The stochastic Schrödinger equation approach to open quantum systems

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Abstract. Under the system-environment interaction the dynamics of the open system can be described by a set of quantum trajectories satisfying some stochastic Schrödinger equation. Such an approach can be extended to the non-Markovian regime by replacing white noise with colored noise. This approach is efficient for simulations with the help of the time-discrete stochastic wave-function methods. As an illustrative example we consider the model of a dissipative qubit. The adaptive Platen method has been derived in order to introduce the colored noise to the iteration algorithm. Also, we test the validity of the approximation based on the Nakajima-Zwanzig method in the stochastic sense. This method is not well studied and needs further investigations.

1. Introduction

A first aim of the theory of open quantum systems is the description of the time evolution of a system S (the open system) interacting with an external environment E. One of the ways to describe the partial dynamics of such a system is to use the generalized master equation for the reduced density matrix $\eta(t)$. In this situation the simple approach is based on the absence of memory effects of the environment and is provided by the Markov approximation. Nevertheless, this approach is no more valid when the memory effects can not be excluded: strong coupling, correlation, and entanglement in the initial S-E state and the system at low temperature. This gives rise to the theory of non-Markovian quantum dynamics, for which a general theory does not exist, but only approaches, for example [1, 2, 3].

Under the system-environment interaction the dynamics of the system can be described by a set of quantum trajectories satisfying some stochastic Schrödinger equation. In this case, the density matrix of the system is recovered as an average over all possible number of trajectories of the state vector $\mathbb{E}[|\psi(t)\rangle\langle\psi(t)|] = \eta(t)$. Such an approach can be extended to the non-Markovian regime by replacing white noise with colored noise [3]. Specifically, the colored noise is represented by an Ornstein-Uhlenbeck process.

We describe the numerical investigation of the dynamics of a non-Markovian dissipative qubit, studied analytically in [3]. The stochastic simulations were done with the help of the extended Platen method.

The results of the simulations are compared with an analytical approximation firstly presented in [4] which is based on the Nakajima-Zwanzig projection method but conceptually is different due to the appearance of the stochastic terms in the non-Markovian master equation. This method is not well studied and needs further investigations.

2. The linear SSE with colored noise and the closed stochastic master equation

In this section we will show two methods, presented recently in [3] and in [4]. Both the methods describe the non-Markovian dynamics. One method is based on the introduction of memory effects with the help of the colored noise and can be used for the simulations. Another method is an analytical approach, that is based on the Nakajima-Zwanzig method utilized to get a closed stochastic master equation. Furthermore, the simulation results will be compared with this analytical approach.

Let us start from the method, presented in [3]. A generic homogeneous linear stochastic differential equation for the non-normalized state $\phi(t)$ with $W = \{W_j(t),\ t \geq 0,\ j = 1, \ldots, d\}$, a continuous d-dimensional Wiener process:

$$\mathrm{d}\phi(t) = K(t)\phi(t)\,\mathrm{d}t + \sum_{j=1}^{d} R_j(t)\phi(t)\,\mathrm{d}B_j(t), \tag{1}$$

where $\phi(0) = \psi_o$, $\psi_0 \in \mathcal{H}$, the coefficients $R_j(t), K(t)$ are (non-random) linear operators on separable, complex Hilbert space $\mathcal{H}$. The normalized vector $\psi(t) = \phi(t)/\left\|\phi(t)\right\|$ corresponds to the conditional state of the system given the observed output up to time t and is often called the *a posteriori state*. For the case of measurement in continuous time the output is not discrete, but it is a whole trajectory of some observed quantity; this brings into play the stochastic processes. Apart from this complication, the linear stochastic Schrödinger equation is an evolution equation for the non-normalized vectors $\phi(t)$.

The stochastic differential equation (1) is to be intended in integral sense and the solution ϕ is the continuous, adapted Itô process [5] satisfying

$$\phi(t) = \psi_0 + \int_0^t K(s)\phi(s)\,\mathrm{d}s + \sum_{j=1}^{d} \int_0^t R_j(s)\phi(s)\,\mathrm{d}W_j(s).$$

The last term in the above equation is a stochastic Itô integral (see [5]). The coefficient in the drift part of (1) has the structure:

$$K(t) = -iH(t) - \frac{1}{2}\sum_{j=1}^{d} R_j(t)^{\dagger} R_j(t), \tag{2}$$

where H is the effective Hamiltonian of the system.

Finally, the *linear stochastic Schrödinger equation* (diffusive type) [6] is given by

$$\mathrm{d}\phi(t) = \left(-\mathrm{i}H(t) - \frac{1}{2}\sum_{j=1}^{d} R_j(t)^{\dagger} R_j(t)\right)\phi(t)\,\mathrm{d}t + \sum_{j=1}^{d} R_j(t)\phi(t)\,\mathrm{d}W_j(t), \tag{3}$$

$$\phi(0) = \psi_0, \quad \psi_0 \in \mathcal{H}, \quad \|\psi_0\| = 1, \qquad H(t) = H(t)^{\dagger}. \tag{4}$$

The extension of the Markovian approach allows to describe the random dynamics for open quantum system with memory by introducing colored noise in the linear stochastic Schrödinger equation. In our case the model represents a dissipative evolution with memory, but without any observation of the quantum system.

The colored stationary Ornstein-Uhlenbeck (O-U) process $X(t)$ is defined by

$$X(t) = e^{-kt}\frac{Z}{\sqrt{2k}} + \int_0^t e^{-k(t-s)}dW(s), \qquad k > 0, \qquad 0 \le s < t < +\infty, \tag{5}$$

and satisfies the stochastic differential equations:

$$dX(t) = -kX(t)dt + dW(t), \qquad X(0) = Z/\sqrt{2k}, \tag{6}$$

where $W(t)$ is a one-dimensional Wiener process and Z is a standard normal random variable. We note, that Z is independent from the Wiener process. The non-Markovianity of the O-U process follows from the fact that its correlation function is no more a δ-function (the Markovian regime is recovered in the limit $k \downarrow 0$):

$$\mathbb{E}[\dot{X}(t)\dot{X}(s)] = \delta(t-s) - \frac{k}{2}e^{-k|t-s|}. \tag{7}$$

Let us consider a one-dimensional driving noise $X(t)$ and three non-random operators C, D and R on $\mathcal{H}$. The starting point is the basic linear stochastic Schrödinger equation

$$\mathrm{d}\phi(t) = \big(A + BX(t)\big)\phi(t)\,\mathrm{d}t + R\phi(t)\,\mathrm{d}X(t), \tag{8}$$

where $X(t)$ is the stationary O-U process. This can be rewritten by changing dX according to its definition:

$$\mathrm{d}\phi(t) = \big(A + X(t)B - kX(t)R\big)\phi(t)\,\mathrm{d}t + R\phi(t)\mathrm{d}W(t), \tag{9}$$

and the initial condition is a wave function $\psi_0 \in \mathcal{H}$, such that $\|\psi_0\|^2 = 1$. To perform the normalisation condition for the probability $\mathbb{E}[\|\phi(t)\|^2] = 1$ we need to impose two self-adjoint operators K and H_0 such that

$$B = -\mathrm{i}K + \frac{k}{2}\left(R + R^\dagger\right), \qquad A = -\mathrm{i}H_0 - \frac{1}{2}R^\dagger R. \tag{10}$$

As a consequence the initial Eq. (8) becomes

$$\mathrm{d}\phi(t) = \left(-\mathrm{i}H(t) - \frac{1}{2}R^\dagger R\right)\phi(t)\,\mathrm{d}t + R\phi(t)\,\mathrm{d}W(t), \tag{11a}$$

$$H(t) := H_0 + X(t)L, \qquad L := K + \frac{\mathrm{i}k}{2}\left(R^\dagger - R\right). \tag{11b}$$

Apart from the randomness introduced by the random Hamiltonian H with colored noise $X(t)$ we have the same situation of the linear (3).

For the case of a random unitary evolution we take $B = 0$ in Eq. (8), which gives also $K = 0$. Moreover, the conditions (10) become

$$R = -\mathrm{i}V, \quad V^\dagger = V, \qquad A = -\mathrm{i}H_0 - \frac{1}{2}V^2.$$

Then, we get

$$L = -kV, \qquad H(t) = H_0 - kX(t)V. \tag{12}$$

As it was demonstrated in [7], the linear stochastic Schrödinger equation reduces to :

$$d\phi(t) = -\mathrm{i}\Big[(H_0 - kX(t)V)\,dt + V dW(t)\Big]\phi(t) - \frac{1}{2}V^2\phi(t)dt. \tag{13}$$

The evolution of the quantum system is completely determined by the time-dependent, random Hamiltonian $H(t)$ of an isolated and closed system incorporating a random environment characterized in terms of O-U process.

Sometimes, it is convenient to study the state corresponding to the statistical operator $\eta(t)$ which is the state we attribute to the system at time t, when the output is not known and this is the second method, derived in [4]. The *a priori* state that corresponds to the master equation (which is not closed) is:

$$\eta(t) = \mathbb{E}[|\psi(t)\rangle\langle\psi(t)|], \tag{14}$$

where $\mathbb{E}$ corresponds to the mean value and $\psi(t) = \phi(t)/\|\phi(t)\|$.

Using the definition (14) and (13) the stochastic master equation is obtained. The closed stochastic master equation has been derived by the adapting Nakajima-Zwanzig method (for full derivation see [4, 7]):

$$\dot{\eta}(t) \simeq \mathcal{L}_0[\eta(t)] + \frac{k}{2}\int_0^t \left[V, e^{(\mathcal{L}_0-k)(t-s)}\left[[V,\eta(s)]\right]\right] ds. \tag{15}$$

The methods presented above will be considered for the model of the dissipative qubit. Also, in the next section it will be shown, how to introduce the colored noise to the simulation algorithm.

3. The simulation

The description of open quantum systems by using stochastic wave-function methods has recently received a great deal of attention. By using the wave function instead of the density matrix, one can significantly speed up computer simulations as the dimension of the system increases [8].

Let us consider the two presented methods on the concrete example, namely the dissipative qubit. For this model we have the following parameters:

$$H_0 = \frac{\omega_0}{2}\sigma_z, \quad \omega_0 > 0, \qquad V = \sqrt{\frac{\gamma}{2}}\sigma_y, \quad \gamma > 0. \tag{16}$$

The linear stochastic Schrödinger equation (13) then becomes:

$$\begin{cases} \mathrm{d}\phi_1(t) = -\frac{1}{2}\left(\frac{\gamma}{2} + \mathrm{i}\omega_0\right)\phi_1(t)\,\mathrm{d}t - \sqrt{\frac{\gamma}{2}}\,\phi_2(t)\,\mathrm{d}X(t), \\ \mathrm{d}\phi_2(t) = -\frac{1}{2}\left(\frac{\gamma}{2} - \mathrm{i}\omega_0\right)\phi_2(t)\,\mathrm{d}t + \sqrt{\frac{\gamma}{2}}\,\phi_1(t)\,\mathrm{d}X(t), \end{cases} \tag{17}$$

and the operator $\mathcal{L}_0$:

$$\mathcal{L}_0[\sigma] = -\frac{i\omega_0}{2}[\sigma_z,\sigma] - \frac{\gamma}{2}[\sigma_y,[\sigma_y,\sigma]].$$

We use the Platen scheme [9] for which it will be convenient to rewrite the system (17) in the matrix Itô form:

$$d\boldsymbol{\phi} = Q\boldsymbol{\phi}dt + C\boldsymbol{\phi}dW, \tag{18}$$

where the corresponding support matrices are:

$$Q = \begin{pmatrix} -1/2(\gamma/2 + i\omega_0) & \sqrt{\gamma/2}kx & 0 \\ -\sqrt{\gamma/2}kx & -1/2(\gamma/2 - i\omega_0) & 0 \\ 0 & 0 & -k \end{pmatrix}, \qquad C = \begin{pmatrix} 0 & -\sqrt{\gamma/2} & 0 \\ \sqrt{\gamma/2} & 0 & 0 \\ 0 & 0 & 1/x \end{pmatrix}, \tag{19}$$

and the vector $\boldsymbol{\phi}$ is

$$\boldsymbol{\phi} = \begin{pmatrix} \phi_1 \\ \phi_2 \\ x \end{pmatrix}. \qquad (20)$$

Here the main difference from the classical Platen scheme is the presence of an O-U process with an extra variable x that have been added to the vector $\boldsymbol{\phi}$ to provide an element of the colored noise.

The Platen scheme has the form:

$$\begin{aligned} \boldsymbol{\phi}_{n+1} &= \boldsymbol{\phi}_n + \frac{1}{2}\left(\boldsymbol{a}(\Upsilon) + \boldsymbol{a}\right)\Delta \\ &\quad + \frac{1}{4}\big(\boldsymbol{b}(R_+) + \boldsymbol{b}(R_-) + 2\boldsymbol{b}\big)\Delta W \\ &\quad + \frac{1}{4}\big(\boldsymbol{b}(R_+) - \boldsymbol{b}(R_-)\big)\{\Delta W^2 - \Delta\}, \end{aligned} \qquad (21)$$

with corresponding:

$$\boldsymbol{a}(\phi) = Q\phi, \qquad \boldsymbol{b}(\phi) = C\phi,$$
$$\Upsilon = \boldsymbol{\phi}_n + \boldsymbol{a}\Delta t + \boldsymbol{b}\Delta W, \qquad R_\pm = \boldsymbol{\phi}_n + \boldsymbol{a}\Delta \pm \boldsymbol{b}\sqrt{\Delta}.$$

Finally, we can extrapolate the results to provide a higher order approximation of the resulting functional. The order 4.0 weak extrapolation [5] has the form:

$$V_{g,4}^{\Delta}(T) = \frac{1}{21}\left[32E(g(Y_T^{\Delta})) - 12E(g(Y_T^{2\Delta})) + E(g(Y_T^{4\Delta}))\right],$$

where E denotes the mean value of the simulated function g with the time steps Δ, 2Δ and 4Δ correspondingly (for our case $\Delta = 0.05$).

The solutions of (15) for different values of k are shown in figure 1. One can see that the memory effects (increasing k) slow down the decay. In figure 2 and figure 3 the analytical approximation (15) is presented together with the simulation of (18). Each simulation was done for 10^4 realisations with the help of the Platen method adapted for the presence of O-U noise, with an additional term in (20), while the initial state was taken as:

$$\eta(0) = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}. \qquad (22)$$

The choice of parameters for figure 2 and figure 3 has been optimized for the simplest case of equation (15).

4. Conclusion

One of the ways to describe the dynamics of an open quantum systems is to use the stochastic Schrödinger equations. The properties of this approach leads to effective computer simulations with the help of stochastic wave-function methods. These methods may also be used to describe systems with memory.

One of the strategies to describe memory effects in the system is to introduce the colored noise. In particular, the colored O-U noise has been added to the linear stochastic Schrödinger equation. This procedure was presented in [3] and was used to perform the simulations. To get the correct results, we adapt the Platen algorithm, with an additional term in (20), due to the presence of the colored noise.

Also, we have tested some approximation, derived in [4]. It is based on the Nakajima-Zwanzig technique but in connection to the stochastic equations. The final master equation was shown and its solution compared with the results of the simulations. The obtained curves show a good agreement for both methods.

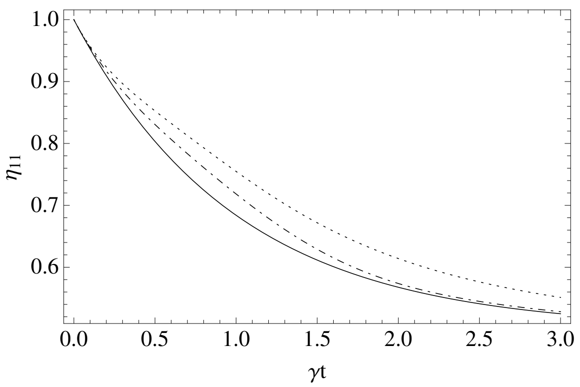

Figure 1. The solutions of (15) for different values of k: $k = 0$ (solid line), $k = 1$ (dot-dashed line), $k = 2$ (dotted line).

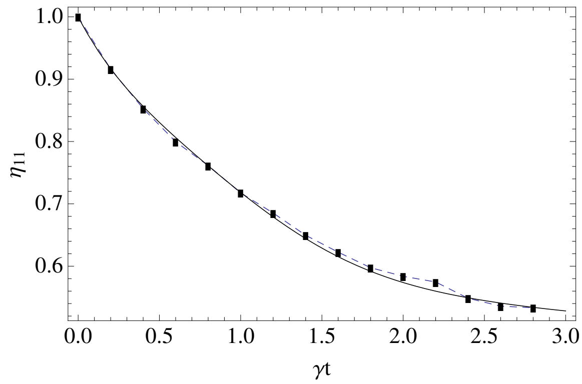

Figure 2. Plot of the mean occupation number of the excited state for the parameters $\gamma = 1, \omega_0 = \sqrt{37}/2, k = 1$. The solid line comes from the analytical approximation (15), while the dashed line and dots show the results of the stochastic simulation of (18).

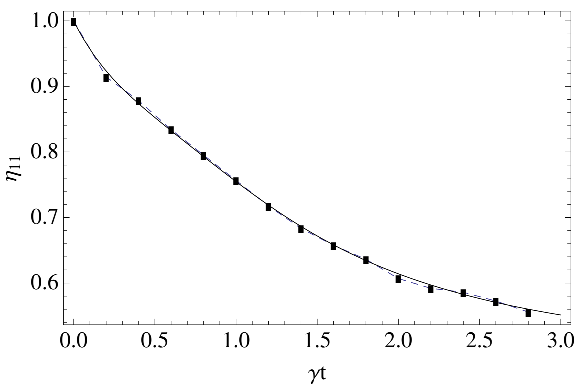

Figure 3. Plot of the mean occupation number of the excited state for the parameters $\gamma = 1, \omega_0 = \sqrt{37}/2, k = 2$. The solid line comes from the analytical approximation (15), while the dashed line and dots show the results of the stochastic simulation of (18).

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