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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. The ensemble average recovers the reduced density matrix without approximation and hence it allows one to determine open system dynamics with strong and non-Markovian environmental effects in a very efficient way. We demonstrate the power of our approach with several illustrative examples. First, we discuss a measurement-type situation, then a two-state system strongly coupled to a non-Markovian environment, exhibiting decays and revivals. Further examples showing the remarkable features of our new approach to non-Markovian open system dynamics are discussed, for instance, the possibility to shift the "Heisenberg cut" between system and environment. [S0031-9007(99)08603-2]

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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. Standard descriptions of open quantum systems very often rely on a weak system-environment coupling, and the validity of the Markov approximation: environmental correlation times are assumed negligibly short compared to the system's characteristic time scale. With new experimental advances on mesoscopic scales, these conditions are too restrictive and appropriate theoretical tools have to be developed to efficiently describe quantum systems in either unavoidable or even designed contact with structured environments. The spontaneous decay of an atom in a photonic band gap material and the output coupling from a Bose Einstein condensate necessary to create an atom laser are just two out of many current topics where standard Markov methods are known to fail [1].

To motivate our result, let us first recall the Markov case. For the numerical solution of a Markov master equation in Lindblad form

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

a breakthrough was achieved through the discovery of Monte Carlo wave function methods [2,3]. These are stochastic Schrödinger equations for states $\psi_t(z)$ (*quantum trajectories*), driven by a classical stochastic process z_t, such that the ensemble mean $M[\cdots]$ recovers the density operator,

$$\rho_t = M[|\psi_t(z)\rangle\langle\psi_t(z)|]\,. \quad (2)$$

Hence, the solution of Eq. (1) is reduced from the matrix space of ρ_t to a much simpler Monte Carlo simulation of quantum trajectories $\psi_t(z)$ in the space of pure states.

For the Markov master Eq. (1), several such *stochastic unravelings* are known. Some involve jumps at random times [2], others have continuous, diffusive solutions [3]. Among the latter is the *quantum state diffusion* (QSD) equation

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

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driven by complex white noise z_t and here written as a Stratonovich stochastic Schrödinger equation [4].

Stochastic unravelings of Markov density operator dynamics have been used extensively over recent years, since they provide useful insight into the dynamics of continuously monitored (individual) quantum processes [5] or into the mechanism of decoherence [6]. Most importantly, they provide a very efficient tool for the numerical solution of the master Eq. (1). It is thus desirable to extend the powerful concept of stochastic unravelings to the more general case of non-Markovian evolution, where the traditional reduced density matrix approach leads to evolution equations that are very difficult to handle in practice [7].

Feynman and Vernon's path integral approach to open systems [8] might be regarded as one of the most fruitful routes to describe open system dynamics beyond the weak-coupling and Markov approximation. In practice this approach suffers from the difficulty of evaluating the remaining double path integral [9], which is why in the Markov case one rather prefers solving a master or even better, a stochastic Schrödinger equation.

As with Feynman and Vernon and most standard models of open system dynamics—particularly in quantum optics—our starting point is a quantum "system" coupled to a set of bosonic oscillators, the "environment," such that the total Hamiltonian reads

$$H_{\rm tot} = H + \sum_\lambda g_\lambda (L a_\lambda^\dagger + L^\dagger a_\lambda) + \sum_\lambda \omega_\lambda a_\lambda^\dagger a_\lambda \,. \tag{4}$$

Here, H is the Hamiltonian of the isolated system and L a system operator describing the coupling to the environmental degrees of freedom (operators $a_\lambda, a_\lambda^\dagger$), g_λ denotes the coupling strength, and ω_λ is the frequency of environmental oscillator λ. In Feynman and Vernon's model we have $L = q$ the position operator. The crucial quantity describing the environmental influence on the system is the response function [8,9]

$$\alpha(t,s) = \sum_\lambda g_\lambda^2 e^{-i\omega_\lambda (t-s)} \tag{5}$$

here for a zero temperature environment, i.e., for an initial state $\Psi_{\rm tot}(t=0) = \psi_0 \otimes |0\rangle \otimes |0\rangle \ldots$. We emphasize, however, that finite temperature can easily be incorporated in our approach [10,11].

We now present a Monte Carlo wave function method that recovers the reduced system dynamics of the model (4) without approximation, in particular, without Markov approximation. A first step towards this goal was made in [11], where the authors derive a linear non-Markovian stochastic Schrödinger equation

$$\frac{d}{dt}\psi_t = -iH\psi_t + L\psi_t z_t - L^\dagger \int_0^t \alpha(t,s)\,\frac{\delta \psi_t}{\delta z_s}\,ds \,, \tag{6}$$

which unravels the exact reduced dynamics of model (4). In (6), $\alpha(t,s)$ is the response function (5) and z_t is colored complex Gaussian noise of zero mean and correlations $M[z_t^* z_s] = \alpha(t,s)$ and $M[z_t z_s] = 0$.

Despite its crucial property of unraveling the reduced dynamics of the model (4), the linear Eq. (6) is of little use from the point of view of applications for two reasons. First, we have to find a way to handle the functional derivative appearing in the memory integral in (6). Second, the linear equation (6) has the drawback of not being norm preserving. In general, in fact, the norm $|\psi_t|$ tends to zero. Thus, in Monte Carlo simulations we are faced with the problem of importance sampling [12].

The first problem can be tackled by observing that applying the functional derivative amounts to applying an operator to the state,

$$\frac{\delta}{\delta z_s}\,\psi_t \equiv \hat{O}(t,s,z)\psi_t \,, \tag{7}$$

where the explicit expression of $\hat{O}(t,s,z)$ can be complicated but, in principle, can be determined consistently from Eq. (6). For specific relevant models, this task is solved (see the examples below and [10]). In the general case, further efforts have to be made to get a (possibly approximate) expression for the $\hat{O}$ operator [13].

We solve the second problem similar to the Markov case [14] by going over to the normalized states and derive the appropriate stochastic Schrödinger equation. Note that this step is far from trivial and requires a non-Markovian dynamical adjustment of the distribution functional of the stochastic process z_t in order to preserve the correct ensemble mean (2). It is maybe the most remarkable result of this Letter that it is nevertheless possible to derive a closed evolution equation for these normalized and "noise-adjusted" states. The quite elaborate derivation can be found in [10] and leads to the desired non-Markovian quantum state diffusion equation

$$\begin{aligned}\frac{d}{dt}\tilde{\psi}_t = {} & -iH\tilde{\psi}_t + (L - \langle L\rangle_t)\tilde{\psi}_t \tilde{z}_t \\ & - \int_0^t \alpha(t,s)\,[\Delta L_t^\dagger \hat{O}(t,s,\tilde{z}) \\ & \qquad - \langle \Delta L_t^\dagger \hat{O}(t,s,\tilde{z})\rangle_t]\,ds\,\tilde{\psi}_t \,.\end{aligned} \tag{8}$$

Here, $\tilde{z}_t$ is the shifted noise $\tilde{z}_t = z_t + \int_0^t \alpha^*(t,s)\langle L^\dagger\rangle_s ds$, and for brevity we use $\Delta L_t^\dagger = L^\dagger - \langle L^\dagger\rangle_t$. Thus, once the operator $\hat{O}(t,s,z)$ from (7) is known, the reduced density operator of the model (4) can be calculated by computing quantum trajectories using the non-Markovian QSD equation (8).

Notice an important property of non-Markovian QSD: there is no need to store the history of the entire trajectory $\psi_t(z)$. Memory integrals over the past are extended over quantum expectation values only, allowing for a very efficient algorithm.

Let us turn to concrete illustrative examples. First, we consider an environment modeling energy measurement, i.e., the coupling in model (4) is through the energy $L = H$. Using (6), it is easy to show that $\hat{O} = H$ in (7), and hence the non-Markovian QSD equation (8) reads

$$\frac{d}{dt}\tilde{\psi}_t = -iH\tilde{\psi}_t - (H^2 - \langle H^2\rangle_t)\tilde{\psi}_t \int_0^t \alpha(t,s)\,ds + (H - \langle H\rangle_t)\tilde{\psi}_t\left(\tilde{z}_t + \int_0^t \alpha(t,s)\,ds\,\langle H\rangle_t\right) \quad (9)$$

with $\tilde{z}_t = z_t + \int_0^t \alpha(t,s)^*\langle H\rangle_s\,ds$. Notice that indeed, (9) reduces to the Markov QSD equation (3) for $\alpha(t,s) \to \delta(t-s)$.

If the environmental correlation $\alpha(t,s)$ goes to zero fast enough as $|t-s| \to \infty$, the asymptotic solution is an eigenstate ϕ_n of H, reached with the expected quantum probability $|\langle\phi_n\,|\,\psi_0\rangle|^2$. Numerical solutions of (9) for the 2-dimensional case $H = \frac{\omega}{2}\sigma_z$ and exponentially decaying correlation are shown in Fig. 1(a) (grey lines). The asymptotic state is either the "up" or the "down" state. The ensemble mean $M[\langle\sigma_z\rangle]$ remains constant (black solid line) as expected from the analytical solution (black dashed line, indistinguishable).

If, however, the environment consists of a finite number of oscillators only, represented by a quasiperiodic correlation function $\alpha(t,s)$, such a reduction to an eigenstate will not occur. Figure 1(b) shows non-Markovian QSD trajectories for an environment consisting of a single harmonic oscillator only. As in Fig. 1(a), the initial superposition of up and down first decays to either of the two states. Since the entire system is quasiperiodic, the initial superposition revives after one period $\omega t = 2\pi$. A similar analysis holds for Schrödinger cat states, where non-Markovian QSD trajectories show decays and revivals as in proposed experiments on reversible decoherence [10,15].

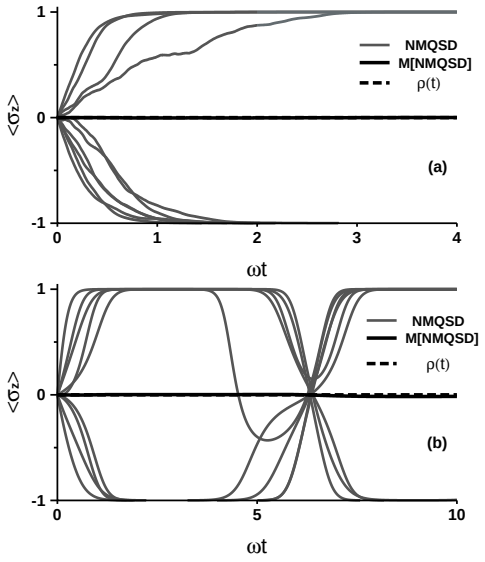

FIG. 1. Non-Markovian quantum trajectories (grey lines) for a spin-$\frac{1}{2}$ system $H = \frac{\omega}{2}\sigma_z$ with $L = H$, and initial $|\psi_0\rangle = (|\uparrow\rangle + |\downarrow\rangle)/\sqrt{2}$. In (a) we choose a decaying environment correlation $\alpha(t,s) = \frac{\gamma}{2}\exp[-\gamma|t-s| - i\Omega(t-s)]$, with $\gamma = \Omega = \omega$. We observe reduction to an eigenstate. In (b) the environment consists of just a single harmonic oscillator, $\alpha(t,s) = \exp[-i\Omega(t-s)]$ with $\Omega = \omega$, where the initial reduction is reversible. In both cases the ensemble mean value over 10 000 runs (black solid line) is in very good agreement with the analytical result (black dashed line, indistinguishable).

As a second example, we consider a dissipative spin-$\frac{1}{2}$ system with $H = \frac{\omega}{2}\sigma_z$ and a coupling $L = g\sigma_-$ (g a coupling constant), modeling the decay of a two-state atom into a structured environment. For an exponentially decaying correlation function with an environmental central frequency Ω and memory time γ^{-1}, the non-Markovian QSD equation (8) reads [10]

$$\frac{d}{dt}\tilde{\psi}_t = -i\,\frac{\omega}{2}\,\sigma_z\tilde{\psi}_t - gF(t)\,(\sigma_+\sigma_- - \langle\sigma_+\sigma_-\rangle_t)\tilde{\psi}_t + g(\sigma_- - \langle\sigma_-\rangle_t)\tilde{\psi}_t[\tilde{z}_t + \langle\sigma_+\rangle_t F(t)] \quad (10)$$

with $\tilde{z}_t = z_t + g\int_0^t \alpha(t,s)^*\langle\sigma_+\rangle_s\,ds$, and $F(t)$ determined through $f(t) = \exp\{-g\int_0^t F(s)\,ds\}$, where

$$\ddot{f} + [\gamma + i(\Omega - \omega)]\dot{f} + \frac{\gamma g^2}{2} f = 0 \quad (11)$$

with initial condition $f(0) = 1$, $\dot{f}(0) = 0$. Depending on the parameters, this leads to overdamped [Fig. 2(a)] or underdamped [Fig. 2(b)] decay of the initial up state to the down state.

In Fig. 2(a) we show non-Markovian quantum trajectories for a fairly short environmental memory time ($\gamma = 5\omega$), describing the nonexponential decay towards the down state. In the limit $\gamma \to \infty$, i.e., very short memory time, we recover the exponential decay as predicted by the Markov approximation. More interesting is the case of long memory, $\gamma = 0.1\omega$ as shown in Fig. 2(b). The oscillatory behavior shows how the two-state system first loses its energy into the environment, but how later some of it is fed back into the system, resulting in an oscillating relaxation. From a traditional point of view, one could look at this case as a two-state system coupled to one oscillator mode, which is then coupled to an environment (Jaynes-Cummings model). Here we show how this problem can be described using quantum trajectories in the space of the two-state system alone. Interestingly, since at discrete times ($\omega t \approx 5, 15, 25, \ldots$) the reduced density operator is the pure down state, each single quantum trajectory has to be the down state as well, as can clearly be seen in Fig. 2(b). We want to remark that this behavior was wrongly described in [10], where we thought that all trajectories remain in the down state once they reach it.

Non-Markovian QSD (8) can be applied to many more standard models of open system dynamics, for instance, a harmonic oscillator ($H = \omega a^\dagger a$) coupled to a finite

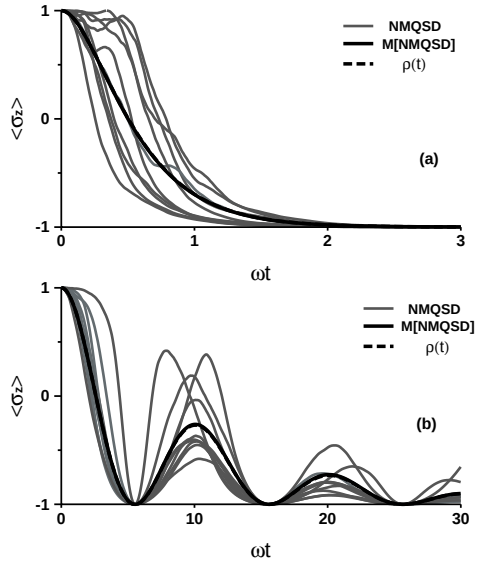

FIG. 2. Non-Markovian quantum trajectories (grey lines) for a damped spin-$\frac{1}{2}$ system $H = \frac{\omega}{2}\sigma_z$, $L = \sqrt{2}\,\sigma_-$, with an exponentially decaying environment correlation $\alpha(t,s) = \frac{\gamma}{2}\exp\times[-\gamma|t-s| - i\Omega(t-s)]$ with $\Omega = \omega$ and $|\psi_0\rangle = |\uparrow\rangle$. In (a) we choose $\gamma = 5\omega$, i.e., fairly short memory and observe an overdamped decay into the down state. In (b) we choose long memory, $\gamma = 0.1\omega$, resulting in an oscillatory relaxation. Note that in this case all individual trajectories coincide at discrete times ($\omega t \approx 5, 15, 25, \ldots$), when the reduced density operator is in the pure down state. The ensemble mean value over 10 000 runs (black solid line) is in very good agreement with the analytical result (black dashed line, indistinguishable).

or infinite number of oscillators. In the rotating wave coupling ($L = a$) this model is of current interest for output coupling to create an atom laser [1]. The Feynman-Vernon coupling corresponds to $L = q$ and leads to the non-Markovian QSD equation for quantum Brownian motion [10,13]. We emphasize that due to its rigorous derivation from the microscopic model (4), our approach is valid for arbitrary environmental correlations $\alpha(t,s)$. Thus, it can be applied to realistic situations (photonic band gaps, atom laser problem), where exponentially decaying correlations—tractable also by pseudomode techniques [1]—can merely serve as a simple first model.

Finally, we point out that non-Markovian QSD allows one to shift the split (the "Heisenberg cut") between system and environment naturally between various positions. Since we treat the total model (4) exactly, we might choose to include a distinguished "environmental" oscillator to be part of the system. Non-Markovian QSD attributes stochastic pure states to a subsystem in a way which depends on the position of the Heisenberg cut, but which is consistent for all possible choices of the cut (see [10] for further elaboration on this property).

In conclusion, we present a non-Markovian unraveling of the dynamics of a quantum system coupled to an environment of harmonic oscillators. Conceptually, we do not rely on a master equation for the reduced density operator but derive our quantum trajectory method straight from the total model including system and environment. In the Markov limit, standard quantum state diffusion (3) is recovered.

For measurementlike interactions, reduction to eigenstates takes place whenever the environment correlation function $\alpha(t,s)$ decreases fast enough. If the environment consists of only a finite number of oscillators, we see decay and revival of the initial superposed state. Non-Markovian effects are visible in the nonexponential decay of a two-state system. For very long environmental memory time, the oscillatory relaxation to the down state is reproduced by our quantum trajectory method. Finally, unravelings corresponding to different positions of the Heisenberg cut between system and environment are mutually compatible. Most of these features are entirely new and have no counterpart in any Markov unraveling. Our approach represents a potentially very powerful tool for the numerical simulation of quantum devices, whenever non-Markovian effects are relevant.

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