Quantum master equation for a system influencing its environment

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We derive a new perturbative quantum master equation for the reduced density matrix of a system interacting with an environment (with a dense spectrum of energy levels). The total system energy (system plus environment) is constant and finite. This equation takes into account the finite energy effects of the environment due to the total energy conservation. This equation is more general than the common perturbative equations used for describing a system in interaction with an environment (like the Redfield equation [1, 2] or the Cohen-Tannoudji one [3]) because these last equations can be deduced from it in the limit of an infinitely large environment. We apply numerically this equation to the spin-GORM model. This model represents the interaction of a two-level system with an environment described by random matrices. We compare our equation with the exact von Neumann equation of the total system and show its superiority compared to the Redfield equation (in the Markovian and non-Markovian cases).

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The study of the quantum dynamics of a system interacting with its environment is an old but still very important problem in quantum mechanics and more specifically in non-equilibrium quantum statistical mechanics. The understanding of such problems is central for the study of very fundamental physical processes such as the relaxation to the thermodynamic equilibrium, the decoherence or the thermalization at the environment temperature. Actually, one of the more general and of the most used equations to describe the dynamics of a system interacting with its environment is the non-Markovian Redfield equation. The other well-known equations used in the past for the study of such systems (the Markovian Redfield equation [1], the Cohen-Tannoudji equation [3] or the Lindblad equation [2]) can be derived from the non-Markovian Redfield equation [2]. The Markovian form of this equation was first derived empirically for understanding NMR experiments [1], but later generalized to the non-Markovian case by deducing it formally by perturbation theory from the von Neumann equation of the total system (system plus environment) [2]. The fundamental assumption in the Redfield theory is that the environment is infinite and therefore not affected by the system. As a consequence of the recent development of nanotechnology, there is an increasing interest for nanometric systems. In nanosystems, one can encounter situations where purely quantum degrees of freedom like the spin are interacting with degrees of freedom that are dense in energy but with an energy distribution that varies on small energy scales sometime of the order of the system energy. In such situations, the Redfield equation is not valid anymore, the infinite environment hypothesis fails and the finite energy effects of the total system have to be taken into account. In this paper the plan is as follows: we derive our new equation, that takes into account the finite energy effects of the total system, we then apply it to the population dynamics of the spin-GORM model (a two-level system interacting in a non-diagonal way with an environment described by Gaussian orthogonal random matrices) and we finally compare it to the exact von Neumann equation for the total system and to the Redfield equation. We will finally conclude presenting the perspectives created by this work. The quantum system that we consider has a simple spectrum (integrable system) given by his Hamiltonian $\hat{H}_S$. Its eigenvalues (respectively its eigenvectors) are given by $\{E_s\}$ (respectively by $\{|s\rangle\}$). The environment is also a quantum system but with a dense spectrum (containing many levels forming a quasi-continuum) given by a Hamiltonian $\hat{H}_B$. Its eigenvalues (respectively its eigenvectors) are given by $\{\epsilon\}$ (respectively by $\{|\epsilon\rangle\}$). The interaction between the system and the environment is generally taken to be the product of a system operator $\hat{S}$ and an environment operator $\hat{B}$. The coupling parameter $\lambda$ measures the intensity of the interaction between the system and the environment. Therefore, the Hamiltonian of the total system is given by $\hat{H}_{tot} = \hat{H}_S + \hat{H}_B + \lambda \hat{S}\hat{B}$. The exact time evolution of the total system is described by the von Neumann equation $\dot{\rho}(t) = -i[H_{tot}, \rho(t)]$, where $\dot{\rho}(t)$ is the density matrix of the total system. The system dynamics is described by the reduced density matrix of the system $\dot{\rho}_S(t) = Tr_B\dot{\rho}(t)$. The total system has a finite constant energy. At initial time, the environment is in a microcanonical state at energy $\epsilon$.

The ansatz in the Redfield derivation is to suppose that the total density matrix evolves keeping the following form:

$$\dot{\rho}(t) = \dot{\rho}_S(t) \otimes \delta(\epsilon - \hat{H}_B). \quad (1)$$

We see that the environment part of the density matrix does not evolves, supposing that the environment is not affected by the dynamics. But as we announced it, we want to include the finite total energy effects in the dynamics. The main idea (the new ansatz) is to suppose that the total density matrix can be described at all times
by a density matrix of the following form:

$$\hat{\rho}(t) = \frac{1}{n(\hat{H}_B)} \sum_{s,s'} |s\rangle\langle s'| P_{ss'}(\hat{H}_B; t),$$

(2)

where $n(\epsilon) = \text{Tr}_B \delta(\epsilon - \hat{H}_B)$ is the smoothed density of states of the environment. The reduced density matrix of the system becomes

$$\bar{\rho}_s(t) = \int d\epsilon \text{Tr}_B \delta(\epsilon - \hat{H}_B) \hat{\rho}(t) = \sum_{s,s'} |s\rangle\langle s'| \int d\epsilon P_{ss'}(\epsilon; t).$$

The only approximation made by the ansatz is that we neglect the contribution to the dynamics coming from the environment coherences. We see that the environment energy can now depend on the system state. Inserting (2) in the von Neumann equation, taking the trace over the environment degrees of freedom and performing a perturbative expansion up to the second order in $\lambda$, one gets our new equation. For the population dynamics, this equation takes the following form:

$$\dot{P}_{ss}(\epsilon; t) = -2\lambda^2 \sum_{s', s} \left[ +\langle s|\hat{S}|s'\rangle \langle s'|\hat{S}|s\rangle P_{ss}(\epsilon; t) \int d\epsilon' F(\epsilon, \epsilon') n(\epsilon') \frac{\sin(E_s - E_{s'} + \epsilon - \epsilon') t}{E_s - E_{s'} + \epsilon - \epsilon'} -\langle s|\hat{S}|s'\rangle \langle s'|\hat{S}|s\rangle P_{ss'}(\epsilon; t) \int d\epsilon' F(\epsilon, \epsilon') n(\epsilon) \frac{\sin(E_s - E_{s'} + \epsilon - \epsilon') t}{E_s - E_{s'} + \epsilon - \epsilon'} \right],$$

(3)

where $F(\epsilon, \epsilon') = |\langle \epsilon|\hat{B}|\epsilon'\rangle|^2$ where the quotes denote a smoothening over the dense spectrum of eigenvalues around $\epsilon$ and $\epsilon'$. Performing the same procedure using Markovian approximation consists in taking the infinite time limit of the time-dependent coefficients of (4) using the property $\lim_{\tau \to \infty} \frac{\sin(\xi)}{\xi} = \pi \delta(\xi)$. Performing this approximation on our new equation (respectively on the non-Markovian Redfield equation) gives the Markovian version of our new equation (respectively the Redfield equation (2)). If one further neglects the contributions of the coherences to the populations evolution and the contributions of the populations to the coherences evolution, one gets a simplified Markovian version of our new equation. This equation takes the following form for the populations dynamics:

$$\dot{P}_{ss}(\epsilon; t) = -2\pi^2 \sum_{s' \neq s} |\langle s|\hat{S}|s'\rangle|^2 F(\epsilon, E_s - E_{s'} + \epsilon) + n(E_s - E_{s'} + \epsilon) P_{ss}(\epsilon; t) + 2\pi^2 \sum_{s' \neq s} |\langle s|\hat{S}|s'\rangle|^2 F(\epsilon, E_s - E_{s'} + \epsilon) n(\epsilon) P_{s's'}(E_s - E_{s'} + \epsilon; t).$$

(4)

Doing the same for the Redfield equation one get the well known Cohen-Tannoudji equation [2]. Our simplified Markovian equation describes the evolution of the total system as a random walk between the states belonging to the same energy shell with transition probabilities given by the Fermi golden rule. This equation may look like the Pauli equation [2] but it describes the time evolution of the distributions of populations over the energy of the environment which is the new feature of our equation. On the other hand, the difference between our simplified Markovian equation (respectively the non-Markovian version of our equation) and the Cohen-Tannoudji equation [2] (respectively the non-Markovian Redfield equation) is the fact that this last equation considers that the environment density of states is not affected by the system energy. This is represented in Fig. 1. We will apply now our equation to the spin-GORM model. This model describes the evolution of a two-level system that interacts in a non-diagonal way with a complex environment. Here, the complexity is supposed to come from many-body interactions like in heavy nuclei or from a classically chaotic dynamics. Therefore, we represent all the environment operators by Gaussian orthogonal random matrices (GORM). The Hamiltonian of the total system is then $\hat{H}_{\text{tot}} = \frac{1}{2} \sigma_z + \frac{1}{\sqrt{8N}} \hat{X} + \lambda \sigma_z \frac{1}{\sqrt{8N}} \hat{X}',$
Energy $\lambda$ 0 0

The semicircular density of states of the environment is given by the Wigner semicircular $n(\epsilon) = \frac{4N}{\pi} \sqrt{\frac{1}{4} - \epsilon^2}$ with the convention that $\sqrt{x}$ for $x < 0$. The smoothed density of states of the nonperturbed total system ($\lambda = 0$) is the sum of two semicircular centered at the two energies $-\frac{\Delta}{2}$ and $\frac{\Delta}{2}$ as depicted in Fig. 2.

In this paper, we restrict ourselves to the study of the small coupling regimes $\lambda \ll 1$ because all the equations discussed in this paper are obtained perturbatively. Another restriction is related to the mean level spacing of the environment. The coupling between the levels (that is of order $\lambda^2$ because the first order in perturbation theory is zero due to the non-diagonal nature of the coupling) has to be of the order or larger than the mean level spacing $1/N$ of the environment to induce a sufficient interaction between the levels belonging to the microcanonical energy shell in order to reach a microcanonical distribution inside these shells. The criterion is therefore $\lambda^2 \geq 1/N$. Of course, the lower bound disappears in the continuum limit $N \to \infty$. The validity domain is shown in Fig. 3. The detailed study of the lower bound of the coupling parameter has been done in [7].

Applying our equation (3) to the spin-GORM model in order to study the system population evolution through $\hat{\sigma}_z$ (difference between the probability of being in the upper state of the system minus the probability of being in the lower one), one gets

$$\langle \hat{\sigma}_z \rangle^{NM}(t) = \int d\epsilon' \left[ P_{++}(\epsilon'; t) - P_{--}(\epsilon' + \Delta; t) \right]$$

where

$$\hat{P}_{\pm \pm}(\epsilon; t) =$$

$-\frac{\lambda^2}{\pi} P_{\pm \pm}(\epsilon; t) \int^{\pm \frac{\Delta}{2}} d\epsilon' \sqrt{\frac{1}{4} - \epsilon'^2} \sin(\pm \Delta + \epsilon - \epsilon')
+ \frac{\lambda^2}{\pi} \sqrt{\frac{1}{4} - \epsilon'^2} \int^{\pm \frac{\Delta}{2}} d\epsilon' P_{\pm \pm}(\epsilon'; t) \sin(\pm \Delta + \epsilon - \epsilon').$

An important remark is that the Markovian and the simplified Markovian version of our equation are the same for the spin-GORM model. Neglecting the coherences contributions to the populations dynamics is not necessary here. This has also the consequence that the Markovian Redfield equation and the Cohen-Tannoudji are the same.

The Markovian version of our equation (5) becomes the following equation for the spin-GORM model:

$$\langle \hat{\sigma}_z \rangle^M(t) = P_{++}(\epsilon; t) - P_{--}(\epsilon + \Delta; t).$$

In this case, we get an analytical solution describing an exponential decay to equilibrium:

$$\langle \hat{\sigma}_z \rangle^M(t) = \left[ \langle \hat{\sigma}_z \rangle^M(0) - \langle \hat{\sigma}_z \rangle^M_{\infty} \right] e^{-\gamma t} + \langle \hat{\sigma}_z \rangle^M_{\infty},$$

where the relaxation rate is given by

$$\gamma = \lambda^2 \left( \frac{1}{4} - \langle \epsilon \rangle^2 + \frac{1}{4} - \langle \epsilon + \Delta \rangle^2 \right),$$

and the equilibrium population by

$$\langle \hat{\sigma}_z \rangle^M_{\infty} = \sqrt{\frac{1}{4} - \langle \epsilon \rangle^2} - \sqrt{\frac{1}{4} - \langle \epsilon + \Delta \rangle^2}.$$

Notice that the relaxation rate and the equilibrium population are independent of the initial condition.

We now start the discussion of the comparison between the different equations based on the numerical simulations of Fig. 4. We always take $\langle \hat{\sigma}_z \rangle^M(0) = 1$ in our numerical simulations. The initial state of the environment is characterized by the energy of the microcanonical distribution $\epsilon$. The width of the energy shell is always $\delta \epsilon = 0.05$. The curves are averages over $\chi = 10$ realizations of GORM of size $N = 2000$ of the Hamiltonian, and over the different eigenstates of the environment energy shell.

As we announced it, our equation is necessary when the system energy $\Delta$ is of the order of magnitude of the energy scale of variation of typical environment smooth density of states: $n(\epsilon + \Delta) \neq n(\epsilon)$. But when $\Delta$ is small enough and therefore $n(\epsilon + \Delta) \approx n(\epsilon)$, our equation reduces to the non-Markovian Redfield equation. This can be well seen comparing Figs. 4A and B. In Fig. 4A, our
Markovian (M) and non-Markovian (NM) equations are very close to the Redfield M and NM ones, but this is not the case anymore in Fig. 4B. Another important point is the validity of the Markovian approximation. This approximation has the effect of constraining the dynamics inside the microcanonical energy shell of the unperturbed spectrum according to the Fermi golden rule. At short time, because $\sin\left(\frac{1}{\Delta + \epsilon - \epsilon'}t\right)$ is not yet a delta function, the non-Markovian equation has the possibility of describing a spread of the probability in energy around the microcanonical energy shell. When the delta contribution to the dynamics is important, the non-Markovian effect are very small, as in Figs. 4A and B, and can only be seen on very short time scales. But when this contribution is small or zero, like in Fig. 4C (because the microcanonical energy shell is not inside the overlapping zone as seen in Fig. 2A), then the non-Markovian effects become very important. In Fig. 4C, the Markovian curves are not represented because they completely miss the dynamics (they predict no evolution $\langle \sigma_z \rangle = 1$). Fig. 4C represents therefore a pure non-Markovian dynamics to which only the non-central part of $\frac{\sin(\pm \Delta + \epsilon - \epsilon')t}{(\pm \Delta + \epsilon - \epsilon')}$ contributes.

We can conclude saying that our new equation is always valid in the small coupling limit independently of the energy ratio between the system and the environment. It is therefore an important equation for the study of nanosystems. This equation reduces to the Redfield equation for very small system energies compared to the energy variations of the environment density of states. It can be shown that it is also in this limit that the equilibrium values of the system populations thermalize to a canonical distribution corresponding to the microcanonical temperature of the environment. The coherences dynamics will be investigated in future work.

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FIG. 4: Two-level system dynamics for the spin-GORM model.

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