Classical limit of master equation for a harmonic oscillator coupled to an oscillator bath with separable initial conditions

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The Wigner transform of the master equation describing the reduced dynamics of the system, of a harmonic oscillator coupled to an oscillator bath, was obtained by Karrlein and Grabert [Phys. Rev. E **55**, 153 (1997)]. It was shown that for some special correlated initial conditions the master equation reduces, in the classical limit, to the corresponding classical Fokker-Planck equation obtained by Adelman [J. Chem Phys. **64**, 124 (1976)]. However, for separable initial conditions the Adelman equations were not recovered. We resolve this problem by showing that, for separable initial conditions, the classical Langevin equations are somewhat different from the one considered by Adelman. We obtain the corresponding Fokker-Planck equation and show that they exactly match the classical limit of the evolution of the Wigner function obtained from the master equation for separable initial conditions. We also discuss why thermal initial conditions correspond to Adelman's solution.

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The concept of "open" quantum systems is a ubiquitous one in that any system can be thought of as being not isolated but being surrounded by a larger system constituting its environment which should effect its dynamics. The theory of open quantum systems provides a natural route for the reconciliation of damping with the process of quantization. Ford, Kac, and Mazur [1] suggested the first microscopic model describing dissipative effects in which the system was assumed to be coupled to an infinite number of harmonic oscillators. Interest in quantum dissipation was intensified by the work of Caldeira and Leggett [2] who used the influence functional approach, developed by Feynman and Vernon [3], to discuss quantum Brownian motion. They considered the case where the system and its environment were initially uncorrelated, the so called separable initial condition. This was generalized to the situation where initial correlations exist between the system and its environment by Hakim and Ambegaokar [4], Smith and Caldeira [5], Grabert, Schramm, and Ingold [6], Chen, Lebowitz, and Liverani [7], and Banerjee and Ghosh [8] among others. The master equation for the quantum Brownian motion of a harmonic oscillator in a bosonic bath of harmonic oscillators was obtained by Haake and Reibold [9] and later by Hu, Paz, and Zhang [10] who used path integral methods in their derivation. A derivation of the Wigner transform of this equation was also given by Halliwell and Yu [11] and a solution of this Fokker-Planck equation with time dependent coefficients was given by Ford and O'Connell [12]. The reduced density matrix of a damped parametric oscillator was obtained by Zerbe and Hanggi [13], for the case of separable initial conditions, from which they obtained the master equation and its corresponding Wigner function.

In a very interesting paper, Karrlein and Grabert [14] studied the master equation for the reduced density matrix of the system for generalized correlated initial conditions. They showed that in general it is not possible to obtain a Liouvillean operator for the master equation of the reduced dynamics of the system under the influence of its environment. However, for some specialized correlated initial conditions like the one discussed by Hakim and Ambegaokar [4], called the thermal initial condition, and for the case of the time evolution of equilibrium correlation functions [6], it is possible to obtain the Liouvillean to describe the reduced system dynamics. In both these cases Karrlein and Grabert [14] obtained the Fokker-Planck equation from the Wigner transform of the master equation. They found that in the classical limit, these equations reduced exactly to the corresponding equation obtained by Adelman [15] for the dissipative dynamics of the classical harmonic oscillator driven by a Gaussian non-Markovian noise. They then considered the case of separable initial conditions and found that in the classical limit the corresponding Fokker-Planck equation does not reduce to the Adelman equation. It was suggested that this indicated a problem with separable initial conditions and that this could affect the long time behavior of the system. We find this a very intriguing as well as an interesting point and in this Brief Report we look at it more closely.

We first point out that the Langevin equation for the system consisting of a harmonic oscillator coupled to a bath of harmonic oscillators with which it is initially uncorrelated, differs from the one used by Adelman [15] by an additional term. This additional term leads to a different Fokker-Planck equation and is the crux that enables us to resolve the issue. We show that the Fokker-Planck equation obtained from the Langevin equation with this additional term is the exact classical limit of the corresponding equation in the quantum regime obtained by Karrlein and Grabert [14]. We also give a brief discussion on why the Langevin equation used by Adelman is the correct classical equation describing a correlated initial state.

We consider a single harmonic oscillator described by the phase space variables (x,p) and with a natural frequency ω_0. The oscillator is coupled to a heat bath modeled by N independent oscillators described by $\{X_\alpha, P_\alpha\}$ and which have

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frequencies $\{\omega_\alpha\}$. We will eventually take the limit $N\to\infty$. The full Hamiltonian is taken to be [16,17]

$$H=\frac{p^2}{2}+\frac{\omega_0^2x^2}{2}+\sum_\alpha\left[\frac{P_\alpha^2}{2}+\frac{\omega_\alpha^2X_\alpha^2}{2}-xc_\alpha X_\alpha\right]. \tag{1}$$

Using the equations of motion for the system and bath variables, the bath variables can be eliminated to yield the following Langevin equation describing the reduced dynamics of the system:

$$\ddot{x}=-\omega^2x-\gamma(t)x(0)-\int_0^t dt'\,\gamma(t-t')\dot{x}(t')+\eta(t), \tag{2}$$

where ω is a shifted frequency given by $\omega^2=\omega_0^2-\Sigma_\alpha c_\alpha^2/\omega_\alpha^2$ and $\gamma(t)=\Sigma_\alpha(c_\alpha^2/\omega_a^2)\cos(\omega_\alpha t)$. The treatment is valid both classically and quantum mechanically. In the quantum case the variables correspond to operators in the Heisenberg representation. Separable initial conditions imply that at $t=0$ the reservoir is isolated and in equilibrium. We then find that the noise correlations are given by

$$\frac{1}{2}\langle\eta(t)\,\eta(t')+\eta(t')\,\eta(t)\rangle=\hbar\,K'(t-t'), \tag{3}$$

where

$$K'(t)=\sum_\alpha\frac{c_\alpha^2}{2\omega_\alpha}\cos\omega_\alpha t\coth\frac{\hbar\omega_\alpha}{2k_BT}. \tag{4}$$

Here we have used the notation in Refs. [6,14]. In the classical limit the noise correlation reduces to the usual fluctuation-dissipation relation $\langle\eta(t)\,\eta(t')\rangle=k_BT\gamma(t-t')$.

The Langevin equation considered by Adelman [15] is similar to Eq. (2). The difference is in the initial condition dependent term $-\gamma(t)x(0)$, the so called initial slip term [18,19] which, as we will see, is crucial in getting the correct Fokker-Planck equation. In order to obtain the Fokker-Planck equation from the above Langevin equation we follow the method used by Adelman [15]. This method relies on a simplification achieved by using the following transformation, from the variables $\{x,p=\dot{x}\}$ to the new variables $\{q_1,q_2\}$

$$\begin{pmatrix}x(t)\\p(t)\end{pmatrix}=\begin{pmatrix}H(t)&G(t)\\\dot{H}(t)&\dot{G}(t)\end{pmatrix}\begin{pmatrix}q_1(t)\\q_2(t)\end{pmatrix}. \tag{5}$$

Here $H(t)$ and $G(t)$ are solutions of the homogeneous part of Eq. (2) for the initial conditions $H(0)=1,\dot{H}(0)=0$ and $G(0)=0,\dot{G}(0)=1$, respectively. The steps required to construct the Fokker-Planck equation using this method are somewhat nontrivial, but for the sake of brevity and compactness we omit them here and refer the interested reader to Ref. [20] for the details. As a result of the analysis we obtain the following Fokker-Planck equation:

$$\frac{\partial P[x,p,t|x(0),p(0),0]}{\partial t}=-p\frac{\partial P}{\partial x}+\gamma_q x\frac{\partial P}{\partial p}+\gamma_p\frac{\partial(pP)}{\partial p}+D_p\frac{\partial^2P}{\partial p^2}+D_q\frac{\partial^2P}{\partial x\,\partial p}, \tag{6}$$

where

$$\gamma_q=\frac{\ddot{G}^2-\dot{G}\dddot{G}}{\dot{G}^2-G\ddot{G}},$$

$$\gamma_p=\frac{G\dddot{G}-\dot{G}\ddot{G}}{\dot{G}^2-G\ddot{G}},$$

$$D_q=\frac{1}{2}\ddot{A}_{11}-A_{22}+\gamma_qA_{11}+\frac{\gamma_p}{2}\dot{A}_{11},$$

$$D_p=\frac{1}{2}\dot{A}_{22}+\frac{\gamma_q}{2}\dot{A}_{11}+\gamma_pA_{22},$$

with

$$A_{11}=-k_BT\left(G^2+\frac{F^2-1}{\omega^2}\right),$$

$$A_{22}=-k_BT(\omega^2G^2+\dot{G}^2-1),$$

and

$$F(t)=1-\omega^2\int_0^t dt'G(t').$$

In the classical limit $\hbar K'(t)\to k_BT\gamma(t)$, which implies that the classical limits of the functions $K_q(t)$ and $K_p(t)$ in Ref. [14] are

$$\hbar K_q(t)\to A_{11},\quad \hbar\,K_p(t)\to A_{22}. \tag{7}$$

With this we immediately see that the coefficients of the equation for the Wigner function, given by Eq. (89) in Ref. [14], reduces in the classical limit, to those in the Fokker-Planck equation given by Eq. (6).

We now briefly comment on the precise reason for the observed correspondence between the Adelman results and the quantum Fokker-Planck equation for the correlated initial conditions considered in Ref. [14]. The Langevin equation used by Adelman also follows from the same microscopic model if, instead of choosing a separable initial condition, we take a correlated initial state which is *prepared* by making measurements on an equilibrium state of the *coupled* system and bath. Classically if we want to describe a similar situation, corresponding to the quantum cases studied in Refs. [14,17], then the corresponding Langevin equation should describe the time evolution of the system's phase space variables $\{x,p\}$ *given* that an initial measurement, in the initial equilibrium state of the *coupled* system and bath, gave the values $\{x(0),p(0)\}$. Starting from the same model of reservoir with the full Hamiltonian given by Eq. (1) we again get an equation in the form of Eq. (2) but the noise correla-

tions are now different since at $t=0$ the bath and system variables are correlated. A simplification occurs if we redefine the noise [17,21] and write $\xi(t)=\eta(t)-\gamma(t)x(0)$. Averaging the bath variables over its distribution, which in this case is given by the *conditional* probability of $\{X_\alpha(0),P_\alpha(0)\}$ given that an initial measurement in the initial equilibrium state on the system gave the values $\{x(0),p(0)\}$, we find that $\xi(t)$ is again a Gaussian stationary process with exactly the same correlations as obtained for $\eta(t)$ for separable initial conditions [17,20,21]. The corresponding Langevin equation is now exactly the equation of Adelman [15]. This shows that the Langevin equation of Adelman is the correct classical equation describing a correlated initial state.

In the literature various initial conditions have been discussed [2,4,6]. These correspond to different and valid physical situations. However, there is some confusion in the literature regarding the importance of initial conditions. The equivalence of the separable and correlated initial conditions was suggested in Ref. [7]. On the other hand, it was noted in Ref. [14] that for separable initial conditions there was no correspondence between the quantum and classical Fokker-Planck equations and hence it was suggested that there could be a problem with separable initial conditions. Our work clarifies this point and shows that a correspondence exists even for factorizing initial conditions. We show that one needs to start with a different Langevin equation [Eq. (2)] than that used by Adelman. Our work highlights the importance of initial conditions in the modeling of physical situations. Depending on the situation to be studied, there is a different process describing the dynamics, the basic point being that correlated and uncorrelated initial conditions lead to different classical Langevin equations and hence to different Fokker-Planck equations.

In conclusion we have shown that for the case of a single harmonic oscillator coupled to a bath of oscillators there is an exact correspondence between the classical Fokker-Planck equation and the quantum equations for the Wigner function both for some special correlated as well as uncorrelated initial conditions.

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