Stochastic Feshbach Projection for the Dynamics of Open Quantum Systems

Valentin Link and Walter T. Strunz
Institut für Theoretische Physik, Technische Universität Dresden, D-01062 Dresden, Germany
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We present a stochastic projection formalism for the description of quantum dynamics in Bosonic or spin environments. The Schrödinger equation in coherent state representation with respect to the environmental degrees of freedom can be reformulated by employing the Feshbach partitioning technique for open quantum systems based on the introduction of suitable non-Hermitian projection operators. In this picture the reduced state of the system can be obtained as a stochastic average over pure state trajectories. The corresponding non-Markovian stochastic Schrödinger equations include a memory integral over the past states. In the case of harmonic environments and linear coupling the approach gives a new form of the established non-Markovian quantum state diffusion (NMQSD) stochastic Schrödinger equation without functional derivatives. Utilizing spin coherent states, the evolution equation for spin environments resembles the Bosonic case with, however, a non-Gaussian average for the reduced density operator.

Introduction.— Fueled by novel applications in the field of quantum information [1, 2], there has been a long-lasting and growing interest in the description of open quantum system dynamics during the last decades [3]. The celebrated Gorini-Kossakowski-Sudarshan-Lindblad equation [4] is a popular tool, mainly due to its simple mathematical structure [5]. However, for this equation to hold one needs to make severe assumptions on the interplay between system and environment, in particular the Markov, or memoryless, approximation. This approximation loses its validity when structured environments or strong system-environment couplings are considered.

Describing non-Markovian open quantum system dynamics is a much more challenging task that inspired the development of several quite distinct theoretical methods [1, 3]. Arguably the most general form of open system evolution equation is the famous Nakajima-Zwanzig master equation [6]. This equation includes memory-effects in the master equation for the reduced density operator $\rho_t$ in the form of an explicit time nonlocal term

$$\partial_t \rho_t = \mathcal{L}_t \rho_t + \int_0^t ds \mathcal{K}_{t,s} \rho_s .$$  

(1)

Here $\mathcal{K}_{t,s}$ is the so-called memory kernel. This equation can be derived microscopically by employing a projection operator technique in the space of Hilbert-space operators. Specifically, one chooses a projector that maps the total state of system and environment onto the reduced system density operator. One is also able to construct a time-convolutionless (TCL) master equation within this formalism [2, 3, 6]. These TCL equations have explicitly time dependent (but time local) generators which are easier to handle than equation (1) with an explicit memory integral. However, non-Markovian TCL master equations may not be well-defined in some cases because they require the existence of a certain operator inverse [6, 10].

The structure of the Nakajima-Zwanzig master equation is very intricate, especially because starting from the form [11], one does not know explicit, general conditions for the memory kernel which ensures that the equation preserves density operators [11]. Recent progress in this topic using special examples can be found in [12]. Approximating the kernel with perturbation theory leads, in general, to loss of positivity [13].

A possible cure for positivity violation are quantum trajectories. The idea is to express the reduced density operator as an average over an ensemble of pure states

$$\rho_t = \mathcal{M}(\langle \psi(z^*) \rangle \langle \psi(z^*) \rangle) ,$$  

(2)

where $\mathcal{M}(\ldots)$ denotes the average with respect to a stochastic variable $z$ such that positivity is guaranteed by construction. A prominent example in the non-Markovian regime is the non-Markovian quantum state diffusion (NMQSD) formalism as introduced in [14]. This theory describes quantum dynamics in environments consisting of Bosonic, harmonic baths with linear coupling to the system. The NMQSD evolution equation for the stochastic pure states $|\psi(z^*)\rangle$ may be quite difficult to solve, since it involves derivatives with respect to the stochastic variable $z$. Nevertheless, the big advantage is that approximations for the stochastic pure states still lead to a reduced density operator $\rho_t$ that is positive by construction, see (2). Apart from their numerical efficiency in applications [15–17], NMQSD and related equations also appear in exactly soluble open quantum system models [18], in non-Markovian generalizations of spontaneous wave function collapse [19], in general Gaussian open quantum system dynamics [20, 21], or in attempts to establish a non-Markovian continuous measurement theory [22, 24].

The aim of this letter is to connect ideas from both, the projection-operator method and the non-Markovian quantum state diffusion formalism thus laying the foundations for a very general non-Markovian quantum trajectory theory well beyond the current status. A Feshbach projection in connection with NMQSD is also used in reference [25], where it is applied within the NMQSD.
formalism. Our results here are very different and more fundamental as we use the projection method to derive a new non-Markovian stochastic evolution equation looking similar to [1]. Remarkably, this new stochastic Schrödinger equation does not involve the problematic functional derivatives of NMQSD. In particular we employ a stochastic variant of the Feshbach projection formalism for open quantum systems that was introduced in reference [26]. In this Feshbach formalism one applies Hilbert space projection operators to the Schrödinger equation of the pure total state of system and environment. One can define creation- and annihilation operators \( z \), which include derivatives with respect to various variables. Most remarkably, with the Feshbach technique we automatically achieve the harmonic Bosonic baths and linear coupling as in NMQSD.

**Stochastic Feshbach projection formalism.** We consider an arbitrary quantum system interacting with an environment consisting of Bosonic modes that need not be harmonic. The total Hilbert space of system and environment is then the product space of the respective subspaces \( \mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_E \). In the environment Hilbert space we can define creation- and annihilation operators \( b_i^\dagger, b_i \) of each mode, satisfying the commutation relation \([b_i, b_j^\dagger] = \delta_{ij}\). Then the Bargmann coherent states \( |z_1 z_2 \ldots \rangle = |z\rangle \) in \( \mathcal{H}_E \) are defined by

\[
|z\rangle = e^{z b_1^\dagger} e^{z^* b_1} \otimes |0\rangle,
\]

where \(|0\rangle\) denotes the vacuum bath state \( b_i |0\rangle = 0 \). The double-bar ket notation is used to emphasize that the Bargmann states are not normalized. These states are analytical in \( z \) and fulfill the completeness relation

\[
1_E = \int \frac{d^2z}{\pi} e^{-|z|^2} |z\rangle \langle z|,
\]

with the integral measure \( \frac{d^2z}{\pi} = \prod_i \frac{d\text{Re} z_i d\text{Im} z_i}{\pi} \). Moreover, coherent states are never orthogonal, their scalar product is

\[
\langle z | z' \rangle = \prod_i e^{z_i z_i'}.
\]

Let \(|\Psi_t\rangle\) be the total state of system and environment satisfying the Schrödinger equation

\[
i \partial_t |\Psi_t\rangle = H(t) |\Psi_t\rangle,
\]

with some completely general Hamiltonian \( H(t) \). As initial condition, for most of the following, we assume a zero temperature bath such that \(|\Psi_0\rangle = |\psi_0\rangle |0\rangle\). Now we switch to the coherent state representation with respect to \( \mathcal{H}_E \), i.e. we consider the states \( \langle z | \Psi_t \rangle \equiv |\psi_t(z^*)\rangle \) in \( \mathcal{H}_S \). The Schrödinger equation in this representation would include derivatives with respect to \( z^* \).

In a quite different spirit we derive a new form of this equation, by employing the Feshbach technique. The non-Hermitian operator

\[ P_{z^*} = 1_S \otimes |0\rangle \langle z| \] (7)

is a projector, \( P_{z^*}^2 = P_{z^*} \), because the overlap of any unnormalized coherent state with the vacuum is one \( \langle z | 0 \rangle = 1 \) according to [26]. As a consequence, \( Q_{z^*} = 1 - P_{z^*} \) is a corresponding orthogonal projector. Crucially, the initial state of the form \( |\Psi_0\rangle = |\psi_0\rangle |0\rangle \) lies in the subspace spanned by \( P_{z^*} \), so that \( Q_{z^*} |\Psi_0\rangle = 0 \). Note that \( P_{z^*} \) maps any state in \( \mathcal{H} \) to the corresponding state in coherent-state representation evaluated at \( z^* \). Thus, the Feshbach method for this particular projector results in a closed evolution equation for \( |\psi_t(z^*)\rangle \),

\[
\partial_t |\psi_t(z^*)\rangle = -i \langle z | H(t) |0\rangle |\psi_t(z^*)\rangle
- \int_0^t ds K_{t,s}(z^*) |\psi_s(z^*)\rangle.
\]

(8)

Remarkably, the only assumption that was necessary to derive this equation is that the initial state of the environment is the vacuum. Otherwise an additional inhomogeneous term would need to be included. The kernel operator (an operator in \( \mathcal{H}_S \)) is given by \( K_{t,s} = \langle z | H(t) W_{t,s}(z^*) Q_{z^*} H(s) |0\rangle \), with the non-unitary evolution operator

\[
W_{t,s}(z^*) = T \exp \left( -i \int_s^t dv Q_{z^*} H(v) \right)
\]

and \( T \) denotes chronological operator ordering. The difficulty of the problem now obviously lies in computing the kernel operator.

Since solving [1] for all coherent state labels \( z^* \) is equivalent to solving the total Schrödinger equation [1], we can easily derive a formula for the reduced system density operator \( \rho_t \). As in NMQSD, by virtue of the completeness relation [2], the latter can be obtained as an ensemble average of pure states according to

\[
\rho_t = \int \frac{d^2z}{\pi} e^{-|z|^2} |\psi_t(z^*)\rangle \langle \psi_t(z^*)|.
\]

(10)

This is nothing but an unraveling of the form [2], when we consider the coherent state labels as Gaussian random variables. Most remarkably, with the Feshbach technique and the choice of non-Hermitian projectors we obtain closed pure state evolution equations for each of these states.

A few remarks about the initial condition \(|\Psi_0\rangle\) are in order. In our formalism it is crucial to have \( Q_{z^*} |\Psi_0\rangle = 0 \) for obtaining homogeneous equations like [1]. This is automatically achieved in the zero-temperature case, but can also be assured for initial states of the form \(|\Psi_0\rangle = |\psi_0\rangle |\xi\rangle\), where \(|\xi\rangle\) is a coherent state of the environment.
Either one performs a unitary displacement or one considers the modified projector

$$P_{z^*} = 1_S \otimes \frac{\langle z \vert \xi \rangle}{\langle z \vert \xi \rangle}.$$  

This is a well-defined object because the overlap of two coherent states is never zero. Starting from the coherent-state initial condition one can also realize a thermal environment by taking a Gaussian mean over the coherent state labels $\xi$. It might also be possible to consider more general mixed initial states by applying the formalism to 'amplitudes' of the total mixed state rather than pure states, similar to what is presented in reference [26]. For the sake of simplicity, we assume the vacuum bath initial condition in the following.

**Spin environments.**– It is possible to generalize the new projection method in order to establish an exact quantum trajectory theory for spin environments (with finite spin quantum number $S$ of a single spin). To this aim we introduce spin coherent states analogous to the Bargmann coherent states [3] for Bosons. Let the ground state of the spin system be the state that satisfies $S_z \vert 0 \rangle = S \vert 0 \rangle$, where $S_z$ denotes the $z$-component of the spin operator. The (scaled) ladder operator $b^\dagger$ of the spin $S$ is given by [27]

$$b^\dagger = \frac{1}{\sqrt{2S}} (S_x - iS_y) = \frac{J}{\sqrt{2S}}, \quad [b, b^\dagger] = \frac{S_z}{S}. \quad (12)$$

Here, contrary to the literature, the operator is defined in such a way that the analogy to the Bosonic environment is obvious. The unnormalized spin coherent state is $\langle z \vert = \exp(b^\dagger z) \vert 0 \rangle$, and the overlap of two such states becomes

$$\langle z \vert z' \rangle = \left(1 + \frac{z^* z'}{2S}\right)^{2S}, \quad (13)$$

leading to the Bosonic results in the limit $S \to \infty$. Note that this implies $\langle z \vert 0 \rangle = 1$ and thus $\vert 0 \rangle \langle z \vert$ is again a projector that can be used in (7). Crucially, there is also a completeness relation of the form

$$1 = \int \frac{d^2z}{\pi} m(|z|^2) \langle z \vert z \rangle. \quad (14)$$

In order for this relation to hold, the first $2S$ moments of the weight function $m$ must satisfy

$$\int_0^\infty d\sigma \sigma^p m(\sigma) = \frac{p! (2S - p)! (2S)^p}{2S!}, \quad (15)$$

with $p = 0, \ldots, 2S$ and the natural choice is $m(|z|^2) = \frac{1 + |z|^2}{2S + 1 + |z|^2}$, reflecting the overlap (13). The projector $P_{z^*}$ and the completeness relation are the only ingredients necessary for the Feshbach method. Thus, all previous equations for Bosonic environments, including the evolution equation (5), can be copied for the spin environment. It is a remarkable feature that within the new formalism the treatment of Bosonic and spin environments is formally identical with, however, a non-Gaussian probability distribution of the coherent state labels $z$ according to (14). While in many cases a spin environment can be described by an effective harmonic bath, this no longer holds true beyond linear response approximation [28].

**Non-Markovian quantum state diffusion, revisited.**– As an important application we consider an environment of harmonic oscillators with frequencies $\omega_i$, coupled linearly to the system with coupling strengths $g_i$. In this model equation (20) is a novel evolution equation for non-Markovian quantum state diffusion and the stochastic interpretation will become very appealing.

In interaction representation with respect to the free environment dynamics the Hamiltonian of this model reads

$$H(t) = H_S \otimes 1_E + \sum_i (g_i e^{i\omega_i t} L \otimes b_i^\dagger + \text{h.c.}). \quad (16)$$

Here $H_S$ is the system Hamiltonian and $L$ an operator in $H_S$. One also defines the zero-temperature bath correlation function by

$$\alpha(t) = \sum_i |g_i|^2 e^{-i\omega_i t}. \quad (17)$$

We briefly recapitulate the usual way to obtain the NMQSD stochastic Schrödinger equation [14]: here, the Schrödinger equation for $\vert \psi_i(t) \rangle$ includes derivatives with respect to the coherent state labels $z^*$. Introducing a complex Gaussian stochastic process via

$$z_i^* = -i \sum_t g_i e^{i\omega_i t} z_i^*, \quad \mathcal{M}(z_i z_i^*) = \alpha(t - s), \quad (18)$$

in a functional picture the Schrödinger equation for $\vert \psi_i(t) \rangle$ becomes the non-Markovian quantum state diffusion (NMQSD) stochastic Schrödinger equation

$$\frac{\partial}{\partial t} \vert \psi_i(t) \rangle = -i H_S \vert \psi_i(t) \rangle + L z_i^* \vert \psi_i(t^*) \rangle$$

$$- L^\dagger \int_0^t ds \alpha(t - s) \frac{\delta}{\delta z_i^*} \vert \psi_i(t^*) \rangle, \quad (19)$$

again assuming the vacuum environment initial condition. Then $\vert \psi_i(t^*) \rangle$ can be interpreted as a functional of $z_i^*$, and $p_i(t)$ is obtained according to (2). The NMQSD equation implies that the influence of the environment on the bath is exclusively characterized by the bath correlation function. Of course, the appearance of the functional derivatives makes solving this equation quite involved (for an application see [13]). A numerically exact treatment is possible using a hierarchy of stochastic pure states (HOPS) [16].

With the new Feshbach formalism we can now derive this equation in a new form including the memory integral. In particular, for Hamiltonian (16), the general
equation (8) becomes
\[
\partial_t |\psi_t(z^*)\rangle = -iH_S |\psi_t(z^*)\rangle + L z^*_t |\psi_t(z^*)\rangle - \int_0^t ds K_{t,s}(z^*) |\psi_s(z^*)\rangle ,
\] (20)
with the Kernel operator \(K_{t,s}(z^*)\). This is a completely new version of the NMQSD evolution equation in closed form that is well defined by construction. It can be seen as the analogue of the Nakajima-Zwanzig equation (11) within the NMQSD formalism. Note that the memory integral term exactly replaces the term with the functional derivative of NMQSD. The kernel operator can now also be interpreted as a functional of \(z^*_t\), which can be seen most easily by expanding this object in powers of the coupling strength. Explicitly up to third order in \(g\) one has
\[
K_{t,s}(z^*) = \alpha(t-s)L^\dagger e^{-iH_S(t-s)}L + \int_s^t dv z^*_v \alpha(t-s)L^\dagger e^{-iH_S(t-v)}Le^{-iH_S(v-s)}L + \ldots .
\]
The Born-like approximation described in (22) corresponds to taking into account only the \(z^*\)-independent first term. If in addition one formally assigns \(\alpha(t) = \kappa \delta(t)\) the usual Markov stochastic Schrödinger equation is retained. In complete analogy to the calculations in [7, 8] for a density operator, in the projection formalism one can also construct TCL evolution equations. In the framework of NMQSD this has become known as the \(O\)-operator substitution [22, 30]. In particular, one defines an operator \(O(t,s,z^*)\) through
\[
\frac{1}{\sqrt{\omega}} |\psi_t(z^*)\rangle = O(t,s,z^*) |\psi_t(z^*)\rangle \quad \text{in} \quad \mathcal{H}_S \quad \text{so that with} \quad \bar{O}_t(z^*) = \int_0^t ds \alpha(t-s)O(t,s,z^*) \quad \text{one can identify}
\]
\[
\int_0^t ds K_{t,s}(z^*) |\psi_s(z^*)\rangle = L^\dagger \bar{O}_t(z^*) |\psi_t(z^*)\rangle ,
\] (21)
i.e. eq. (20) becomes time-local. While the existence of \(K_{t,s}(z^*)\) is guaranteed by construction, \(\bar{O}_t(z^*)\) may not exist for certain times.

To fill these concepts with life we apply our formalism to a Jaynes-Cummings-type model. In particular, the model describes a two level system with Hamiltonian \(H_S = \omega \sigma^+_s \sigma^-_s\) coupled to a bath of harmonic oscillators in rotating wave approximation \(L = \sigma_-\). For this model one can easily compute the kernel operator \(K_{t,s}\) and obtain the new evolution equation
\[
\partial_t |\psi_t(z^*)\rangle = -i\omega \sigma^+_s \sigma^-_s |\psi_t(z^*)\rangle + z^*_t \sigma^-_s |\psi_t(z^*)\rangle - \int_0^t ds \alpha(t-s)\sigma^+_s \sigma^-_s |\psi_t(z^*)\rangle ,
\] (22)

We can use the new time-nonlocal form of the stochastic Schrödinger equation to obtain its TCL version. For that we make the ansatz \(\bar{O}_t = \bar{f}_t \sigma_-\), which yields
\[
\partial_t |\psi_t(z^*)\rangle = -i\omega \sigma^+_s \sigma^-_s |\psi_t(z^*)\rangle + z^*_t \sigma^-_s |\psi_t(z^*)\rangle - \bar{f}_t \sigma^+_s \sigma^-_s |\psi_t(z^*)\rangle .
\] (23)
We multiply both (22) and (23) from the left by \(\sigma_-\). Comparing both expressions gives
\[
\bar{f}_t = \int_0^t ds \alpha(t-s)\frac{\psi^+_s}{\psi^*_t} ,
\] (24)
with the complex-valued function \(\psi^+_t\) satisfying the nonlocal differential equation
\[
\partial_t \psi^+_t = -i \omega \psi^+_t - \int_0^t ds \alpha(t-s)\psi^*_s .
\] (25)
This result can also be obtained by using a Heisenberg operator technique, without knowledge of (22) [30]. Here it arises quite naturally from the structure of the new evolution equation. Note that \(\bar{O}_t\) is ill-defined whenever \(\psi^*_t = 0\), whereas \(K_{t,s} = \alpha(t-s)\sigma^+_s \sigma^-_s\) is always well defined. With the operator \(\bar{O}_t\) at hand it is also easily possible to derive the corresponding TCL master equation for this model, see reference [30].

**Conclusions.**—With the aim to describe non-Markovian quantum dynamics, we have introduced a new formalism applicable to quantum systems in environments consisting of Bosonic modes or spins. The very general formalism arises from a Feshbach-like projection operator technique based on a stochastic ensemble of non-Hermitian projectors in the environment Hilbert space. In particular, when the Bosonic or spin modes are initially in the vacuum state, the quantum state in the coherent state-representation with respect to the environmental degrees of freedom satisfies the new evolution equation (8).

We applied the formalism to an environment of harmonic oscillators linearly coupled to the system. For this model we recover the non-Markovian quantum state diffusion (NMQSD) stochastic Schrödinger equation in a closed form (20), where the functional derivative with respect to the stochastic trajectory is replaced by a memory integral over the past state. Structurally, the projection method provides a new access to the NMQSD formalism that makes the non-Markovian nature of this equation much more apparent. While the new equation is always well defined, this is not true for the TCL version of the NMQSD stochastic Schrödinger equation arising from the \(O\)-operator method, as we have seen based on the simple example of the Jaynes-Cummings-type model. It should be stressed that for the formalism no restrictions on the total Hamiltonian are made. Thus the ‘environment’ could also describe an interacting Bosonic many-body system. There is currently a huge interest in nonequilibrium dynamics of many-body quantum systems in the context of ultracold atomic gases (see, for instance
and we believe that the current work opens a door for a quantum open system point of view of these dynamics. For applications in this field one needs to find suitable approximations for the memory kernel operator. Since the formula for the reduced state has the form of a stochastic unraveling, an approximated kernel still leads to a positive reduced density operator, in contrast to the Nakajima-Zwanzig method, where approximations typically lead to loss of positivity. By introducing quantum spin states analogous to the Bargmann coherent states one can also apply the formalism when the environment consists of spins. Notably, this leads to evolution equations whose form is identical to the ones for Bosonic environments with, however, a non-Gaussian distribution of the random variables $z^*$.  

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