Description of Quantum Noise by a Langevin Equation

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We derive an equation of motion for a fully observed classical system which is coupled to a quantum companion whose degrees of freedom are only partially observed. Our purpose is to discuss the nature of the quantum noise by using a generalization of the Langevin equation.

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Both the question of the ultimate sensitivity of measurement devices¹ and that of detection of quantum behavior on a macroscopic scale ² require an understanding of the properties of quantum noise. It has been suggested that quantum noise can be accounted for through the phenomenological Langevin equation³

$$m\ddot{q} + \gamma \dot{q} + \partial V(q) / \partial q = \xi(t). \tag{1}$$

The particle coordinate q is acted upon by deterministic forces (including a damping term proportional to the velocity) and by a Gaussian stochastic force. The quantum nature of this random variable is reflected in its correlation function, which—in accordance with the (quantum) fluctuationdissipation equation—is

$$\int_{-\infty}^{+\infty} dt \left\langle \xi(t)\xi(0) \right\rangle e^{i\omega t} = \gamma \hbar \,\omega \coth \hbar \,\omega / 2kT.$$
(2)

In the classical limit $\hbar \omega \ll kT$ this becomes the standard Gaussian noise, with $\langle \xi(t)\xi(0) \rangle = 2kT\delta(t)\gamma$.

Formal motivations for such a quantum Langevin

equation were given in the literature.^{4,5} However, doubts regarding its validity, and questions related to its interpretation outside the classical regime, have not been completely settled. One of the problems is that the noise appears to provide energy even at zero temperature.⁶ Such behavior is unacceptable since at absolute zero the system causing the noise must be in its ground state, and no energy can be extracted from it. Furthermore, results obtained from (1) and (2) depend on the magnitude of an arbitrarily imposed high-frequency cutoff. Since in a well-formulated theory the system that is responsible for dissipation and noise has a natural cutoff frequency, which is the frequency of its highest elementary excitation, there should be no need to impose it arbitrarily. Finally, we mention that the noise is correlated on a time scale given by \hbar/kT , and these correlations have to be taken into account carefully.

Microscopic models designed to produce Eq. (1) in the appropriate limit are typically based on the Hamiltonian

$$H = \frac{p^2}{2m} + V(q) + \sum_{i=1}^{N} f_i(q) Q_i + \sum_{i=1}^{N} \frac{P_i^2}{2M_i} + \frac{M_i \Omega_i^2 Q_i^2}{2},$$
(3)

representing a particle coupled to a set of N-independent oscillators. If the initial state of the oscillators is incompletely specified (e.g., if they are in thermal equilibrium at a temperture T) and/or if their final state is not measured, they provide quantum noise in the classical equation for q(t).

In what follows we want to point out certain general features of the quantum noise problem viewed as the problem of deriving the equation of motion for a fully observed classical system (i.e., the particle) coupled to a partially observed quantum companion (i.e., the set of oscillators). These features are general and the model (3) is used for illustration only. We will arrive at a description similar in spirit to that of Eqs. (1) and (2) but differing in the fact that we more explicitly keep track of the properties of the quantum companion. This elucidates the meaning of the quantum noise, and avoids the shortcomings of the phenomenological theory mentioned above.

Since we found it useful to use the classical Langevin equation as a guide, we outline briefly its properties.⁷ We start from the equations of motion corresponding to the classical version of the Hamiltonian given by Eq. (3), solve exactly for Q(t), and, using this solution, eliminate Q(t) from the equation for motion for q(t). This leads to the Langevin equation

$$m\ddot{q}(t) + \frac{\partial V}{\partial q} - \frac{\partial}{\partial q} f(q(t)) \frac{1}{M\Omega} \int_{t_1}^t \sin\Omega(t-\tau) f(q(\tau)) d\tau = -\frac{\partial}{\partial q} f(q(t)) Q_0(t) = \xi(t)$$
(4)

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where

$$Q_0(t) = [\dot{Q}(t_1)/\Omega] \sin \Omega (t - t_1) + Q(t_1) \cos \Omega (t - t_1)$$

To simplify the notation we use one oscillator only;

the extension to N oscillators is straightforward. In fact, if we want to produce genuine dissipation we have to couple to an infinite set of oscillators. By choosing their spectral density and coupling as

$$\frac{\pi}{2}\sum_{i=1}^{N}\frac{[\partial f_i(q)/\partial q]^2}{M_i\Omega_i}\delta(\omega-\Omega_i)=\gamma\omega,$$

independent of q, we can model the velocityproportional damping of Eq. (1).⁸ On the other hand, the Hamiltonian (3) may be used to model the interaction of a particle with a surface, distorted by thermally excited phonons. In this case $f_i(q) = -N^{-1/2} \partial V(q)/\partial q$ and the spectral distribution is that of the phonons (e.g., a Debye spectrum).

In those cases where we know only the probability that prior to the collision $Q(t_1)$ and $\dot{Q}(t_1)$ have given values, the quantity $\xi(t)$ is a stochastic variable. If at $t = t_1$ the oscillator was in equilibrium with a thermostat, then $\xi(t)$ is a Gaussian variable whose correlation function satisfies the classical limit (since the oscillator is classical) of the fluctuation-dissipation theorem.

A suggestive, but unsatisfactory, method to quantize Eq. (4) is to retain *classical dynamics* (i.e., the form of the equation of motion) but to describe the statistical properties of the random force by use of quantum statistical correlation functions. We call the resulting equations the quantum statistical Langevin equations (QSLE). This amounts to the use of, for the correlation function of $Q_0(t)$, the form

$$\frac{1}{2} \langle \hat{Q}_0(t) \hat{Q}_0(0) + \hat{Q}_0(0) \hat{Q}_0(t) \rangle$$

= $(\hbar/2M\Omega) \coth(\hbar \Omega/2kT) \cos(\Omega t)$

which satisfies the general (quantum) fluctuationdissipation theorem. The QSLE is very similar to the phenomenological equation. However, the frequency of the oscillator (or, for many oscillators, the largest oscillator frequency) appears as a natural cutoff. $-t_1$).

To understand the meaning and the limitations of QSLE we go a step further and suggest a Langevin equation in which quantum *dynamics effects* are also incorporated (referred to in what follows as the quantum dynamic Langevin equation). This should have the form

$$m\ddot{q} + \partial V/\partial q = \mathcal{F}_{IF}(\{q\}).$$
(5)

The key element here is the new force $\mathscr{F}_{IF}(\{q\})$ which is a functional of the particle trajectory $\{q(t)\}$ and depends on the initial and final states I and F of the quantum companion (i.e., the oscillator, in the simple model). This is a Langevin equation since we do not fix the initial or the final state of the quantum companion; all we know about them is the probability P_I that prior to the collision the companion is in the state I, and the transition probability $W_{I \to F}(\{q\}_{IF})$ that the collision with the particle, moving along the trajectory $\{q\}_{IF}$, will take the companion into the state F. The average value for any mechanical quantity $A(q,\dot{q})$ characterizing the classical particle is

$$\langle A \rangle = \sum_{F} \sum_{I} P_{I} W_{I \to F} A \left(\{q\}_{IF}, \{\dot{q}\}_{IF} \right).$$
(6)

Note that we must pick I and F, determine \mathcal{F}_{IF} , solve Eq. (5) to get $\{q\}_{IF}$, evaluate P_I and $W_{I \to F}(\{q\}_{IF})$, and calculate $\langle A \rangle$ from Eq. (6). This is reminiscent of the classical theory except that the noise source is no longer the uncertainty in $Q(t_1)$ and $\dot{Q}(t_1)$. In the quantum case there are two different noise sources: a *statistical* one which appears through P_I , reflecting the uncertainty in the initial state I, and a quantum dynamical one which appears through W_{IF} , reflecting the quantum mechanical uncertainty of whether a quantum transition from a specified initial state I to a final state F occurs. This second noise source has no classical analog.

The new force $\mathcal{F}_{IF}(\{q\})$ is required by rather general considerations: If the collision takes the quantum companion from *I* to *F*, there must be a force to slow down the particle such that energy is conserved according to

$$\frac{1}{2}m\dot{q}(t_2)^2 + V(q(t_2)) - \frac{1}{2}m\dot{q}(t_1)^2 - V(q(t_1)) = \hbar \Omega(n_I - n_F).$$
⁽⁷⁾

Here t_1 and t_2 are prior and post collision times, respectively, and n_I and n_F are the initial- and final-state energy quantum numbers of the companion. Thus we must have different "Newton equations" for each conceivable quantum transition of the companion.

Probably there is no general systematic and rigorous method for deriving an equation of the form (5), since there is no hybrid mechanics in which some degrees of freedom are treated classically and others quantum mechanically. Here we propose a method for obtaining an expression for \mathcal{F}_{IF} , based on Feynman's path-integral formulation.⁹ Other, more heuristic procedures, were outlined elsewhere.¹⁰

We start with the time-dependent Green's function written as a path integral:

$$\langle q_2, F | \exp\{-iH(t_2 - t_1)/\hbar\} | q_1, I \rangle = \int_{q_1}^{q_2} \mathscr{D}(q) \exp\{iS_0(q)/\hbar\} K_{IF}(\{q\}),$$
(8)

with

$$K_{IF}(\{q\}) = \int dQ_2 \phi_F^*(Q_2) \int dQ_1 \phi_I(Q_1) \int_{Q_1}^{Q_2} \mathscr{D}(Q) \exp[iS(q,Q)/\hbar].$$
(9)

Here $\phi_I(Q) \equiv \langle Q | I \rangle$ and $\phi_F(Q) = \langle Q | F \rangle$ are the initial- and final state wave functions of the companion, and $S_0(q)$ and S(Q,q) are the action of the particle and of the companion interacting with the particle, respectively. If we now write the complex amplitude $K_{IF}(\{q\})$ in "polar" form,

$$K_{IF}(\{q\}) = W_{I \to F}^{1/2}(\{q\}) \exp[i\mathcal{S}_{IF}(\{q\})],$$
(10)

we can regard $\mathscr{S}_{IF}(\{q\})$ as an addition to the particle action $S_0(\{q\})$. In the spirit of the work of Feynman and Hibbs^{9a} and of Pechukas and Davis,^{9b} we postulate that the generalized Hamiltonian principle follows from the stationary phase condition¹¹

$$\delta[S_0(\lbrace q \rbrace) + \mathscr{S}_{IF}(\lbrace q \rbrace)]/\delta q(t) = 0.$$

This Hamilton principle leads to

$$m\ddot{q} + \partial V/\partial q = \delta \mathscr{G}_{IF}(\{q\})/\delta q(t)$$

(11)

Moreover, since $K_{IF}(\{q\})$ is the probability amplitude that, under the influence of the trajectory $\{q\}$, the companion undergoes the transition $I \rightarrow F$, the quantity $W_{I \rightarrow F}(\{q\})$ appearing in Eq. (10) is identified with the transition probability appearing in Eq. (6).

For the model described by the Hamiltonian (3) these quantities can be computed by standard methods.^{9a} We obtain

$$W_{I \to F}(\{q\}) = \exp[-|\alpha(\{q\})|^2] |f_{IF}\{q\}|^2,$$
(12)

with

$$f_{IF} = (n_F!)^{-1/2} (n_I!)^{-1/2} \sum_{r=0}^{\min(n_F, n_I)} {n_F \choose r} {n_I \choose r} r! [i\alpha(\{q\})]^{n_I - r} [i\alpha(\{q\})^*]^{n_F - r}$$

and

$$\alpha(\{q\}) = (2M\hbar \Omega)^{-1/2} \int_{t_1}^{t_2} \exp(-i\Omega\tau) f(q(\tau)) d\tau.$$
(13)

The equation of motion corresponding to Eq. (11) is

$$m\ddot{q}(t) + \frac{\partial V}{\partial q} - (M\Omega)^{-1} \frac{\partial f(q(t))}{\partial q} \int_{t_1}^t d\tau \sin\Omega(t-\tau) f(q(\tau)) = \eta_{IF}(t),$$
(14)

with

$$\eta_{IF}(t) = -(2M\Omega)^{-1} \frac{\partial f(q(t))}{\partial q} \int_{t_1}^{t_2} d\tau \sin\Omega (t-\tau) f(\tau) \\ \times \left[1 - (n_F - n_I) 2\hbar M\Omega \left(\int_{t_1}^{t_2} d\tau_2 \int_{t_1}^{t_2} d\tau_1 f(q(\tau_2)) f(q(\tau_1)) \cos\Omega (\tau_2 - \tau_1) \right)^{-1} \right].$$
(15)

We have written the Eq. (14) [i.e., we split \mathcal{F}_{IF} of Eq. (5)] so that the left-hand side looks exactly like the friction appearing in the classical Langevin equation; correspondingly one can interpret $\eta_{IF}(t)$ as a quantum generalization of the random force $\xi(t)$. However, there is no compelling way of splitting \mathcal{F}_{IF} into friction and random force. For example, one may argue that the first term of $\eta_{IF}(t)$ is not stochastic since the only stochastic variables are n_I and n_F . Moreover, we observe that it is the last term in $\eta_{IF}(t)$ that accounts for the energy loss by the particle, and hence the dissipation; therefore

one might want to call that term friction.

It is straightforward to show that the equation of motion has all the general properties that we have requested when we commented on the general equation, (5). The conservation laws are satisfied. In particular, if the particle-oscillator interaction vanishes at t_1 and t_2 we can integrate Eq. (14) and recover the energy balance Eq. (7). The work done by the "classical friction" term, appearing on the left-hand side of Eq. (14), is exactly canceled by the work done by the first term of η_{IF} [Eq. (15)]. We

also mention that in the limit $n_I = 0$, the general expression W_{IF} in Eq. (12) reduces to a Poisson distribution in n_F with average $|\alpha\{q\}|^2$.

Another interesting feature of the force \mathcal{F}_{IF} is its dependence on the whole particle trajectory, in an apparent violation of causality. However strange, this feature is required by the fact that we have fixed the final state of the quantum companion, which, through the energy conservation condition Eq. (7), fixes the final velocity $\dot{q}(t)$; thus in order to guide the particle to its correct final velocity the force \mathscr{F}_{IF} must be a functional of the whole trajectory. In practical applications this means that the trajectory corresponding to a fixed set (I,F) must be computed self-consistently, either by a successive iteration of Eqs. (14) and (15), or by calculating the trajectory with the aid of the variational principle preceding Eq. (11).

Finally, the most interesting features, as far as quantum noise is concerned, are the statistical properties of η_{IF} . By using the definition (6) of the average we find that $\langle \eta_{IF}(t) \rangle = 0$ and, neglecting terms which vanish upon time averaging,

$$\left\langle \eta_{IF}(t)\eta_{IF}(t')\right\rangle = \frac{\hbar}{2M\Omega} \frac{\partial f(q(t))}{\partial q} \frac{\partial f(q(t'))}{\partial q} \cos\left[\Omega(t-t')\right] \coth\left[\frac{h\Omega}{2kT}\right].$$
(16)

Again, the correlation function of a system coupled to N oscillators is the sum of N such terms. In particular, with the choice of coupling and spectral density as given in the text after Eq. (4) we recover the correlation function.¹²

The quantum dynamic Langevin equation resembles in many aspects that of Koch, van Harlingen, and Clarke,³ Sebastian⁴ and Schmid.⁵ The latter two follow Feynman and Vernon¹³ and consider an average functional, which takes into account the effect of the quantum companion on the observed variable. Within a semiclassical approximation, this functional is equivalent to an equation of motion, containing a Gaussian random variable with a quantum correlation function. This stochastic force simulates the effect of the companion in an average way, but does not depend on the initial and the final state. The nature of this "average" is ambiguous and we are unable to understand it fully, while in the procedure suggested here the origin of the noise is directly related to the dynamics of the excitation of the quantum companion and the fact that the latter is incompletely measured. Furthermore, the present formulation quarantees that the conservation laws are satisfied; in particular, the system cannot extract energy from the companion at 0 K.

We emphasize that the general features of quantum noise introduced here go beyond the Hamiltonian (3), which was used for illustration and to make connection to past work. If Eq. (3) is used, numerical calculations are feasible,¹⁴ and we plan to publish them shortly. Beyond the quantum noise problem the model discussed here is useful in dealing with atom-surface scattering and trapping by phonon or electron-hole pair excitations,¹⁰ in the low-temperature limit when quantum effects become important.

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¹See, e.g., R. H. Koch, D. J. van Harlingen, and J. Clarke, Appl. Phys. Lett. **38**, 380 (1981); M. Ketchen, IEEE Trans. Magn. **17**, 387 (1981).

²See, e.g., J. Kurkijärvi, Phys. Lett. **88A**, 241 (1982). ³R. H. Koch, D. J. van Harlingen, and J. Clarke, Phys.

Rev. Lett. **45**, 2132 (1980).

⁴K. L. Sebastian, Chem. Phys. Lett. **81**, 14 (1981).

⁵A. Schmid, J. Low Temp. Phys. **49**, 608 (1982).

⁶R. F. Voss and R. A. Webb, Phys. Rev. B **24**, 7447 (1981).

⁷S. A. Adelman and J. D. Doll, Acc. Chem. Res. **10**, 378 (1977); J. C. Tully, Annu. Rev. Phys. Chem. **31**, 319 (1980).

⁸A. O. Caldeira and A. J. Leggett, Phys. Rev. Lett. **46**, 211 (1981), and Ann. Phys. (N.Y.) **149**, 374 (1983).

^{9(a)}R. P. Feynman and A. R. Hibbs, *Quantum Mechanics and Path Integrals* (McGraw-Hill, New York, 1965).

^{9(b)}P. Pechukas and J. P. Davis, J. Chem. Phys. 56, 4970 (1972).

¹⁰K. M. Leung, G. Schön, P. Rudolph, and H. Metiu, to be published.

¹¹This stationary phase condition is not a strict expansion in powers of \hbar . Rather $N\hbar$, where N is the number of the oscillators, is considered of order 1. In fact, $\sum_{i}^{N} \Omega_{i} (n_{i}^{i} - n_{i}^{j})$ is the macroscopic energy absorbed by the oscillators.

¹²We obtained (16) ignoring the implicit dependence of $W_{I \to F}$ and η_{IF} on I and F which arises through their functional dependence on the trajectory $\{q\}_{IF}$. This is well justified in the limit of \hbar small and N large, where $\{q\}$ depends only weakly on transitions of individual oscillators.

 13 R. P. Feynman and F. L. Vernon, Ann. Phys. (N.Y.) **24**, 118 (1963).

¹⁴G. Schön, M. Golan, and H. Metiu, unpublished.