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# Langevin and Master Equation in Quantum Mechanics

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The behavior of a system in contact with a heat bath can be described either by a Langevin equation or by an equation for its density matrix. As both descriptions inevitably involve approximations, it is not evident that their results coincide. It is shown here by explicit calculation that they do. The main complication is that in the Langevin equation the random force is multiplied by a nonconstant factor, which itself feels the fluctuations. In an alternative formulation of the Langevin approach this complication is avoided.

**KEY WORDS:** Quantum Langevin equation; quantum master equation.

## 1. INTRODUCTION

In classical mechanics the relationship between the Langevin equation and the Fokker–Planck equation is well known,(1) but in quantum mechanics it is less obvious. In this article we shall derive explicitly both equations and compare the results. The Fokker–Planck equation takes the form of an equation for the density matrix, which in this connection is usually called the quantum master equation.

Consider a quantum system S, with Hamiltonian $H_S$, in interaction with a bath B of harmonic oscillators, whose Hamiltonian is

$$H_B = \sum k_n a_n^\dagger a_n$$

Here $a_n^\dagger$ and $a_n$ are the creation and annihilation operators of the $n$th bath oscillator and the $k_n$ are their frequencies. The frequencies are supposed to be densely distributed along the positive real axis. The interaction between

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It is a pleasure to dedicate this work to Matthieu Ernst on the occasion of his 60th birthday.

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S and B is given by a Hamiltonian $H_{\rm I}$, which is a product, $H_{\rm I}=\lambda SB$, of an operator $S$ referring to the system, and a bath operator

$$B=\sum v_n(a_n+a_n^\dagger)$$

The $v_n$ are coupling constants and $\lambda$ is a parameter that scales the strength of the interaction. Thus the total Hamiltonian of the combined system is

$$H_{\rm T}=H_{\rm S}+\sum k_n a_n^\dagger a_n+\lambda S\sum v_n(a_n+a_n^\dagger) \tag{1}$$

In Section 2 we derive an equation that expresses the time derivative of the density matrix $\rho_{\rm S}$ of the system S, which is obtained from the density matrix of the total system by eliminating the bath variables in a well-known way. An expansion to order $\lambda^2$ turns this into an equation for $\rho_{\rm S}$ alone, which is the quantum master equation. From this equation it is possible to find an equation for the rate of change of the expectation value of an arbitrary system operator $G$.

In Section 3 an equation for $G$ is obtained resembling a Langevin equation, but its random term contains a prefactor, which has the effect that the average is not zero. It is essential to compute the average of this term in order to obtain an equation for the time dependence of the average of $G$. The resulting average of $\dot{G}(t)$ then agrees with that obtained from the master equation.

In Section 4 an alternative derivation of the Langevin equation is given and the results are shown to agree with those of Sections 2 and 3.

Section 5 contains a number of remarks and comments.

## 2. THE QUANTUM MASTER EQUATION

Let $\rho_{\rm T}$ be the density matrix of the total system S + B. It obeys the exact evolution equation

$$\dot{\rho}_{\rm T}=-i[H,\rho_{\rm T}]\equiv\mathscr{L}\rho_{\rm T}=(\mathscr{L}_{\rm S}+\mathscr{L}_{\rm B}+\lambda\mathscr{L}_{\rm I})\,\rho_{\rm T} \tag{2}$$

$\mathscr{L}$ stands for a superoperator acting on the space of operators $\rho$. We are interested in the density matrix $\rho_{\rm S}$ of the system S alone, obtained from $\rho_{\rm T}$ by taking the trace over the bath. The method for obtaining an approximate equation for $\rho_{\rm S}$ alone is well known,(1,2) but we shall briefly summarize it here.

Define the projection superoperator $\mathscr{P}$ by its action on any operator in the total Hilbert space:

$$\mathscr{P}\rho_{\rm T}=\rho_{\rm B}^{\rm e}\,{\rm Tr}_{\rm B}\,\rho_{\rm T}=\rho_{\rm B}^{\rm e}\rho_{\rm S}$$

where $\rho_{\mathrm{B}}^{\mathrm{e}}$ is the density matrix that describes the equilibrium state of the bath. Note the identities

$$\mathcal{P}\mathcal{L}_{\mathrm{S}}=\mathcal{L}_{\mathrm{S}}\mathcal{P}, \qquad \mathcal{P}\mathcal{L}_{\mathrm{B}}=\mathcal{L}_{\mathrm{B}}\mathcal{P}=0, \qquad \mathcal{P}\mathcal{L}_{\mathrm{I}}\mathcal{P}=0$$

The meaning of the last one is that the average of the interaction term vanishes, which is the case in most applications.

Equation (2) can be split into two coupled equations for $\mathcal{P}\rho_{\mathrm{T}}$ and $(1-\mathcal{P})\,\rho_{\mathrm{T}}=\mathcal{Q}\rho_{\mathrm{T}}$:

$$\delta_t\mathcal{P}\rho_{\mathrm{T}}=\mathcal{L}_{\mathrm{S}}\mathcal{P}\rho_{\mathrm{T}}+\lambda\mathcal{P}\mathcal{L}_{\mathrm{I}}\mathcal{Q}\rho_{\mathrm{T}} \tag{3a}$$

$$\delta_t\mathcal{Q}\rho_{\mathrm{T}}=\mathcal{Q}\mathcal{L}\mathcal{Q}\rho_{\mathrm{T}}+\lambda\mathcal{Q}\mathcal{L}_{\mathrm{I}}\mathcal{P}\rho_{\mathrm{T}} \tag{3b}$$

Solving the second line yields

$$\mathcal{Q}\rho_{\mathrm{T}}(t)=\lambda\int_0^t e^{\mathcal{Q}\mathcal{L}\mathcal{Q}(t-t')}\,\mathcal{Q}\mathcal{L}_{\mathrm{I}}\mathcal{P}\rho_{\mathrm{T}}(t')\,dt' \tag{4}$$

The initial value $\mathcal{Q}\rho_{\mathrm{T}}(0)$ vanishes because we assume that at some initial time $t=0$ the density matrix factorizes and the bath is in equilibrium:

$$\rho_{\mathrm{T}}(0)=\rho_{\mathrm{S}}(0)\otimes\rho_{\mathrm{B}}^{\mathrm{e}} \tag{5}$$

Substitute (4) into (3a) to get an equation for $\rho_{\mathrm{S}}(t)$ by itself,

$$\dot{\rho}_{\mathrm{S}}(t)=\mathcal{L}_{\mathrm{S}}\rho_{\mathrm{S}}(t)+\lambda^2\,\mathrm{Tr}_{\mathrm{B}}\,\mathcal{L}_{\mathrm{I}}\int_0^t e^{\mathcal{Q}\mathcal{L}\mathcal{Q}\tau}\mathcal{Q}\mathcal{L}_{\mathrm{I}}\mathcal{Q}\rho_{\mathrm{B}}^{\mathrm{e}}\rho_{\mathrm{S}}(t-\tau)\,d\tau$$

The second term is multiplied by $\lambda^2$, so that in the exponent the interaction term may be neglected ("Born approximation")

$$\dot{\rho}_{\mathrm{S}}(t)=\mathcal{L}_{\mathrm{S}}\rho_{\mathrm{S}}(t)+\lambda^2\int_0^t \{\mathrm{Tr}_{\mathrm{B}}\,\mathcal{L}_{\mathrm{I}}e^{\mathcal{L}_{\mathrm{S}}\tau}e^{\mathcal{L}_{\mathrm{B}}\tau}\mathcal{Q}\mathcal{L}_{\mathrm{I}}\rho_{\mathrm{B}}^{\mathrm{e}}\}\,\rho_{\mathrm{S}}(t-\tau)\,d\tau \tag{6}$$

This is not just an *ad hoc* approximation, but an essential step; under the integral the evolution is treated as unperturbed.(3) The quantity in curly brackets is a superoperator acting on $\rho_{\mathrm{S}}(t-\tau)$, which works out to

$$-\mathrm{Tr}_{\mathrm{B}}[SB,\,e^{\mathcal{L}_{\mathrm{S}}\tau}e^{\mathcal{L}_{\mathrm{B}}\tau}[SB,\,\rho_{\mathrm{B}}^{\mathrm{e}}\rho_{\mathrm{S}}(t-\tau)]]$$

The exponentials move the time forward in $\rho_{\mathrm{S}}$, but backward in the observables $S$ and $B$,

$$-\mathrm{Tr}_{\mathrm{B}}[SB,\,[S_0(-\tau)\,B_0(-\tau),\,\rho_{\mathrm{B}}^{\mathrm{e}}\rho_{\mathrm{S}}(t)]]$$

The subscript zero indicates evolution according to the unperturbed $\mathscr{L}_S+\mathscr{L}_B\equiv\mathscr{L}_0$ (in other words, the interaction representation). Thus

$$B_0(t)=\sum v_n\{a_n(0)\,e^{-ik_nt}+a_n^\dagger e^{ik_nt}\} \tag{7}$$

The double commutators work out to

$$\begin{aligned}&SS_0(-\tau)\,\rho_S(t)\langle BB_0(-\tau)\rangle^e-S\rho_S(t)\,S_0(-\tau)\langle B_0(-\tau)\,B\rangle^e\\&-S_0(-\tau)\,\rho_S(t)\,S\langle BB_0(-\tau)\rangle^e+\rho_S(t)\,S_0(-\tau)\,S\langle B_0(-\tau)\,B\rangle^e\end{aligned}$$

The angular brackets $\langle\ \rangle^e$ indicate an average over the equilibrium distribution $\rho_B^e$ of the bath. One easily finds

$$\begin{aligned}\langle BB_0(-\tau)\rangle^e&=\sum v_n^2\left(\frac{e^{-ik_n\tau}}{1-e^{-\beta k_n}}+\frac{e^{ik_n\tau}}{e^{\beta k_n}-1}\right)\\&=\Gamma_c(\tau)-i\Gamma_s(\tau)\end{aligned}$$

where

$$\Gamma_c(\tau)=\sum v_n^2\cos k_n\tau\coth(\tfrac{1}{2}\beta k_n),\qquad \Gamma_s(\tau)=\sum v_n^2\sin k_n\tau$$

and $\beta$ indicates the bath temperature. Similarly

$$\langle B_0(-\tau)\,B\rangle^e=\Gamma_c(\tau)+i\Gamma_s(\tau)$$

After some algebra one obtains

$$\begin{aligned}\dot\rho_S(t)=\mathscr{L}_S\rho_S(t)&+i\lambda^2\int_0^t\Gamma_s(\tau)[S,[S_0(-\tau),\rho_S(t)]]_+\,d\tau\\&-\lambda^2\int_0^t\Gamma_c(\tau)[S,[S_0(-\tau),\rho_S(t)]]\,d\tau\end{aligned} \tag{8}$$

where $[\cdots]_+$ denotes the anticommutator.

This is the quantum master equation for the density matrix $\rho_S(t)$. From it one can determine for any observable $G$ referring to the system S how its average $\langle G\rangle(t)=\mathrm{Tr}_S\,G\rho_S(t)$ evolves. Multiply (6) with $G$ and take the trace over S:

$$\begin{aligned}\delta_t\langle G\rangle(t)=-\langle\mathscr{L}_SG\rangle(t)&+i\lambda^2\int_0^t\Gamma_s(\tau)\langle[[G,S],S_0(-\tau)]_+\rangle(t)\,d\tau\\&-\lambda^2\int_0^t\Gamma_c(\tau)\langle[[G,S],S_0(-\tau)]\rangle(t)\,d\tau\end{aligned} \tag{9}$$

This consequence of the quantum master equation can be compared to the average given by the Langevin equation derived in the next two sections.

## 3. THE LANGEVIN EQUATION

We denote by $S(t)$, $G(t)$, $a_n(t)$, etc., the Heisenberg operators whose time dependence is determined by the total Hamiltonian (1). Thus

$$\begin{aligned}\dot{G}(t) &= i[H_{\mathrm{T}}, G(t)] \\ &= i[H_{\mathrm{S}}(t), G(t)] + i\lambda[S(t), G(t)] \sum v_n\{a_n(t) + a_n^\dagger(t)\} \\ \dot{a}_n(t) &= -ik_n a_n(t) - i\lambda v_n S(t)\end{aligned}$$

The latter equation can be solved to give

$$a_n(t) = a_n(0)\, e^{-ik_n t} - i\lambda v_n \int_0^t e^{ik_n(t-t')} S(t')\, dt'$$

Substitution in the former yields

$$\begin{aligned}\dot{G}(t) = i[H_{\mathrm{S}}(t), G(t)] + L(t) - 2i\lambda^2[S(t), G(t)]& \\ \times \sum v_n^2 \int_0^t \sin k_n(t-t')\, S(t')\, dt'& \qquad (10\mathrm{a})\end{aligned}$$

$$L(t) = i\lambda[S(t), G(t)]\, B_0(t) \qquad (10\mathrm{b})$$

where $B_0(t)$ is the same expression as given in (7).

This equation resembles a Langevin equation, but it is still exact; solving it would be tantamount to solving the Schrödinger equation for the total system. It is necessary to apply an approximation by neglecting all terms of higher order than $\lambda^2$. Accordingly we replace on the second line of (10a) the Heisenberg operators by their interaction representation:

$$S_0(t) = e^{-\mathscr{L}_{\mathrm{S}} t} S(0), \qquad G_0(t) = e^{-\mathscr{L}_{\mathrm{S}} t} G(0)$$

This turns Eq. (10) into a true Langevin equation. The fluctuating force $L(t)$, however, does not have an average equal to zero, owing to the commutator that multiplies $B_0(t)$. We have to find this average to order $\lambda^2$.

The exact time dependence of the commutator in (10b) is given by

$$[S(t), G(t)] = e^{-(\mathscr{L}_0 + \lambda\mathscr{L}_1)t}[S(0), G(0)], \qquad \mathscr{L}_0 = \mathscr{L}_{\mathrm{S}} + \mathscr{L}_{\mathrm{B}}$$

We use the operator identity

$$e^{-(\mathscr{L}_0+\lambda\mathscr{L}_1)t} = e^{-\mathscr{L}_0 t} - \int_0^t e^{-\mathscr{L}_0(t-\tau)}\lambda\mathscr{L}_1 e^{-(\mathscr{L}_0+\lambda\mathscr{L}_1)}\,d\tau$$

$$= e^{-\mathscr{L}_0 t} - \lambda\int_0^t e^{-\mathscr{L}_0(t-\tau)}\mathscr{L}_1 e^{-\mathscr{L}_0\tau}\,d\tau + \mathcal{O}(\lambda^2) \qquad (11)$$

When this is substituted into (10b) the first term is

$$i[S_0(t), G_0(t)]\, B_0(t)$$

The average of this term over the initial bath distribution vanishes because $B_0(t)$ is linear in the $a_n$, $a_n^\dagger$, while $S_0(t)$, $G_0(t)$ are independent of the bath. The second term, however, yields

$$\langle L(t)\rangle^{\mathrm{e}} = -\lambda\int_0^t [S_0(t-\tau), [S_0(t), G_0(t)]]\langle B_0(t-\tau)\, B_0(t)\rangle^{\mathrm{e}}\, d\tau$$

$$= -\lambda\int_0^t [S_0(t-\tau), [S_0(t), G_0(t)]]\{\Gamma_c(\tau) + i\Gamma_s(\tau)\}\, d\tau$$

Substitution in (10a) finally gives

$$\delta_t\langle G(t)\rangle^{\mathrm{e}} = i[H_S(t), \langle G(t)\rangle^{\mathrm{e}}]$$

$$-\lambda^2\int_0^t \Gamma_c(\tau)[S_0(t-\tau), [S_0(t), G(t)]]\, d\tau$$

$$-i\lambda^2\int_0^t \Gamma_s(\tau)[S_0(t-\tau), [S_0(t), G(t)]]_+\, d\tau$$

When this is averaged over $\rho_S(0)$ one obtains the same formula as the result (9) of the master equation treatment. Note that in this equation $S_0(t)$ may be replaced with $S(t)$, and $G_0(t)$ with $\langle G(t)\rangle^{\mathrm{e}}$, because that makes no difference in this order of $\lambda$.

## 4. ALTERNATIVE DERIVATION OF THE LANGEVIN EQUATION

An alternative derivation of the Langevin equation may be obtained as follows. Define a projection superoperator $\mathscr{P}^\dagger$ acting on the *observables* $C$ in the total Hilbert space by taking their bath average[4, 5]

$$\mathscr{P}^\dagger C = \mathrm{Tr}_{\mathrm{B}}(\rho_{\mathrm{B}}^{\mathrm{e}} C) = \langle C\rangle^{\mathrm{e}}$$

It is the adjoint of the projector $\mathscr{P}$ in Section 2. The evolution of any operator $C$ is

$$\dot{C}(t) = \mathscr{L}^{\dagger} C(t) = -\mathscr{L} C(t) = i[H_{\mathrm{T}}, C(t)]$$

Note the identities

$$\mathscr{P}^{\dagger}\mathscr{L}_{\mathrm{S}} = \mathscr{L}_{\mathrm{S}}\mathscr{P}^{\dagger}, \qquad \mathscr{P}^{\dagger}\mathscr{L}_{\mathrm{B}} = 0, \qquad \mathscr{P}^{\dagger}\mathscr{H}_{\mathrm{I}} = 0$$

Consider an observable $G$ in the system space. Our aim is to derive a Langevin equation for its Heisenberg representation $G(t)$. Introduce the quantity

$$K(t) = -e^{-\mathscr{Q}^{\dagger}\mathscr{L}t} Q^{\dagger}\mathscr{L}G$$

which will turn out to be the fluctuating force. One has

$$-\mathscr{L}G = i[H_{\mathrm{S}}, G] + i\lambda[H_{\mathrm{I}}, G]$$

$$-\mathscr{P}^{\dagger}\mathscr{L}G = i[H_{\mathrm{S}}, G]$$

Hence

$$K(t) = e^{-\mathscr{Q}^{\dagger}\mathscr{L}t} i\lambda[H_{\mathrm{I}}, G] = e^{-\mathscr{Q}^{\dagger}\mathscr{L}t}\{\dot{G} - i[H_{\mathrm{B}}, G]\} \tag{12}$$

With the aid of the identity (11) one may write

$$K(t) = \dot{G}(t) - i[H_{\mathrm{S}}, G](t) + \int_0^t e^{-\mathscr{L}(t-\tau)}\mathscr{P}^{\dagger}\mathscr{L}K(\tau)\,d\tau$$

which is the same as

$$\begin{aligned}\dot{G}(t) &= K(t) + i[H_{\mathrm{S}}, G](t)\\ &\quad - \lambda^2 \int_0^t e^{-\mathscr{L}(t-\tau)} \langle [H_{\mathrm{I}}, e^{-\mathscr{Q}^{\dagger}\mathscr{L}t}[H_{\mathrm{I}}, G]]\rangle^{\mathrm{e}}\,d\tau\end{aligned}$$

This is an exact equation for $G(t)$. In order to obtain the Langevin equation the $\tau$ dependence must be approximated by replacing $\mathscr{L}$ with $\mathscr{L}_0$; we have

$$\begin{aligned}\dot{G}(t) &= K(t) + i[H_{\mathrm{S}}, G](t)\\ &\quad - \lambda^2 \int_0^t e^{-\mathcal{L}t} \langle [S_0(-\tau)\, B_0(-\tau), [SB, G]] \rangle^{\mathrm{c}}\, d\tau\\ &= K(t) + i[H_{\mathrm{S}}, G](t)\\ &\quad - i\lambda^2 \int_0^t \Gamma_s(\tau) [S_0(-\tau), [S, G]]_+ (t)\, d\tau\\ &\quad - \lambda^2 \int_0^t \Gamma_c(\tau) [S_0(-\tau), [S, G]](t)\, d\tau \qquad (13)\end{aligned}$$

This is an operator equation in the total space of system plus bath. It is a Langevin equation for $G(t)$.

In order to compare this equation with the master equation we average it over the initial distribution (5). First the average over $\rho_{\mathrm{B}}^{\mathrm{c}}$ yields

$$\begin{aligned}\langle \dot{G}(t) \rangle^{\mathrm{c}} &= i\langle [H_{\mathrm{S}}, G](t) \rangle^{\mathrm{c}}\\ &\quad + i\lambda^2 \int_0^t \Gamma_s(\tau) \langle \{ [[G, S], S_0(-\tau)]_+ \}(t) \rangle^{\mathrm{c}}\, d\tau\\ &\quad - \lambda^2 \int_0^t \Gamma_c(\tau) \langle \{ [[G, S], S_0(-\tau)] \}(t) \rangle^{\mathrm{c}}\, d\tau\end{aligned}$$

This is an operator in the system space alone. Finally the average over $\rho_{\mathrm{S}}(0)$ yields an equation which is identical to that obtained in Section 2. Note that the bath average of the fluctuating force $\langle K(t) \rangle^{\mathrm{c}}$ vanishes according to (12).

## 5. DISCUSSION

Our first remark is meant to emphasize the crucial role of the "Born approximation." In each of the three preceding sections the derivation consisted in first rewriting the exact equation in a suitable form, and subsequently replacing under the integral the actual time evolution by the unperturbed one. Without this step one is stuck with a formally correct equation, but of no use, because it cannot be solved and none of the familiar features of damping and fluctuations can be recognized in it.

A second remark is that what is here called the Langevin equation is actually much more general than the familiar one describing Brownian motion. Equations (10) and (13) are formulated for any system observable

$G$ rather than just for the velocity.(6) Let us take the special case of a one-dimensional particle in potential $V(Q)$, with an interaction as in (1) in which $S=Q$; and let us apply (13) to the observable $G=P$. The last line of (13) vanishes and one gets

$$\dot{P}(t) = -V'(Q(t)) + 2\lambda^2 \int \Gamma_s(\tau)\, Q(t-\tau)\, d\tau + K(t)$$

$$K(t) = -\lambda B_0(t)$$

After partial integration this reduces to the well-known Langevin equation with memory.

The third remark is that Eqs. (8) and (13) are not yet satisfactory inasmuch as the integrations over $\tau$ extend from 0 to $t$, and therefore still refer to the initial time [at which the initial condition (5) has been imposed]. It is therefore necessary to make sure that the memory kernels $\Gamma_s$ and $\Gamma_c$ decay within a finite correlation time $\tau_c$. This will be the case if the bath frequencies $k_n$ and the coupling constants $v_n$ are smoothly spread out. Moreover, it is necessary that the bath temperature is not so low that the relevant oscillators are frozen out by the Planck factor. Under these conditions the integrations over $\tau$ may be extended to infinity without serious error.

An extreme way to meet the smoothness requirement is the "Ohmic case," defined by $v_n^2/k_n$ having a constant density $\gamma$ in the frequency scale. One then has

$$\Gamma_s(\tau) = -\pi\gamma\delta(\tau)$$

$$\Gamma_c(\tau) = \gamma \int_0^{\infty} k \cos k\tau \coth \tfrac{1}{2}\beta k \, dk$$

The latter reduces for small $\beta$ to

$$\Gamma_c(\tau) \approx (2\pi\gamma/\beta)\, \delta(\tau)$$

where $\delta(\tau)$ stands for a sharp peak with width $\tau_c \sim \hbar/k_B T$. Thus in this case the master equation (8) reduces to

$$\begin{aligned}\dot{\rho}_S = \mathscr{L}_S \rho_S - \pi\lambda^2\gamma k_B T[S, [S, \rho_S]]\\ + \tfrac{1}{2}\pi\lambda^2\gamma[S, [[H_S, S], \rho_S]]_+ \qquad (14)\end{aligned}$$

The final remark concerns the Kossakowski–Lindblad condition,(7) which is a general requirement of the form that any evolution equation for

$\rho_S$ must have in order to be Hermitian and positive definite with unit trace. This requirement is obeyed by the first two terms of (14), but not by the last one, nor by the general equation (8). In fact it has been found that the expansion in the interaction leads to a violation of that requirement,^(2,8) except for the harmonic oscillator.^(1) A remedy has been proposed by Davies,^(9) but the present authors do not feel that they have really understood this difficulty.

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