Open System Dynamics with Non-Markovian Quantum Trajectories

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A non-Markovian stochastic Schrödinger equation for a quantum system coupled to an environment of harmonic oscillators is presented. Its solutions, when averaged over the noise, reproduce the standard reduced density matrix without any approximation. We illustrate the power of this approach with several examples, including exponentially decaying memory correlations and extreme non-Markovian periodic cases, where the ‘environment’ consists of only a single oscillator. The latter case shows the decay and revival of a ‘Schrödinger cat’ state. For strong coupling to a dissipative environment with memory, the asymptotic state can be reached in a finite time. Our description of open systems is compatible with different positions of the ‘Heisenberg cut’ between system and environment.

The dynamics of open quantum systems is a very timely problem, both to address fundamental questions (quantum decoherence, measurement problem) as well as to tackle the more practical problems of engineering the quantum devices necessary for the emerging fields of nanotechnology and quantum computing. So far, the true dynamics of open systems has almost always been simplified by the Markov approximation: environmental correlation times are assumed negligibly short compared to the system’s characteristic time scale.

For the numerical solution of Markovian open systems, described by a master equation of Lindblad form

$$\frac{d}{dt}\rho_t = -i[H, \rho_t] + \frac{1}{2} \sum_m \left[ (L_m \rho_t L_m^\dagger + [L_m, \rho_t L_m^\dagger]) \right]$$  \hspace{1cm} (1)

(where $\rho_t$ denotes the density matrix, $H$ the system’s Hamiltonian and the operators $L_m$ describe the effect of the environment in the Markov approximation), a breakthrough was achieved through the discovery of stochastic unravellings $^{[1,2]}$. These are stochastic Schrödinger equations for states $\psi_t(z)$, driven by a certain classical noise $z_t$ with distribution functional $P(z)$. Crucially, the ensemble mean $\bar{M} \ldots$ over the noise recovers the density operator,

$$\rho_t = \bar{M}\left[ \left| \psi_t(z) \right\rangle \left\langle \psi_t(z) \right| \right].$$  \hspace{1cm} (2)

Hence, the solution of eq.(1) is reduced from a problem in the matrix space of $\rho$ to a much simpler Monte Carlo simulation of quantum trajectories $\psi_t(z)$ in the state space.

For the Markov master eq.(1), several such unravellings are known. Some involve jumps at random times $^{[1]}$; others have continuous, diffusive solutions $^{[3]}$. They have been used extensively over recent years, as they provide useful insight into the dynamics of continuously monitored (individual) quantum processes $^{[4]}$, or into the mechanism of decoherence $^{[4]}$. In addition, they provide an efficient tool for the numerical solution of the master eq.(1). It is thus desirable to extend the powerful concept of stochastic unravellings to the more general case of non-Markovian evolution.

The simplest unravellings are linear stochastic Schrödinger equations. In the Markov case $^{[1]}$, for a single $L$, the linear equation

$$\frac{d}{dt}\psi_t = -iH\psi_t + L\psi_t \circ z_t - \frac{1}{2}L^\dagger L\psi_t,$$  \hspace{1cm} (3)

provides such an unravelling, where, $z_t$ is a complex-valued Wiener process of zero mean and correlations $M[z_t^* z_s] = \delta(t - s)$, $M[z_t z_s] = 0$, and where $\circ$ denotes the Stratonovich product $^{[5]}$.

However, eq.(1) is of limited value, since the norm $\|\psi_t(z)\|$ of its solutions tends to 0 with probability 1 and to infinity with probability 0, such that the mean square norm is constant. To be really useful, one should find unravellings in terms of the normalized states

$$\tilde{\psi}_t(z) = \frac{\psi_t(z)}{\|\psi_t(z)\|}.$$

which requires a redefinition of the distribution of the noise $P(z) \rightarrow \bar{P}_t(z) \equiv \|\psi_t(z)\|^2 P(z)$ $^{[6]}$ so that eq.(2) remains valid for the normalized solutions:

$$\rho_t = \bar{M}_t \left[ \tilde{\psi}_t(z) \left\langle \tilde{\psi}_t(z) \right| \right].$$  \hspace{1cm} (5)

Now $^{[1]}$ can be interpreted as an unravelling of the mixed state $\rho_t$ into an ensemble of pure states. For the Markov unravelling $^{[1]}$, the normalized states $\tilde{\psi}_t$ satisfy the non-linear Quantum State Diffusion (QSD) equation $^{[7]}$:

$$\frac{d}{dt}\tilde{\psi}_t = -iH\tilde{\psi}_t + (L - \left\langle L \right\rangle_{t})\tilde{\psi}_t \circ (z_t + \left\langle L^\dagger \right\rangle_{t})$$

$$- \frac{1}{2}(L^\dagger L - \left\langle L^\dagger L \right\rangle_{t})\tilde{\psi}_t,$$

where $\left\langle L \right\rangle_{t} \equiv \left\langle \tilde{\psi}_t|L|\tilde{\psi}_t \right\rangle$. Contrary to eq.(3), eq.(6) provides an efficient Monte-Carlo algorithm for the numerical solution of eq.(5).

In this Letter we present for the first time a nonlinear non-Markovian stochastic Schrödinger equation that unravels the dynamics of a system interacting with an arbitrary ‘environment’ of a finite or infinite number of harmonic oscillators, without any approximation. In the Markov limit, this unraveling reduces to QSD $^{[1]}$ and will therefore be referred to as non-Markovian Quantum State Diffusion. Other authors have treated non-Markovian open systems effectively with Markovian unravellings: either the system has in fact been influenced by a second Markovian environment in addition to the...
original non-Markovian one or, alternatively, fictitious modes have been added to the system \([\mathcal{H}].\) In our approach, the ‘system’ remains unaltered, and the unravelling is genuinely non-Markovian.

Below we summarize the general theory, which will be presented in detail elsewhere \([\text{3}].\) and we present four examples: First, we consider a ‘measurement-like’ environment. Then, a dissipative environment with exponentially decaying environment correlations is discussed. Remarkably, here the asymptotic state can be reached in a finite time. In the third example we consider an ‘environment’ consisting of only a single oscillator. This example is thus periodic, that is extremely non-Markovian. It shows the decay and revival of a ‘Schrödinger cat’ state. Finally, the fourth example shows that the description of a subsystem in terms of non-Markovian QSD is independent of the ‘Heisenberg cut’, that is independent of where precisely the boundary between system and environment is set.

Our starting point is the non-Markovian generalization of the linear stochastic equation \([\text{3}].\) derived in \([\text{3}].\)

\[
\frac{d}{dt}\psi_t = -i\mathcal{H}\psi_t + L\psi_t z_t - L^\dagger \int_0^t \alpha(t,s) \frac{\delta \psi_t}{\delta z_s} ds,
\]

which unravels the exact reduced dynamics of a system coupled to an environment of harmonic oscillators. Here, \(z_t\) is colored complex Gaussian noise of zero mean and correlations

\[
\begin{align*}
M[z^*_t z_s] &= \alpha(t,s), & M[z_t z_s] &= 0.
\end{align*}
\]

The Hermitian \(\alpha(t,s) = \alpha^*(s,t)\) is the environment correlation function \([\text{3}].\) The functional derivative under the memory integral in \([\text{3}].\) indicates that the evolution of the state \(\psi_t\) at time \(t\) is influenced by its dependence on the noise \(z_s\) at earlier times \(s.\) In \([\text{3}].\) we show that it amounts to applying an operator to the state, \(\delta\)

\[
\frac{\delta}{\delta z_s} \psi_t \equiv \hat{O}(s,t,z) \psi_t,
\]

where the explicit expression of \(\hat{O}(s,t,z)\) can be determined consistently from eq.\([\text{3}].\)

Just as in the Markov limit, to be really useful, one has to find the corresponding non-linear non-Markovian QSD equation for the normalized states \([\text{3}].\) This quite elaborate derivation can be found in \([\text{3}].\) and leads to

\[
\frac{d}{dt} \hat{\psi}_t = -i\mathcal{H}\hat{\psi}_t + (L - \langle L \rangle\hat{\psi}_t)\hat{z}_t - L^\dagger \int_0^t \alpha(t,s) \hat{O}(s,t,z) ds,
\]

which is the basic equation of non-Markovian QSD. Here, \(\hat{z}_t\) is the shifted noise \(\hat{z}_t = z_t + \int_0^t \alpha(t,s) ds\), and for brevity we use \(L^\dagger = L^\dagger L = H.\)

Let’s turn to concrete examples of non-Markovian QSD \([\text{3}].\) First, we consider an environment modeling energy measurement: \(L = L^\dagger = H.\) It is easy to prove that \(\hat{O} = H \) in \([\text{3}].\) and hence \([\text{3}].\) reads

\[
\frac{d}{dt} \hat{\psi}_t = -i\mathcal{H}\hat{\psi}_t - (H^2 - \langle H^2 \rangle)\hat{\psi}_t \int_0^t \alpha(t,s) ds
\]

\[
+ (H - \langle H \rangle)\hat{\psi}_t \left( z_t + \int_0^t \alpha(t,s) ds \right).
\]

Notice that indeed, \([\text{3}].\) reduces to the Markov QSD equation \([\text{3}].\) for \(\alpha(t,s) \to \delta(t-s).\)

If the correlation \(\alpha(t,s)\) decreases fast enough, the asymptotic solution of \([\text{3}].\) is an eigenstate \(\phi_0\) of \(\mathcal{H}\), reached with the expected quantum probability \(|\langle \phi_0 | \psi_0 \rangle|^2.\) Numerical solutions of \([\text{3}].\) for the 2-dimensional case \(H = \hat{\sigma}_z\) and exponentially decaying correlation are shown in Fig.1a (solid lines). The asymptotic state is either the ‘up’ or the ‘down’ state. The ensemble mean \(M[\sigma_z]\) remains constant (dashed line) as expected from the analytical solution (dot-dashed line). Note, however, that if the environment consists of a finite number of oscillators, represented by a quasi-periodic correlation function \(\alpha(t,s)\), such a reduction to an eigenstate will not occur (see our third example).

As a second example, we consider a dissipative spin with \(H = \hat{\sigma}_z\), and \(L = \lambda \sigma_\perp.\) We choose exponentially decaying correlations \(\alpha(t,s) = \gamma e^{-|t-s| - \alpha(t-s)}\) with an environmental central frequency \(\Omega\) and memory time \(\gamma^{-1}\). The non-Markovian QSD equation \([\text{3}].\)

\[
\frac{d}{dt} \hat{\psi}_t = -i\omega (\mathcal{H}\hat{\psi}_t - \lambda F(t)(\sigma_+ \sigma_- - \langle \sigma_+ \sigma_- \rangle) \hat{\psi}_t
\]

\[
+ \lambda (\sigma_- - \langle \sigma_- \rangle) \hat{\psi}_t \left( z_t + \lambda \int_0^t \alpha(t,s) \sigma_\perp ds + \langle \sigma_\perp \rangle \right) F(t)
\]

with \(F(t)\) determined from

\[
\frac{d}{dt} F(t) = -\gamma F(t) + (i(\omega - \Omega) F(t) + \lambda F(t)^2 + \frac{\lambda \gamma}{2},
\]

and initial condition \(F(0) = 0.\) The equation for \(F(t)\) can be solved analytically \([\text{3}].\) It is worth mentioning the case of exact resonance, \(\omega = \Omega.\) Two regimes should be distinguished. First, when \(\gamma > 2\lambda^2\) (short memory compared to coupling strength), \(F(t)\) tends to \(\left(\gamma - \sqrt{\gamma^2 - 2\gamma^2}\right) / (2\lambda)\). Hence, for large \(\gamma,\) one recovers Markov QSD \([\text{3}].\) For longer memory times or stronger coupling, \(\gamma < 2\lambda^2,\) things are very different: \(F(t)\) diverges to infinity when the time \(t\) approaches \(t_c = \frac{\pi}{2} \arctan(\gamma / \sqrt{2\gamma^2 - \gamma^2}) / (2\lambda).\)

All realizations \(\psi_t(z)\) reach the down state in a finite time and remain there! In Fig.1b we show quantum trajectories from \([\text{3}].\) (solid lines), their ensemble mean value \(M[\sigma_z(t)]\) (dashed line), and the analytical mean value (dot-dashed), which is almost indistinguishable. The reduction time in this case is \(\omega t_c = \frac{\pi}{2} \approx 4.71.\) This is the first example of a continuous quantum state diffusion that reaches its asymptotic state in a finite time, which was proven impossible for Markovian diffusions \([\text{3}].\)

Our third example is a harmonic oscillator coupled to a finite or infinite number of oscillators initially in their ground states. Here, the non-Markovian QSD eq.\([\text{3}].\) takes the same form \([\text{3}].\) where the Hamiltonian is \(\omega a^\dagger a\) and where \(\sigma_-\) (\(\sigma_+\)) has to be replaced by the annihilation (creation) operator \(a\) (\(a^\dagger\)). The resulting equation preserves coherent states. More interesting is the case of an initial superposition of two symmetric coherent states, known as a ‘Schrödinger cat’ \([\text{3}].\) If the environment correlation \(\alpha(t,s)\) decays, so does the ‘cat’. However, if the environment consists of only a finite number of oscillators, then the ‘cat’ will first decay, due to the localization property of QSD, but since the entire system is quasiperiodic, the ‘cat’ will then revive! In Fig.2 we show contour
plots of the evolution of the $Q$-function of such a ‘cat’, in the extreme case where the environment consists of a single oscillator $\alpha(t, s) = e^{-i\xi z(t-s)}$. Apart from an overall spiraling motion due to the ‘system’ Hamiltonian, the ‘cat’ state first decays but later revives. Our non-Markovian QSD equation thus provides a nice illustration of proposed experiments on reversible decoherence.

As a last example we consider a case where the split between system and environment can be shifted naturally between two positions, see Fig.3. A spin (Hamiltonian $H_1$) and a distinguished harmonic oscillator ($H_2$) are linearly coupled ($H_{12}$). Moreover, the spin is coupled ($H_1$) to a heat bath ($H_{env}$) at zero temperature. We can either consider the quantum state of the spin-oscillator system coupled to a heat bath, or the quantum state of the spin coupled to a heat bath and coupled to the distinguished oscillator. In the first case, we can apply the Markov QSD description, i.e., a family of spin-oscillator states $\psi_\xi(t)$ indexed by a complex Wiener process $\xi$. In the second case, using non-Markovian QSD, we have a family of spin states $\phi_\xi(t, z)$ indexed by the same $\xi$ and also by the noise $z$, due to the distinguished oscillator ‘environment’ with correlation $M[z z^*] = e^{-i\omega_2(t-s)}$.

Let us study a shift of the ‘Heisenberg cut’: compare the states $\phi_\xi(t, z)$ of the spin averaged over the noise $z$, with the mixed state obtained by tracing out (Tr$_2$) the oscillator from the spin-oscillator states $\psi_\xi(t)$. We prove in that the states corresponding to both descriptions are equal:

$$M_z[\langle \phi_\xi(t, z) | \phi_\xi(t, z) \rangle] = \text{Tr}_2[|\psi_\xi(t)\rangle \langle \psi_\xi(t)|].$$

(14)

This illustrates the general fact that non-Markovian QSD attributes stochastic pure states to a system in a way which depends on the position of the Heisenberg cut, but which is consistent for all possible choices of the cut.

In conclusion, we present the first non-Markovian unravelling of the dynamics of a quantum system coupled to an environment of harmonic oscillators, which can thus be simulated by classical complex noise. In the Markov limit, standard Quantum State Diffusion is recovered. We emphasize that non-Markovian QSD reproduces the true evolution of the system taking into account the exact unitary dynamics of system and environment. The power of this new approach represents a new efficient tool for the numerical simulation of quantum devices, whenever non-Markovian effects are relevant.

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**FIGURE CAPTIONS**

**FIG. 1.** Non-Markovian quantum trajectories (solid lines) for a spin $\frac{1}{2}$ system $H = \frac{\omega}{2} \sigma_x$ with an exponentially decaying environment correlation $\alpha(t,s) = \frac{\gamma}{2} \exp(-\gamma|t-s|-i\Omega(t-s))$, where we choose $\gamma = \omega$. The ensemble mean value over 10000 runs (dashed line) is in very good agreement with the analytical result (dot-dashed line). We show (a) a measurement-like interaction $L = \lambda \sigma_z$ with $\Omega = 0$, and (b) a dissipative interaction $L = \lambda \sigma_z$ on resonance $\Omega = \omega$, where each trajectory reaches the ground state in a finite time $\omega t_c = \frac{1}{2} \pi \approx 4.71$. In both cases we choose a coupling strength $\lambda = \omega$ and an initial state $|\psi_0\rangle = 3|\uparrow\rangle + 2|\downarrow\rangle$.

**FIG. 2.** Reversible decoherence of an initial symmetric ‘Schrödinger cat’ state $|\psi_0\rangle = |\alpha\rangle + |\alpha\rangle$ with $\alpha = 2$. The contour plots show the $Q$-function of a non-Markovian quantum trajectory of a harmonic oscillator (ω) ‘system’, coupled to just a single ‘environment’ oscillator $(\Omega = 0.5\omega)$. The coupling strength between the two oscillators is $0.1\omega$, and the time step between two successive plots is $0.47/\omega$.

**FIG. 3.** ‘Spin - single oscillator - heat bath’ system. First, we consider the ‘spin - single oscillator’ as the ‘system’ with state $\psi_t(\xi)$, coupled to the heat bath with noise $\xi_t$. Alternatively, we can consider the ‘spin’ as the ‘system’ $\phi_t(\xi,z)$, coupled to the ‘single oscillator + heat bath’ environment (noises $(\xi_t, z_t)$). In non-Markovian QSD, both descriptions are possible and lead to the same reduced spin state.
$H_{12}$

Spin

$\phi_t(\xi, Z)$

Single oscillator

$H_2$

$Z_t$

$H_{env}$

Bath of oscillators

$\xi_t$