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On the Quantum Langevin Equation

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The quantum Langevin equation is the Heisenberg equation of motion for the (operator) coordinate of a Brownian particle coupled to a heat bath. We give an elementary derivation of this equation for a simple coupled-oscillator model of the heat bath.

KEY WORDS: Langevin equation; quantum stochastic processes; Brownian motion; heat bath; coupled oscillators.

1. INTRODUCTION

Some 20 years ago, in a paper written jointly with Peter Mazur, we presented a discussion of the statistical mechanics of a coupled-oscillator model of a heat bath.(1) This model enabled us to obtain the quantum mechanical form of the Langevin equation for a Brownian particle moving in an external potential. Our purpose here is to repeat this derivation, using a different, some would say simpler, oscillator model of the heat bath. Repeating the discussion will enable us to lay a different emphasis on certain aspects of the derivation and of the equation itself, aspects that have become of interest in the intervening years.

As in our earlier paper, for simplicity we restrict our considerations to a particle moving in one dimension; it will be seen that this is not an essential restriction. In this case the quantum Langevin equation is the (Heisen-

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berg) equation of motion for the particle coordinate operator $x(t)$ and takes the form

$$m\ddot{x} + \zeta\dot{x} + V'(x) = F(t) \tag{1}$$

where $V(x)$ is the external potential and $F(t)$ is an operator-valued random force, with (symmetric) correlation

$$\frac{1}{2}\langle F(t)\,F(0) + F(0)\,F(t)\rangle = \frac{\zeta}{\pi}\int_0^\infty d\omega\,\hbar\omega\coth(\hbar\omega/2kT)\cos\omega t \tag{2}$$

and with commutator

$$[F(t), F(0)] = \frac{-2i\hbar\zeta}{\pi}\int_0^\infty d\omega\,\omega\sin\omega t = 2i\hbar\zeta\delta'(t) \tag{3}$$

In addition $F(t)$ has the Gaussian property: correlations of an odd number of factors of F vanish, and symmetric correlations of an even number of factors are equal to the sum of products of pair correlations, the sum being over all pairings.

We shall have more to say about this remarkable equation in Section 3. Here we only emphasize that it is a *contracted* description of the particle motion. The heat bath, which we shall see must have an infinite number of degrees of freedom, is described by a single parameter ζ, the friction constant. This parameter (together with the absolute temperature T) specifies the statistical properties of the random force, as given by the correlation, as well as its commutator.

In the next section we introduce the model and give a succinct derivation of the above results. As with our earlier model, with it we are able to carry through what we call the program of Gibbs. To paraphrase our earlier paper, this program goes as follows.

(i) Solve the mechanical equations of motion for the system consisting of the Brownian particle coupled to the heat bath. The solution will consist of explicit expressions for the dynamical variables at time t in terms of their initial values.

(ii) Assume that the initial variables of the heat bath are somehow statistically distributed, in our case according to the canonical ensemble.

(iii) Show that the coordinate operator for the Brownian particle then satisfies the quantum Langevin equation.

This last step in the program has a pair of aspects that should perhaps be emphasized. The first is that the quantum Langevin equation is a limiting, idealized equation, which is only approximately correct for any real system. This means therefore that it can be obtained as an exact consequence of the program only by specializing the model, i.e., by making special assumptions about the parameters of the model. The second aspect is that for short times the description that results from steps (i) and (ii) will in general reflect the assumed initial state of the heat bath. It is only after a short relaxation period, during which initial transients decay and the particle "forgets" the initial state, that the quantum Langevin equation, characterized by the friction constant above, can arise.

2. THE MODEL AND THE DERIVATION OF THE EQUATIONS

The model we consider is that of the Brownian particle surrounded by a large number of independent heat bath particles, each attached to the Brownian particle by a spring. The Hamiltonian of the system is then

$$H=\frac{p^2}{2m}+V(x)+\sum_j\left[\frac{p_j^2}{2m_j}+\frac{1}{2}k_j(q_j-x)^2\right] \tag{4}$$

Here x and p are the coordinate and momentum operators of the Brownian particle, while q_j and p_j are those of the jth heat bath particle. The mass of this jth heat bath particle is m_j and the spring attaching it to the Brownian particle has spring constant k_j. Finally, $V(x)$ is the potential energy of the external force on the Brownian particle.

We should emphasize that this model is by no means original, it appears in one guise or another frequently in the literature.[2] The earliest appearance we have found is in a paper by Magalinskij,[3] although we have not made a careful search and there may well be earlier appearances.

To this Hamiltonian we must append the canonical (equal-time) commutation relations:

$$[x, p]=i\hbar, \qquad [q_j, p_k]=i\hbar\delta_{jk} \tag{5}$$

and all other commutators vanish. The equations of motion for the time-dependent (Heisenberg) operators are then obtained using the Heisenberg equation:

$$i\hbar\dot{O}=[O, H] \tag{6}$$

which gives the time derivative (denoted by the superposed dot) of an arbitrary operator O. We then get

$$\dot{x}=(1/m)\,p, \qquad \dot{p}=-V'(x)+\sum_j k_j(q_j-x) \tag{7}$$

for the Brownian particle, and

$$\dot{q}_j = (1/m_j)\, p_j, \qquad \dot{p}_j = -k_j(q_j - x) \tag{8}$$

for the jth heat bath particle.

The oscillator equations (8) are simple to solve and we can write

$$q_j(t) = q_j(0) \cos \omega_j t + p_j(0)(\sin \omega_j t)/m_j \omega_j + x(t) - x(0) \cos \omega_j t - \int_0^t dt' \cos \omega_j(t-t')\, \dot{x}(t') \tag{9}$$

where the natural frequency of the oscillator is

$$\omega_j = (k_j/m_j)^{1/2} \tag{10}$$

When this result is put in the right-hand side of the particle equations (7), they can be written in the form

$$m\ddot{x} + \int_0^t dt'\, B(t-t')\, \dot{x}(t') + V'(x) + B(t)\, x(0) = F(t) \tag{11}$$

where the force operator $F(t)$ is given by

$$F(t) = \sum_j \left[q_j(0)\, k_j \cos \omega_j t + p_j(0)\, \omega_j \sin \omega_j t\right] \tag{12}$$

and where

$$B(t) = \sum_j k_j \cos \omega_j t \tag{13}$$

Note that in Eq. (11) the initial variables of the heat bath, i.e., the $q_j(0)$ and $p_j(0)$, occur in $F(t)$; otherwise only the variables of the particle occur. With this result we have completed step (i) in the program outlined in the introduction.

In the next step we introduce the statistical average over the initial variables of the heat bath. We do this by assuming that at $t = 0$ the oscillators are canonically distributed with respect to the free oscillator Hamiltonian:

$$H_O = \sum_j \left(\tfrac{1}{2} p_j^2/m_j + \tfrac{1}{2} k_j q_j^2\right) \tag{14}$$

We therefore introduce the expectation for an arbitrary operator O:

$$\langle O \rangle \equiv \mathrm{Tr}\{O \exp(-H_O/kT)\}/\mathrm{Tr}\{\exp(-H_O/kT)\} \tag{15}$$

where the (partial) trace is with respect to the coordinates of the oscillators. It is straightforward to show that[1,4]

$$\langle q_j(0)\, q_k(0)\rangle = \frac{\langle p_j(0)\, p_k(0)\rangle}{(m_j\omega_j)^2} = \delta_{jk}\frac{\hbar \coth(\hbar\omega_j/2kT)}{2m_j\omega_j}$$
$$\langle q_j(0)\, p_k(0)\rangle = -\langle p_k(0)\, q_j(0)\rangle = \frac{1}{2}\, i\hbar\delta_{jk} \qquad (16)$$

In addition we have the Gaussian property: the expectation of an odd number of factors of the $q_j(0)$ and $p_j(0)$ vanishes; the expectation of an even number of factors is the sum of products of pair expectations with the order of the factors preserved. With these results we find for the symmetric correlation of the force operator (12),

$$\tfrac{1}{2}\langle F(t)\, F(t') + F(t')\, F(t)\rangle$$
$$= \sum_j \tfrac{1}{2} k_j \hbar\omega_j \coth[\hbar\omega_j(2kT) \cos \omega_j(t-t')] \qquad (17)$$

and, of course, $F(t)$ has the Gaussian property, which follows from the corresponding property of the products of the $q_j(0)$ and $p_j(0)$. Finally, from the canonical commulation rules (5) we find

$$[F(t), F(t')] = -i\hbar \sum_j k_j\omega_j \sin \omega_j(t-t') \qquad (18)$$

With these results we have carried out step (ii) of our program.

Equation (11) together with the properties of the force operator we have just obtained is not yet the quantum Langevin equation, although it begins to look close. Comparing the second term in (11) with the corresponding term in the quantum Langevin equation (1), we see that they will be the same if

$$B(t) = 2\zeta\delta(t) \qquad (19)$$

Comparing this with the expression (13) for $B(t)$ in terms of the frequencies and force constants of the bath oscillators, we see that $B(t)$ cannot be of this form unless there are an infinite number of oscillators in the bath and their frequencies are continuously distributed. In that case we can write

$$B(t) = \int_0^\infty d\omega\, N(\omega)\, k(\omega) \cos \omega t \qquad (20)$$

where $N(\omega)\, d\omega$ is the number of oscillators whose natural frequency is between ω and $\omega + d\omega$ and $k(\omega)$ is the (average) force constant of the oscillators whose frequency is ω. Now, if we compare (19) and (21) we see that to obtain the former we must choose

$$N(\omega)\, k(\omega) = 2\zeta/\pi \tag{21}$$

Thus, the force-constant-weighted spectrum of oscillator frequencies must be uniform, corresponding to white noise. When we make this same choice of the spectrum in the formulas (17) and (18) they become exactly the formulas (2) and (3), respectively. Thus, with this choice of the spectrum, Eq. (11) becomes exactly the quantum Langevin equation (1) except for the added term

$$B(t)\, x(0) = 2\zeta x(0)\, \delta(t) \tag{22}$$

on the left-hand side. It is at this point that we complete the third step in our program by asserting that the general quantum Langevin equation will arise out of a model calculation such as ours only after a short relaxation period. In our model the duration of this period is infinitesimal, so that after any finite interval of time we obtain the quantum Langevin equation. We should emphasize that this last step is, so to speak, an artifact of the method; it is required only because one has for convenience made very special assumptions about the initial state of the system.

3. REMARKS

We conclude with a few brief remarks upon the quantum Langevin equation and its derivation. The first is that the equation is somehow universal. We mean this in the same sense as the classical Langevin equation is regarded as universal: there are a number of nontrivial examples of systems that, at least approximately, satisfy the equation and the form of the equation is the same for all. In particular here "form of the equation" means that the operator force must have the Gaussian property and that the correlation and commutator must have the forms (2) and (3), respectively.

Since we have derived the quantum Langevin equation (either here or in our earlier paper) only for very special oscillator models, one might wonder to what extent we have demonstrated the universality of the equation. The answer, of course, is that we have not. Rather, the logic is reversed: *if* there is a universal description, then it must be of the form we have obtained.

In fact, one can do a bit more. Elsewhere, in a separate paper by one of us (G.W.F.), it will be shown that in fact the forms (2) and (3) of the correlation and the commutator are a general result of the fluctuation-dissipation theorem and are therefore independent of model. On the other hand, the Gaussian property of the force operator does not seem to follow from such general considerations, but is implied by the models.

However, there is a more compelling reason to believe in the universal character of the form of the equation. That is, only with this form—by which we mean Eq. (1), the correlation (2), the commutator (3), *and* the Gaussian property of the force operator $F(t)$—does one have the approach to the correct equilibrium state. To be specific, the stationary solution of (1) should correspond to the equilibrium state. In particular, if one forms the moments of this solution, then in the weak coupling limit (i.e., $\zeta \to 0$) they should correspond to the canonical distribution among the levels of the particle in a potential $V(x)$. Explicitly, one should be able to demonstrate the result

$$\lim_{\zeta \to 0} \langle x(t)^N \rangle = \sum_n e^{-E_n/kT} (\psi_n, x^N \psi_n) \Big/ \sum_n e^{-E_n/kT} \tag{23}$$

where $x(t)$ is the stationary solution of the quantum Langevin equation (1), while on the right-hand side the ψ_n are the normalized eigenfunctions and E_n the corresponding eigenvalues of the Schrödinger equation:

$$\left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \right] \psi_n = E_n \psi_n \tag{24}$$

In fact, to prove this in general is an open problem. It has, however, been shown by Benguria and Kac that it holds to third order in perturbation for the perturbed harmonic oscillator.[5,6]

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