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Non-Markovian Wave Function Simulations of Quantum Brownian Motion*

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Abstract. The non-Markovian wave function method (NMWF) using the stochastic unravelling of the master equation in the doubled Hilbert space is implemented for quantum Brownian motion. A comparison between the simulation and the analytical results shows that the method can be conveniently used to study the non-Markovian dynamics of the system.

Keywords: stochastic Schrödinger equation, open quantum systems, non-Markovian dynamics, Monte Carlo wave function methods
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1. Introduction

The theory of open quantum systems has recently received a huge deal of attention because it allows both to address fundamental questions such as the quantum measurement problem and to investigate the effect of decoherence and dissipation in the emerging quantum technologies [1]. One of the most common assumptions for describing open quantum systems is the so-called Born–Markov approximation which basically consists in neglecting memory effects of the reservoir. In other words one assumes that the correlation time of the reservoir, characterizing the time scale on which the reservoir memory would feed back to the system, is much shorter than the typical relaxation time of the system.

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When such condition is satisfied it is possible to derive a master equation describing the time evolution of the dissipative system for times longer than the correlation time of the reservoir. Under this approximation the resulting equation of motion for the reduced density matrix of the system is called Markovian master equation.

In 1976 Lindblad [2] and Gorini–Kossakowski–Sudarshan [3], demonstrated independently the most general form for a Markovian master equation, known thereafter as Lindblad form. Their theorem ensures that the density matrix satisfying a Lindblad master equation is positive at all times. A Lindblad master equation can be numerically solved by means of the powerful Monte Carlo Wave Function (MCWF) simulation methods [4–7] to study the system dynamics. These methods are based on stochastic Schrödinger equations for the state (quantum trajectories), driven by a classical stochastic process, such that the ensemble mean of the quantum trajectories recovers the density operator.

The Markovian approximation, however, does not hold for systems interacting with structured reservoirs, such as atoms decaying in photonic band gap materials or atom lasers [8]. Such physical systems, indeed, are usually characterized by reservoir correlation times longer than their typical relaxation times. In order to describe correctly their time evolution, therefore, one needs to develop approaches not based on the Markovian assumption. Another reason motivating the study of non-Markovian descriptions of the dynamics is that, very recently, the potential interest of non-Markovian reservoirs for quantum information processing has been demonstrated [9] and a non-Markovian description of quantum computing, showing the limits of the Markovian approach, has been presented [10].

Non-Markovian generalized master equations are, in general, extremely difficult to treat, even numerically. For this reason recently some methods extending the concept of stochastic unravelling from Markovian to non-Markovian evolution have been presented [11,12]. In this paper we focus on the non-Markovian wave function method (NMWF) using the stochastic unravelling of the master equation in the doubled Hilbert space [1, 11]. We describe how to implement the NMWF method for the study of quantum Brownian motion. We use Monte Carlo (MC) methods both to confirm the validity of the involved analytical solution and to demonstrate that these methods can be used to study the heating dynamics of a quantum Brownian particle in very general conditions. One might think that it is straightforward to apply MC methods, e.g. the NMWF method, once the master equation of the system and the corresponding jump operators are known. However, there exist situations in which the MC simulations become exceedingly heavy from the computer resource point of view [13, 14]. In this paper we show that, in our case, MC methods can be used conveniently to study numerically the non-Markovian system dynamics.

The paper is structured as follows. In Section 2 we review the NMWF method in the doubled Hilbert space. In Section 3 we apply the method to study quantum Brownian motion. Finally in Section 4 conclusions are presented.

2. Non-Markovian Wave Function Simulations in the Doubled Hilbert Space

The most general form of the master equation obtained from time-convolutionless projection operator technique reads [1, 11]

$$\frac{\partial}{\partial t}\rho\left(t\right)=A\left(t\right)\rho\left(t\right)+\rho\left(t\right)B^{\dagger}\left(t\right)+\sum_{i}C_{i}\left(t\right)\rho\left(t\right)D_{i}^{\dagger}\left(t\right), \tag{1}$$

with time-dependent linear operators $A\left(t\right)$, $B\left(t\right)$, $C_{i}\left(t\right)$, and $D_{i}\left(t\right)$. The unravelling of the master equation can be implemented by using the method of stochastic unravelling in the doubled Hilbert space [1] $\widetilde{\mathcal{H}}=\mathcal{H}_{S}\oplus\mathcal{H}_{S}$, where the state of the system is described by a pair of stochastic state vectors

$$\theta\left(t\right)=\left(\begin{array}{c}\phi\left(t\right)\\ \psi\left(t\right)\end{array}\right). \tag{2}$$

The time evolution of $\theta\left(t\right)$ can be described as a piecewise deterministic process (PDP) [1]. The deterministic part of the PDP is obtained by solving the following differential equation

$$\frac{\partial}{\partial t}\theta\left(t\right)=\left[F\left(t\right)+\frac{1}{2}\sum_{i}\frac{\left\|J_{i}\left(t\right)\theta\left(t\right)\right\|^{2}}{\left\|\theta\left(t\right)\right\|^{2}}\right]\theta\left(t\right), \tag{3}$$

with

$$F\left(t\right)=\left(\begin{array}{cc}A\left(t\right) & 0\\ 0 & B\left(t\right)\end{array}\right) \tag{4}$$

and

$$J_{i}\left(t\right)=\left(\begin{array}{cc}C_{i}\left(t\right) & 0\\ 0 & D_{i}\left(t\right)\end{array}\right), \tag{5}$$

where $A\left(t\right)$, $B\left(t\right)$, $C_{i}\left(t\right)$, and $D_{i}\left(t\right)$ are the operators appearing in Eq. (1).

The stochastic part of the PDP is described in terms of jumps inducing transitions of the form

$$\theta\left(t\right)\rightarrow\frac{\left\|\theta\left(t\right)\right\|}{\left\|J_{i}\left(t\right)\theta\left(t\right)\right\|}\left(\begin{array}{c}C_{i}\left(t\right)\phi\left(t\right)\\ D_{i}\left(t\right)\psi\left(t\right)\end{array}\right). \tag{6}$$

The jump rate for channel i is given by

$$P_{i}(t)=\frac{\left\|J_{i}\left(t\right)\theta\left(t\right)\right\|^{2}}{\left\|\theta\left(t\right)\right\|^{2}}. \tag{7}$$

Finally, the solution for the reduced density matrix is obtained as

$$\rho(t)=\int D\theta D\theta^{*}|\phi\rangle\langle\psi|\tilde{P}[\theta,t], \tag{8}$$

where $\tilde{P}[\theta,t]$ denotes the probability density functional and the integration is carried out over the doubled Hilbert space $\widetilde{\mathcal{H}}$ [1, 11].

3. Implementation of the Method for QBM

The dynamics of a harmonic oscillator linearly coupled with a quantized reservoir, modelled as an infinite chain of quantum harmonic oscillators, is described, in the secular approximation, by means of the following generalized master equation [15, 16]

$$\frac{d\rho_S(t)}{dt} = \frac{\Delta(t)+\gamma(t)}{2}\left[2a\rho_S(t)a^\dagger - a^\dagger a\rho_S(t) - \rho_S(t)a^\dagger a\right] + \frac{\Delta(t)-\gamma(t)}{2}\left[2a^\dagger\rho_S(t)a - aa^\dagger\rho_S(t) - \rho_S(t)aa^\dagger\right]. \tag{9}$$

In the previous equation, a and $a^\dagger$ are the annihilation and creation operators, and $\rho_S(t)$ the density matrix of the system harmonic oscillator. The time dependent coefficients $\Delta(t)$ and $\gamma(t)$ appearing in the master equation are known as diffusion and dissipation coefficient, respectively [15, 16].

The doubled Hilbert space state vector for the quantum Brownian particle reads

$$\theta(t) = \begin{pmatrix} \phi\,(t) \\ \psi\,(t) \end{pmatrix} = \begin{pmatrix} \sum_{n=0}^{\infty}\phi_n(t)|n\rangle \\ \sum_{n=0}^{\infty}\psi_n(t)|n\rangle \end{pmatrix}, \tag{10}$$

where $\phi_n(t)$ and $\psi_n(t)$ are the probability amplitudes in the Fock state basis.

By comparing Eq. (1) with the master equation (9), the operators $A(t)$ and $B(t)$ in Eq. (4) have to be chosen as

$$A(t) = B(t) = -i\omega_0 a^\dagger a - \frac{1}{2}\left\{\left[\Delta(t)+\gamma(t)\right]a^\dagger a + \left[\Delta(t)-\gamma(t)\right]aa^\dagger\right\}. \tag{11}$$

Accordingly, the operators C_i and D_i are

$$C_1(t) = D_1(t) = \sqrt{|\Delta(t)-\gamma(t)|}a^\dagger,$$
$$C_2(t) = D_2(t) = \sqrt{|\Delta(t)+\gamma(t)|}a \tag{12}$$

and the corresponding operators J_i, given by Eq. (5) become

$$J_1(t) = \sqrt{|\Delta(t)-\gamma(t)|}\begin{pmatrix} \operatorname{sgn}\left[\Delta(t)-\gamma(t)\right]a^\dagger & 0 \\ 0 & a^\dagger \end{pmatrix}$$
$$J_2(t) = \sqrt{|\Delta(t)+\gamma(t)|}\begin{pmatrix} \operatorname{sgn}\left[\Delta(t)+\gamma(t)\right]a & 0 \\ 0 & a \end{pmatrix}. \tag{13}$$

When the system dynamics and occupation of the states is restricted to the two lowest Fock states the equations resemble closely the ones used for the study of Jaynes–Cummings model with detuning [11].

The statistics of the quantum jumps is described by the waiting time distribution function $F_w(\tau)$ which represents the probability that the next jump occurs within the time interval $[t, t+\tau)$. $F_w(\tau)$, derived from the properties of the stochastic process, reads

$$F_w(\tau) = 1 - \exp\left[-\int_0^\tau \sum_{i=1,2} P_i(s)\, ds\right], \tag{14}$$

where for channel 1 (jump up, the system absorbs a quantum of energy from the environment)

$$P_1(t) = \frac{|\Delta(t) - \gamma(t)|}{\|\theta(t)\|^2} \sum_{n=0}^{\infty} (n+1) \left[|\phi_n(t)|^2 + |\psi_n(t)|^2\right], \tag{15}$$

and for channel 2 (jump down, the system emits a quantum of energy into the environment)

$$P_2(t) = \frac{|\Delta(t) + \gamma(t)|}{\|\theta(t)\|^2} \sum_{n=0}^{\infty} n \left[|\phi_n(t)|^2 + |\psi_n(t)|^2\right]. \tag{16}$$

When the jump occurs, the choice of the decay channel is made according to the factors $P_1(t)$ and $P_2(t)$. The times at which the jumps occur are obtained from Eq. (14) by using the method of inversion [1].

For very low temperatures, the non-Markovian behaviour of the heating function of the quantum Brownian particle may occur when $\langle n \rangle$ is of the order of 10^{-10}, see Fig. 1. To reach such an accuracy, a MC simulation for the estimation of $\langle n \rangle$ would require more than 10^{10} realizations to be generated. This problem may be circumvented by an appropriate scaling of the time dependent coefficients $\Delta(t) \pm \gamma(t)$ of the master equation. The method is based upon the following considerations. Let us look at the properties of the Hilbert space path integral solution of the stochastic process corresponding to the unravelling of Eq. (1). The Hilbert space path integral representation is essentially the expansion of the propagator of the stochastic process $T[\theta, t|\theta_0, t_0]$ in the number of quantum jumps [1]:

$$T[\theta, t|\theta_0, t_0] = \sum_{N=0}^{\infty} T^{(N)}[\theta, t|\theta_0, t_0], \tag{17}$$

where N denotes the number of jumps, and $T^{(N)}$ are the N jump contributions to the propagator. As long as in the time evolution period of interest there is maximally one jump per realization, it can be shown that, in the weak coupling limit and for the initial conditions used here, the relevant contribution to the propagator is given by the first two terms $T^{(0)}$, $T^{(1)}$. In this case the expectation value of an arbitrary operator O is given by

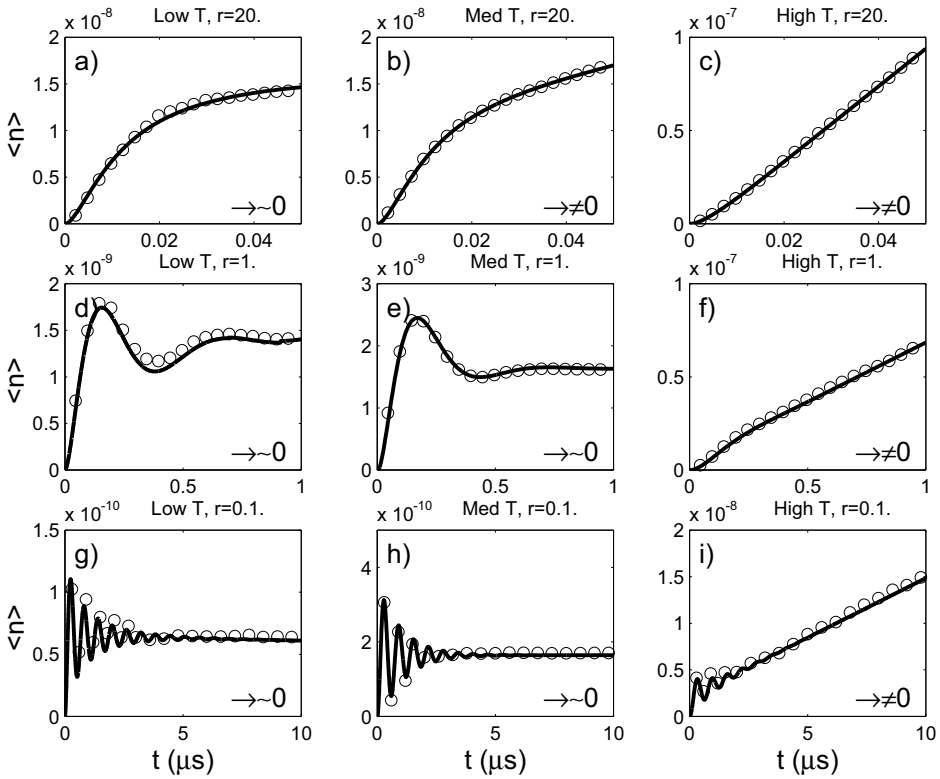

Fig. 1. Dynamics of the heating function $\langle n(t)\rangle$ in the short time non-Markovian regime. For the high T, graphics (c), (f), (i), we have used $r_0 = \omega_0/KT = 0.1$; for the intermediate T, graphics (b), (e), (h) we have used $r_0 = \omega_0/KT = 1$; for low T, graphics (a), (d), (g), we have used $r_0 = \omega_0/KT = 100$. We indicate with solid line the analytic solution and with circles the simulations performed using the NMWF method. In the right-lower corner of all graphics we indicate whether the asymptotic long time value of the heating function is null (zero T reservoir) or not

$$\langle O\rangle(t) = \int D\theta D\theta^* \langle\phi(t)|O|\psi(t)\rangle \left\{T^{(0)}[\theta,t|\theta_0,t_0] + T^{(1)}[\theta,t|\theta_0,t_0]\right\}. \qquad (18)$$

The contribution from $T^{(0)}$ gives the initial expectation value $\langle O\rangle(0)$ plus a term which is directly proportional to the decay coefficients $\Delta \pm \gamma$. Since $T^{(1)}$ is also directly proportional to the decay coefficients we get as a result that the change in the expectation value is also proportional to the decay coefficients

$$\langle O\rangle(t) - \langle O\rangle(0) \propto \Delta \pm \gamma. \qquad (19)$$

Thus, to ease the numerics and still to obtain the correct result, it is possible to speed up the decay by multiplying the coefficients $\Delta \pm \gamma$ with some suitable factor β, and to do the corresponding scaling down by dividing the calculated ensemble average by the same factor at the end of the simulation. For the heating function the validity of the scaling can be seen directly from the analytic solution (see Ref. [17]). The scaling allows to reduce the ensemble size for the estimation of the heating function from the unpractical 10^{10} to the more practical 10^4–10^5.

In Fig. 1 we compare the NMWF simulations with the analytic solution obtained using the method discussed in [18] for different values of the reservoir parameters. In more detail, we vary the temperature of the reservoir and the ratio $r = \omega_c/\omega_0$ between the reservoir cut-off frequency and the frequency of the system oscillator [17]. For all the different regimes considered we obtain a very good agreement between the simulations and the analytical results, thus confirming the usefulness of the NMWF simulation method for the study of the non-Markovian dynamics of a paradigmatic model of the theory of open quantum systems, namely the QBM model.

4. Conclusions

In this paper we have discussed how to implement the non-Markovian wave function method (NMWF) using the stochastic unravelling of the master equation in the doubled Hilbert space for QBM. Starting from the time convolutionless master equation in the secular approximation, the stochastic unravelling is derived, and the short time non-Markovian dynamics of the system is simulated by averaging over many quantum trajectories. A comparison between the simulation and the analytical results for different regimes of the system-reservoir parameter space shows that the method can be conveniently used to study the non-Markovian dynamics of the system.

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Note

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References

1. H.-P. Breuer and F. Petruccione, *The Theory of Open Quantum systems*, Oxford University Press, Oxford, 2002.

2. G. Lindblad, *Comm. Math. Phys.* **48** (1976) 119.
3. V. Gorini, A. Kossakowski and E.C.G. Sudarshan, *J. Math. Phys.* **17** (1976) 821.
4. J. Dalibard, Y. Castin and K. Mølmer, *Phys. Rev. Lett.* **68** (1992) 580.
5. K. Mølmer, Y. Castin and J. Dalibard, *J. Opt. Soc. Am. B* **10** (1993) 524.
6. M.B. Plenio and P.L. Knight, *Rev. Mod. Phys.* **70** (1998) 101, and references therein.
7. H.J. Carmichael, *An Open System Approach to Quantum Optics*, Springer-Verlag, Berlin, 1993.
8. J.J. Hope, *Phys. Rev. A* **55** (1997) R2531; G.M. Moy, J.J. Hope and C.M. Savage, *Phys. Rev. A* **59** (1999) 66; S. John and T. Quang, *Phys. Rev. Lett.* **74** (1994) 3419.
9. D. Ahn, J. Lee, M.S. Kim and S.W. Hwang, *Phys. Rev. A* **66** (2002) 012302.
10. R. Alicki, M. Horodecki, P. Horodecki and R. Horodecki, *Phys. Rev. A* **65** (2002) 062101.
11. H.P. Breuer, B. Kappler and F. Petruccione, *Phys. Rev. A* **59** (1999) 1633.
12. W.T. Strunz, L. Diósi, N. Gisin and T. Yu, *Phys. Rev. Lett.* **83** (1999) 4909.
13. J. Piilo, K.-A. Suominen and K. Berg-Sørensen, *Phys. Rev. A* **65** (2002) 033411.
14. J. Piilo, *J. Opt. Soc. Am. B* **20** (2003) 1135.
15. F. Intravaia, S. Maniscalco and A. Messina, *Eur. Phys. J. B* **32** (2003) 97.
16. S. Maniscalco, F. Intravaia, J. Piilo and A. Messina, *J. Opt. B: Quantum and Semiclass. Opt.* **6** (2004) S98.
17. S. Maniscalco, J. Piilo, F. Intravaia, F. Petruccione and A. Messina, *Phys. Rev. A* **70** (2004) 032113.
18. F. Intravaia, S. Maniscalco and A. Messina, *Phys. Rev. A* **67** (2003) 042108.