{2m_\lambda \omega_\lambda}} (b_\lambda + b^\dagger_\lambda)$ we identify the quantities entering the basic Hamiltonian (15) to be $g_\lambda = G_\lambda \sqrt{\frac{\hbar}{2m_\lambda \omega_\lambda}}$ and the coupling operator is $L = L^\dagger = q/\hbar$. The system Hamiltonian is the harmonic

$$H = \frac{p^2}{2M} + \frac{1}{2} M \Omega^2 q^2.$$

(48)

For the quantum bath correlation function (19) of this model at temperature $T$ one finds the force-force correlation

$$\alpha(t-s) = \langle (B(t) + B^\dagger(t))(B(s) + B^\dagger(s)) \rangle_{\text{env}}$$

$$= \sum_{\lambda} \frac{\hbar G_\lambda^2}{2m_\lambda \omega_\lambda} \left[ \coth \left( \frac{\hbar \omega_\lambda}{2k_B T} \right) \cos \omega_\lambda(t-s) - i \sin \omega_\lambda(t-s) \right].$$

(49)

Introducing a spectral density of bath oscillators

$$J(\omega) = \sum_{\lambda} \frac{G_\lambda^2}{2m_\lambda \omega_\lambda} \delta(\omega - \omega_\lambda)$$

(50)

one usually writes

$$\alpha(t-s) = \hbar \int_0^\infty d\omega J(\omega) \left[ \coth \left( \frac{\hbar \omega}{2k_B T} \right) \cos \omega(t-s) - i \sin \omega(t-s) \right].$$

(51)

Often the so-called Ohmic case is chosen with $J(\omega) = M \gamma \omega f_\omega(\omega/\Lambda)$ with some cutoff function $f_\omega(x)$, e.g. $f_\omega(x) \simeq e^{-x}$ and $\Lambda$ a cutoff frequency. We stress, however, that the following results are valid for any spectral density $J(\omega)$.

B. Master equation

It is well known that the model (17) allows the derivation of an exact convolutionless master equation for the reduced density operator (34, 36, 37). It may be written in the form

$$\dot{\rho}_t = \frac{1}{i\hbar} [H, \rho_t] + \frac{a(t)}{2i\hbar} [q^2, \rho_t] + \frac{b(t)}{2i\hbar} q, [p, \rho_t] + \frac{c(t)}{\hbar^2} [q, [q, \rho_t]] - \frac{d(t)}{\hbar^2} [q, [q, \rho_t]]$$

(52)
with real time dependent coefficients $a(t), b(t), c(t)$ and $d(t)$. The physical meaning of these terms (drift terms $a(t)$ (frequency renormalization), $b(t)$ (damping term) and diffusion terms $c(t), d(t)$) becomes apparent from the Wigner representation of equation \((52)\), for which the reader is referred to the literature \cite{31, 32, 34, 35, 36, 37, 38}. In \cite{34} the derivation of \((52)\) was based on the generator of the time evolution, while in \cite{37, 38}, the authors used path integrals. In Section V we show how the master equation \((52)\) follows directly from the stochastic Schrödinger equation which we discuss next.

\section*{C. Stochastic Schrödinger equation}

Our stochastic Schrödinger equation approach allows a rigorous treatment of model \cite{37}. The replacement of the functional derivative with an operator $O(t, s, z^*)$ in \cite{10} can be established without any approximation, and thus a convolutionless exact stochastic Schrödinger equation \((21)\) may be found. Here, however, we have to allow for an explicit noise dependence. It turns out \cite{15} that the ansatz

\begin{equation}
O(t, s, z^*) = \frac{1}{\hbar} \left( f(t, s) q + \frac{1}{M \Omega} g(t, s) p - i \frac{\partial}{\partial s} \int_0^t ds' j(t, s, s') z^*_s \right),
\end{equation}

with complex functions $f(t, s), g(t, s)$, and $j(t, s, s')$ to be determined is a solution of the general evolution equation \cite{14}. We learn from this example that in general, the functional derivative in \cite{14} may indeed introduce a dependence on the whole history of the noise $z^*_s$.

The functions $f(t, s), g(t, s)$ and $j(t, s, s')$ in \cite{15} have to satisfy the evolution equations

\begin{equation}
\begin{aligned}
\partial_t f(t, s) &= \Omega g(t, s) - 2i g(t, s) F(t) + i f(t, s) G(t) + i J(t, s), \\
\partial_t g(t, s) &= -\Omega f(t, s) - i g(t, s) G(t), \quad \text{and} \\
\partial_j j(t, s, s') &= -i g(t, s) J(t, s, s'),
\end{aligned}
\end{equation}

where we introduced the integrated functions

\begin{equation}
\begin{aligned}
F(t) &= \frac{1}{M \Omega \hbar} \int_0^t ds \alpha(t - s) f(t, s), \\
G(t) &= \frac{1}{M \Omega \hbar} \int_0^t ds \alpha(t - s) g(t, s), \quad \text{and} \\
J(t, s') &= \frac{1}{M \Omega \hbar} \int_0^t ds \alpha(t - s) j(t, s, s').
\end{aligned}
\end{equation}

While $f, g$, and $j$ are dimensionless complex functions, the integrated expressions $F, G$, and $J$ are defined such as to have dimension inverse time: typically, these latter functions turn out to be proportional to a damping rate $\gamma$. The evolution equations \cite{51} have to be solved with boundary conditions

\begin{equation}
\begin{aligned}
f(t = s, s) &= 1, \quad g(t = s, s) = 0, \quad j(t = s, s, s') = 0, \quad \text{and} \\
j(t = s, s', s) &= -g(s, s'),
\end{aligned}
\end{equation}

for all $s$ and $s'$. The first three conditions arise from the initial condition \cite{18} for the operator $O(t, s, z^*) = L = q/\hbar$, the last condition arising from the solution of \cite{19}. The relevant integrated operator \cite{20} turns out to be

\begin{equation}
\tilde{O}(t, z^*) = M \Omega F(t) q + G(t) p - i \int_0^t ds J(t, s) z^*_s
\end{equation}

with time dependent coefficients from \cite{51}.

The resulting linear, convolutionless non-Markovian stochastic Schrödinger equation \cite{21} for the Brownian motion of a harmonic oscillator \cite{48} with a coupling to the environment through position $L = q/\hbar$ thus reads

\begin{equation}
\begin{aligned}
\hbar \partial_t \psi_t &= -i \hbar \psi_t + q \left( z^*_t - \tilde{O}(t, z^*) \right) \psi_t \\
&= -i \hbar \psi_t + q \left( z^*_t - M \Omega F(t) q - G(t) p + i \int_0^t ds J(t, s) z^*_s \right) \psi_t.
\end{aligned}
\end{equation}

The process $z^*_t$ is a complex Gaussian process with the finite temperature correlation function $\alpha(t - s)$ from \cite{51}. Just like the exact master equation \cite{52}, the exact stochastic NMQSD equation \cite{53} is valid for arbitrary bath correlation...
function $\alpha(t - s)$, and thus for any temperature, environmental spectral density, or coupling strength between the harmonic oscillator and its environment.

This example demonstrates clearly that the evolution of quantum trajectories $\psi_t(z^*)$ may indeed depend on the whole history of the noise. Simulations of the Brownian motion model discussed here may be found in [55].

From our construction, it is clear that the ensemble of quantum trajectories of the exact equation (58) evolves according to the exact master equation (52). In the next Section [11] we set out to establish this connection directly.

As $\mathcal{O}(t, z^*)$ depends on the noise, the simple result (56) for the evolution of the reduced density operator $\rho_t$ is not applicable, and further effort is required. As a first step, we show in the next Section how a Heisenberg operator approach helps to gain more insight into result [52] for the operator $\mathcal{O}(t, s, z^*)$ replacing the functional derivative.

## D. Heisenberg method

Major clarification is achieved once we investigate the dependence of the functions $f(t, s)$, $g(t, s)$, and $j(t, s, s')$ in [31] on $s$ rather than $t$. The key step arises from the Heisenberg operator approach as explained in Section (II D) see also [24]. Here, the challenge is to find a suitable expression for

$$Q(s) \equiv \langle z|U_t q(s)|0\rangle = \hbar O(t, s, z^*) \langle z|U_t|0\rangle,$$

similar to expressions (31) and (32). Clearly, $Q(s)$ depends on the time $t$, but we here regard it as a function of $s$ and thus may investigate the $s$-dependence of the desired operator $\mathcal{O}(t, s, z^*)$. Not surprisingly, the Heisenberg equation of motion for $q(s)$ leads to $\partial_s Q(s) = \langle z|U_t \partial_s q(s)|0\rangle = \frac{\hbar}{M} \langle z|U_t p(s)|0\rangle$ and therefore we investigate the second order derivative. Note that required final values are

$$Q(s = t) = \langle z|U_t|0\rangle$$

For the second order derivative we find from (47) with $g = \lambda$ with $\lambda = \sqrt{\frac{\hbar}{2m\omega_\lambda}} G_\lambda$

$$\partial^2_s Q(s) = -\Omega^2 Q(s) - \frac{1}{M} \sum_\lambda \lambda e^{-i\omega_\lambda s} \langle z|U_t b_\lambda(s)|0\rangle + \frac{1}{M} \sum_\lambda \lambda e^{i\omega_\lambda s} \langle z|U_t b_\lambda^\dagger(s)|0\rangle.$$

As before in Section (II D), integrating the Heisenberg equation of motion for the environmental annihilation operator $b_\lambda(s)$, we see that

$$\langle z|U_t a_\lambda(s)|0\rangle = \frac{i}{\hbar} g_\lambda \int_0^s ds' e^{i\omega_\lambda s'} \langle z|U_t q(s')|0\rangle,$$

where use is made of the fact that the initial $b_\lambda(0)|0\rangle = b_\lambda|0\rangle = 0$.

The adjoint $b_\lambda^\dagger(s)$ in (61) is dealt with in similar fashion. Here, however, we make use of the fact that at the final time $t$ the overall expression becomes simple: $\langle z|U_t b_\lambda^\dagger(t)|0\rangle = z_\lambda^* \langle z|U_t|0\rangle$. Thus, we integrate the Heisenberg equation of motion for $b_\lambda^\dagger(s)$ given the final value at $s = t$ to get $b_\lambda^\dagger(s) = b_\lambda^\dagger(t) - \frac{i}{\hbar} g_\lambda \int_s^t ds' e^{-i\omega_\lambda s'} q(s')$, and find

$$\langle z|U_t b_\lambda^\dagger(s)|0\rangle = z_\lambda^* \langle z|U_t|0\rangle - \frac{i}{\hbar} g_\lambda \int_s^t ds' e^{-i\omega_\lambda s'} \langle z|U_t q(s')|0\rangle.$$

All that remains to be done is combining the results (61), (62), and (63) to obtain a linear second order differential equation for $Q(s)$:

$$\partial^2_s Q(s) + \Omega^2 Q(s) - \frac{i}{M \hbar} \int_0^s ds' \alpha(s - s') Q(s') - \frac{i}{M \hbar} \int_s^t ds' \alpha(s' - s) Q(s') = -\frac{i}{M} z_\lambda^* \langle z|U_t|0\rangle,$$

for $s \in [0, t]$ with a fixed final time $t$, and final values (60).

With expression (63), the derived second order differential equation for $Q(s)$ translates into an equation for the desired operator $\mathcal{O}(t, s, z^*)$. Considered as a function of the time $s$, at fixed $t$, we find

$$\partial^2_s \mathcal{O}(t, s, z^*) + \Omega^2 \mathcal{O}(t, s, z^*) - \frac{i}{M \hbar} \int_0^s ds' \alpha(s - s') \mathcal{O}(t, s', z^*) - \frac{i}{M \hbar} \int_s^t ds' \alpha(s' - s) \mathcal{O}(t, s', z^*) = -\frac{i}{M \hbar} z_\lambda^* \langle z|U_t|0\rangle.$$
with final values from (60)

\[ O(t, s = t, z^*) = \frac{1}{\hbar} \Phi_t, \quad \text{and} \quad \partial_s O(t, s, z^*)|_{s=t} = \frac{1}{M\hbar} p. \]  

(66)

As before in (53), we write the operator \( O(t, s, z^*) \) in the form

\[ O(t, s, z^*) = \frac{1}{\hbar} \left( \phi_t(s)q + \frac{1}{M\Omega} \phi_t(s)p - \frac{i}{M\Omega} \int_0^t ds' \chi_t(s, s')z_{s'}^* \right), \]  

(67)

where we introduced three \( s \)-dependent complex functions \( \phi_t(s), \psi_t(s) \) and \( \chi_t(s, s') \) at a fixed time \( t \). Obviously, from (65), the first two of them satisfy the homogeneous equation

\[ \partial_s^2 \phi_t(s) + \Omega^2 \phi_t(s) - \frac{i}{M\hbar} \int_0^s ds'' \alpha(s-s'')\phi_t(s'') - \frac{i}{M\hbar} \int_s^t ds'' \alpha(s''-s)\phi_t(s'') = 0. \]  

(68)

While for \( \phi_t \) we demand the final values

\[ \phi_t(s = t) = 1 \quad \text{and} \quad \partial_s \phi_t(s)|_{s=t} = 0 \]  

(69)

to satisfy (68), \( \psi_t(s) \) has final values

\[ \psi_t(s = t) = 0 \quad \text{and} \quad \partial_s \psi_t(s)|_{s=t} = \Omega. \]  

(70)

The function \( \chi_t(s, s') \) in (67) is nothing but Green’s function that satisfies

\[ \partial_s^2 \chi_t(s, s') + \Omega^2 \chi_t(s, s') - \frac{i}{M\hbar} \int_0^s ds'' \alpha(s-s'')\chi_t(s'', s') - \frac{i}{M\hbar} \int_s^t ds'' \alpha(s''-s)\chi_t(s'', s') = \Omega \delta(s-s') \]  

(71)

with final values

\[ \chi_t(s = t, s') = 0 \quad \text{and} \quad \partial_s \chi_t(s, s')|_{s=t} = 0 \]  

(72)

for all \( s' \in [0, t] \).

The result (67) for the operator \( O(t, s, z^*) \) reflects our ansatz (53) that solved evolution equation (19) with respect to \( t \). Clearly, we identify the functions \( f(t, s) = \phi_t(s), g(t, s) = \psi_t(s), \) and \( j(t, s, s') = \chi_t(s, s') \). All conditions (50) on the functions \( f, g, j \) are met by (69), (70), and (72). One may even derive their evolution equations (54) regarded as a function of \( t \) from the corresponding evolution equations (55) and (56), when considered as functions of \( s \), see appendix A for an example. For numerical applications as in (55), the evolution equations with respect to \( t \) are the ones of interest. In order to derive the convolutionless master equation for this quantum Brownian motion model, however, it turns out that the evolution equation of \( O(t, s, z^*) \) with respect to \( s \) from (67) is the right starting point, as will be explained in the next section.

V. QB M MASTER EQUATION

In the last Section we have established the evolution equation with respect to \( s \) for the operator \( O(t, s, z^*) \) entering the exact convolutionless stochastic Schrödinger equation (65). We are now in the position to derive the corresponding convolutionless master equation from the general expression (59).

\[ \partial_t \rho_t = -\frac{i}{\hbar} [H, \rho_t] + \frac{1}{\hbar}[q, \mathcal{M} \{ P_t \hat{O}^\dagger (t, z^*) \}] + \frac{1}{\hbar}[\mathcal{M} \{ \hat{O}(t, z^*) P_t \}, q] \]  

(73)

which for the Quantum Brownian motion case we display here with coupling operator \( L = q/\hbar \).

We saw previously how knowledge about the operator \( O(t, s, z^*) \) replacing the functional derivative in our stochastic Schrödinger equation, puts us in a position to derive a closed convolutionless master equation. In particular, as soon as the operator \( O(t, s, z^*) \) is independent of the noise, we get \( \mathcal{M} \{ \hat{O}(t) P_t \} = \hat{O}(t) \rho_t \) and (50) provides the convolutionless master equation (56) for \( \rho_t \). In our current example, however, \( \hat{O}(t, z^*) \) does depend on the noise and we show next how to proceed in this case.
Starting point is the evolution equation \([56]\) for the operator \(O(t, s, z^*)\) as a function of \(s\). For the master equation \([73]\), we need an expression for the ensemble mean
\[
\mathcal{M}\left\{ \tilde{O}(t, z^*)P_t \right\} = \int_0^t ds \alpha(t - s) \mathcal{M}\{O(t, s, z^*)P_t\} = \int_0^t ds \alpha(t - s) R(t, s)
\]
with
\[
R(t, s) = \mathcal{M}\{O(t, s, z^*)P_t\}.
\]

Upon taking the mean \(\mathcal{M}\{\ldots P_t\}\) of equation \([56]\), we see from its definition \([75]\) that \(R(t, s)\) satisfies the second order differential equation
\[
\frac{\partial^2}{\partial t^2} R(t, s) + \Omega^2 R(t, s) - \frac{i}{\hbar} \int_s^t ds' \alpha(s - s') R(t, s') = \frac{1}{\hbar} \mathcal{M}\{z^*_s P_t\}.
\]

Next we have to find an expression for \(\mathcal{M}\{z^*_s P_t\}\), which again follows from Novikov’s theorem \([51]\) as in \([84]\). We may express the resulting functional derivative in terms of the operator \(O(t, s, z^*)\) and get
\[
\mathcal{M}\{z^*_s P_t\} = \int_0^t ds' \alpha^*(s - s') \mathcal{M}\{P_t O(t, s, z^*)\} = \int_0^t ds' \alpha^*(s - s') R^1(t, s').
\]

A closed equation for the operator \(R(t, s)\) as a function of \(s\) results:
\[
\frac{\partial^2}{\partial t^2} R(t, s) + \Omega^2 R(t, s) - \frac{i}{\hbar} \int_s^t ds' \alpha(s - s') R(t, s') \]
\[
- \frac{i}{\hbar} \int_s^t ds' \alpha(s' - s) R(t, s') = \frac{1}{\hbar} \mathcal{M}\{r_0(t, s, z^*)\}.
\]

Required final values are
\[
R(t, s = t) = \frac{1}{\hbar} q \rho_t, \quad \text{and} \quad \partial_s R(t, s)|_{s=t} = \frac{1}{\hbar} \rho_t,
\]
as one can easily see from \([60]\).

In fact, it is clear that equation \([78]\) with final values \([80]\) may be satisfied by an expression of the form
\[
R(t, s) = \frac{1}{\hbar} \left\{ k(t, s) q \rho_t + \frac{1}{\Omega} \ell(t, s) \rho_t + m(t, s) \rho_t \rho + \frac{1}{\Omega} n(t, s) \rho p \right\},
\]
where \(k(t, s), \ell(t, s), m(t, s),\) and \(n(t, s)\) are complex functions whose \(s\)-dependence follows from equation \([78]\) with appropriate final values at \(s = t\) from \([79]\). As an example, we get \(k(t, s = t) = 1\) and \(\partial_s k(t, s)|_{s=t} = 0.\) In Appendix \([13]\) we show how to determine all four functions.

Now that we know \(R(t, s) = \mathcal{M}\{O(t, s, z^*)P_t\}\) from \([80]\), the closed master equation for the reduced density operator follows immediately from the general expression \([78]\) with \([74]\). After some rearrangements, we indeed arrive at the more familiar form \([92]\), with time dependent coefficients
\[
a(t) = \frac{2}{\hbar} \text{Im} \left( \int_0^t ds \alpha(t - s) (k(t, s) + m(t, s)) \right)
\]
\[
b(t) = \frac{2}{\hbar \Omega} \text{Im} \left( \int_0^t ds \alpha(t - s) (\ell(t, s) + n(t, s)) \right)
\]
\[
c(t) = \frac{1}{\Omega} \text{Re} \left( \int_0^t ds \alpha(t - s) (n(t, s) - \ell(t, s)) \right)
\]
\[
d(t) = \text{Re} \left( \int_0^t ds \alpha(t - s) (k(t, s) - m(t, s)) \right)
\]

In appendix \([13]\) we discuss these expressions in more detail, establishing the connection to earlier derivations of the master equation \([52]\). Crucially, we here show explicitly that it follows from the corresponding convolutionless stochastic Schrödinger equation \([58]\).
VI. CONCLUSION

Exactly soluble models are valuable tools. They allow us to discuss approximation schemes, show the transitions in the qualitative behaviour when parameters are changed over a wide range, and last not least provide insight into different theoretical approaches.

Our non-Markovian stochastic Schrödinger equation approach offers a new method for handling open quantum systems. In this paper we use this framework as a theoretical tool to derive convolutionless non-Markovian master equations. Most interestingly, the exact master equation for quantum Brownian motion of a harmonic oscillator, coupled to a bath of oscillators is derived from the corresponding convolutionless non-Markovian stochastic Schrödinger equation. In both approaches, non-Markovian properties are encoded in time-dependent coefficients.

The problem how to describe non-Markovian open quantum system dynamics efficiently is a difficult one. As further underlined in this papers, we believe that our non-Markovian stochastic Schrödinger equation approach offers a useful alternative framework to the existing ones.

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APPENDIX A: EVOLUTION EQUATION WITH RESPECT TO TIME t

It is interesting to see the connection between the evolution equations [63] with respect to t for \( f(t,s) = \phi_t(s), g(t,s) = \psi_t(s) \) and \( j(t,s,s') = \chi_t(s,s') \) and the differential equations [65] and [70] for the same functions with respect to s. In fact, here we show how to derive the former from the latter.

Consider \( g(t,s) = \psi_t(s) \) as an example. We showed in Section 14.2 that this function solves [65] which we here display again for convenience:

\[
\partial^2_s \psi_t(s) + \Omega^2 \psi_t(s) - i \frac{\hbar}{\Delta} \int_0^t ds'' \alpha(s - s'') \psi_t(s'') - i \frac{\hbar}{\Delta} \int_s^t ds'' \alpha(s'' - s) \psi_t(s'') = 0. \tag{A1}
\]

Taking the time derivative of this equation with respect to t, and using the final condition \( \psi_t(s = t) = 0 \) from [70], we find that \( \partial_t \psi_t(s) \) satisfies the very same equation [A1]. Therefore, as \( \{ \phi_t(s), \psi_t(s) \} \) forms a basis of solutions, there exists a relation of the form

\[
\partial_t \psi_t(s) = c_1(t) \phi_t(s) + c_2(t) \psi_t(s) \tag{A2}
\]

with suitable coefficients \( c_1(t) \) and \( c_2(t) \). These have to be determined from the final values at \( s = t \). From [63] and [70] we get

\[
c_1(t) = \partial_t \psi_t(s = t) \tag{A3}
\]

\[
c_2(t) = \frac{1}{\Omega} \partial_t \partial_s \psi_t(s) \bigg|_{s=t}.
\]

These expressions are easily evaluated: first, from \( \psi_t(s = t) = 0 \), we get \( \partial_t \psi_t(s = t) + \partial_s \psi_t(s)|_{s=t} = 0 \) and thus \( c_1(t) = -\partial_s \psi_t(s)|_{s=t} = -\Omega \) according to [70]. Secondly, we use the trivial identity

\[
\partial_s \psi_t(s) = \partial_s \psi_t(s)|_{s=t} - \int_s^t ds'' \left( \partial^2_s \psi_t(s)|_{s=s''} \right) \tag{A4}
\]

\[
= \Omega - \int_s^t ds'' \left( \partial^2_s \psi_t(s)|_{s=s''} \right).
\]
Take the derivative with respect to $t$ and then set $s = t$ to find

$$
\left. \partial_t \partial_s \psi_t(s) \right|_{s=t} = -\partial^2_s \psi_t(s) \bigg|_{s=t} = \Omega^2 \psi_t(s = t) - \frac{i}{M\hbar} \int_0^t ds'' \alpha(t - s'') \psi_t(s'') \\
= -\frac{i}{M\hbar} \int_0^t ds'' \alpha(t - s'') \psi_t(s''),
$$

where use is made of the evolution equation (A1) and the condition (C0). Thus, with (A3), $c_2(t) = -\frac{i}{M\hbar} \int_0^t ds'' \alpha(t - s'') \psi_t(s'')$ which may be written as $c_2(t) = -iG(t)$ using definition (C3). We see that with $c_1(t) = -\Omega$ and $c_2(t) = -iG(t)$, relation (A2) is nothing but the evolution equation for $\psi_t(s) = g(t, s)$ in (B4) as derived from the “consistency condition” (C1).

**APPENDIX B: TIME DEPENDENT COEFFICIENTS**

From the second order differential equation (18) for the operator $R(t, s)$ which we here display again for convenience,

$$
R(t, s) = \frac{1}{\hbar} \left\{ k(t, s)\rho_\ell + \frac{1}{M\Omega} \ell(t, s)p_\rho + m(t, s)\rho_\ell q + \frac{1}{M\Omega} n(t, s)\rho_\ell p \right\},
$$

we get (coupled) differential equations for the coefficients $k(t, s)$, $\ell(t, s)$, $m(t, s)$, and $n(t, s)$ as functions of $s$. The final values at $s = t$ for all four functions are determined from the conditions (C3) on $R(t, s)$.

It turns out useful to replace the four unknown functions by the linear combinations appearing in the final result (B1), which we define as

$$
w(t, s) \equiv k(t, s) + m(t, s) \quad (B2)
$$
$$
x(t, s) \equiv \ell(t, s) + n(t, s) \quad (B3)
$$
$$
y(t, s) \equiv k(t, s) - m(t, s) \quad (B3)
$$
$$
z(t, s) \equiv n(t, s) - \ell(t, s)
$$

They all satisfy uncoupled second order differential equations. For $w(t, s)$ we find from (18)

$$
\partial^2_s w(t, s) + \Omega^2 w(t, s) - \frac{i}{M\hbar} \int_0^s ds' \alpha(s - s')w(t, s')
\quad - \frac{i}{M\hbar} \int_s^t ds' \alpha(s' - s)w(t, s') = -\frac{i}{M\hbar} \int_0^t ds' \alpha(s' - s)w^*(s'),
$$

and the identical equation for $x(t, s)$. Required final values are

$$
w(t, s = t) = 1, \quad \partial_s w(t, s)|_{s=t} = 0 \quad (B4)
$$
$$
x(t, s = t) = 0, \quad \partial_s x(t, s)|_{s=t} = \Omega.
$$

For $y(t, s)$ (and also $z(t, s)$) we get a similar equation with a different sign on the right hand side:

$$
\partial^2_s y(t, s) + \Omega^2 y(t, s) - \frac{i}{M\hbar} \int_0^s ds' \alpha(s - s')y(t, s')
\quad - \frac{i}{M\hbar} \int_s^t ds' \alpha(s' - s)y(t, s') = \frac{i}{M\hbar} \int_0^t ds' \alpha(s' - s)y^*(s'),
$$

here with final values

$$
y(t, s = t) = 1, \quad \partial_s y(t, s)|_{s=t} = 0 \quad (B6)
$$
$$
z(t, s = t) = 0, \quad \partial_s z(t, s)|_{s=t} = -\Omega.
$$

It turns out that matters simplify once we separate real- and imaginary parts of the four functions $w, x, y, z$. For the bath correlation function we write

$$
\alpha(t - s) = \nu(t - s) + i\hbar\eta(t - s). \quad (B7)
$$
Thus, microscopically, from its definition (12) we have
\[ \eta(t - s) = - \sum_{\lambda} \frac{G_{\lambda}^2}{2m_\lambda \omega_{\lambda}} \sin \omega_{\lambda}(t - s) = - \int_0^\infty d\omega J(\omega) \sin \omega(t - s). \] (B8)

This kernel turns out to be crucial for the classical equation of motion of the underlying model (17), as will be clarified shortly.

For the imaginary part of \( w(t,s) \) we get from (18)
\[ \partial_x^2 w_I(t,s) + \Omega^2 w_I(t,s) + \frac{2}{M} \int_s^t ds' \eta(s - s')w_I(t,s') = 0 \] (B9)
and the very same equation for the imaginary part of \( x(t,s) \). With final values \( w_I(t,t) = 0, \partial_s w_I(t,s)|_{s=t} = 0 \) and \( x_I(t,t) = 0, \partial_s x_I(t,s)|_{s=t} = 0 \) the solutions are trivial:
\[ w_I(t,s) \equiv 0 \text{ for all } s \]
\[ x_I(t,s) \equiv 0 \text{ for all } s. \] (B10)

Next we consider the real parts \( w_R(t,s), x_R(t,s) \). With (14) and (18) we arrive at
\[ \partial_x^2 w_R(t,s) + \Omega^2 w_R(t,s) + \frac{2}{M} \int_s^t ds' \eta(s - s')w_R(t,s') = 0 \] (B11)
and the same equation for \( x_R(t,s) \). Required final values are
\[ w_R(t,s = t) = 1, \quad \partial_s w_R(t,s)|_{s=t} = 0 \]
\[ x_R(t,s = t) = 0, \quad \partial_s x_R(t,s)|_{s=t} = \Omega. \] (B12)

Similarly, we find for the real and imaginary part of the function \( y(t,s) \) the following equations:
\[ \partial_x^2 y_R(t,s) + \Omega^2 y_R(t,s) + \frac{2}{M} \int_s^t ds' \eta(s' - s)y_R(t,s') = 0 \] (B13)
\[ \partial_x^2 y_I(t,s) + \Omega^2 y_I(t,s) + \frac{2}{M} \int_s^t ds' \eta(s - s')y_I(t,s') = \frac{2}{Mr} \int_s^t ds' \nu(s - s')y_R(t,s'). \]

As before, real and imaginary part of \( z(t,s) \) satisfy the same equations. Required “final values” are
\[ y_R(t,t) = 1, \quad \partial_s y_R(t,s)|_{s=t} = 0 \]
\[ y_I(t,t) = 0, \quad \partial_s y_I(t,s)|_{s=t} = 0 \]
\[ z_R(t,t) = 0, \quad \partial_s z_R(t,s)|_{s=t} = -\Omega \]
\[ z_I(t,t) = 0, \quad \partial_s z_I(t,s)|_{s=t} = 0. \] (B14)

The real parts of all four functions may nicely be expressed using the special solution \( q(s) \) of equation (13),
\[ \partial_x^2 q(s) + \Omega^2 q(s) + \frac{2}{M} \int_s^s ds' \eta(s - s')q(s') = 0 \] (B15)
with initial values
\[ q(0) = 0, \quad \partial_s q(s)|_{s=0} = \Omega. \] (B16)

Equation (B15) is nothing but the classical equation of motion for the position \( q(s) \) of the underlying model (17), provided the environmental oscillators all start with initial values \( q\lambda(0) = 0, \quad \dot{q}\lambda(0) = 0 \). Note that \( q(s) \) satisfies the same equation (B15) with \( \dot{q}(0) = \Omega \) and \( \ddot{q}(0) = 0 \).

It is customary to write equation (B15) in the more familiar form
\[ \partial_x^2 q(s) + \Omega^2 q(s) + \int_0^s ds' \gamma_{\text{el}}(s - s') \dddot{q}(s') = 0 \] (B17)
with the classical damping kernel \( \gamma_{cl}(s - s') \) defined through \( \frac{1}{\hbar} \eta(t - s) \equiv \partial_t \gamma_{cl}(t - s) \).

In terms of this classical solution \( q(s) \) simple inspection shows that

\[
w(t, s) = w_R(t, s) = \frac{\dot{q}(s)t - q(s)q(t)}{(\dot{q}(t))^2 - q(t)\dot{q}(t)}, \tag{B18}\]

\[
x(t, s) = x_R(t, s) = \frac{\Omega q(s)t - \dot{q}(s)q(t)}{(\dot{q}(t))^2 - q(t)\dot{q}(t)},
\]

\[
y_R(t, s) = \frac{1}{\Omega} \dot{q}(t - s),
\]

\[
z_R(t, s) = \dot{q}(t - s).
\]

While the imaginary parts of \( w(t, s) \) and \( x(t, s) \) are zero, the expressions for \( y_I(t, s) \) and \( z_I(t, s) \) are more involved. We find

\[
y_I(t, s) = \frac{2}{M \Omega^2 \hbar} \int_0^s ds' \int_0^t ds'' \nu(s' - s'') \dot{q}(t - s'') q(s - s') \tag{B19}\]

\[- \frac{2}{M \Omega^2 \hbar} \int_0^t ds' \int_0^t ds'' \nu(s' - s'') \dot{q}(s'') [w(t, s)q(s') + x(t, s)\dot{q}(s')/\Omega],\]

\[
z_I(t, s) = \frac{2}{M \Omega \hbar} \int_0^s ds' \int_0^t ds'' \nu(s' - s'') q(t - s'') q(s - s') \tag{B19}\]

\[- \frac{2}{M \Omega \hbar} \int_0^t ds' \int_0^t ds'' \nu(s' - s'') q(s'') [w(t, s)q(s') + x(t, s)\dot{q}(s')/\Omega].\]

The first line in each expression is simply the inhomogeneity on the right hand side of equations \( B13 \), in convolution with Green’s function \( q(s - s')/\Omega \). The second lines, respectively, are solutions of the homogeneous equations and serve to satisfy the final conditions \( B14 \).

Finally, let us make contact to earlier derivations of the time dependent coefficients. For brevity we concentrate on the drift coefficients \( a(t) \) and \( b(t) \) in the master equation \( B2 \). As \( w(t, s) \) and \( x(t, s) \) are real, using \( B1 \) and \( B7 \), \( a(t) \) and \( b(t) \) may be written in the form

\[
a(t) = 2 \int_0^t ds \eta(t - s)w_R(t, s) \tag{B20}\]

\[
b(t) = \frac{2}{M \Omega} \int_0^t ds \eta(t - s)x_R(t, s).
\]

With expressions \( B18 \), and using the evolution equation \( B18 \) for both, \( q(s) \) and \( \dot{q}(s) \), we may write the drift coefficients in the form

\[
a(t) = -M\Omega^2 + M \frac{(\dot{q}(t))^2 - \dot{q}(t)\dot{q}(t)}{(\dot{q}(t))^2 - q(t)\dot{q}(t)} \tag{B21}\]

\[
b(t) = \frac{q(t)\dot{q}(t) - \dot{q}(t)\dot{q}(t)}{(\dot{q}(t))^2 - q(t)\dot{q}(t)}.
\]

Expressions similar to these may also be found in the literature \( 34, 37, 59, 40 \).

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