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DERIVATION OF THE QUANTUM LANGEVIN EQUATION

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Abstract

The phenomenological approach to the Langevin equation breaks down for quantum systems. It is necessary to take into account explicitly an external bath, which causes the damping and fluctuations. The question then is whether there exists an autonomous equation of motion for the system itself, with or without a memory kernel. Some simple cases are listed and for one case the derivation of Langevin's equation is carried out. It is compared to the exact result, which leads to the following conclusions. The equation is true only to the lowest order in the interaction between system and bath. In general there is a memory kernel but in two special cases the damping reduces to a simple proportionality with a friction coefficient ("Ohmic case"). © 1997 Elsevier Science B.V.

1 The phenomenological approach.

In linear systems fluctuations are customarily described by adding a Langevin term [1,2,3]. The classical example is the Brownian particle, whose velocity obeys (for unit mass)

$$\dot{v} = -\gamma v + L(t). \quad (1)$$

The Langevin term is assumed to be a random function of time whose stochastic properties are

$$\langle L(t) \rangle = 0, \quad \langle L(t)L(t') \rangle = C\delta(t-t'), \quad L \text{ Gaussian.} \quad (2)$$

Consequently the solution of (1), with given $v(0)$, is also a stochastic function. Equation (1) can be solved [4]. One finds for $t \gg \gamma^{-1}$ that $\langle v^2 \rangle = C/2\gamma$; as this must be equal to κT one obtains the fluctuation-dissipation relation $C = 2\gamma\kappa T$. Hence it appears that the fluctuations are fully determined once one knows the macroscopic phenomenological equation, including the damping. This I shall call the *phenomenological approach*. It has been tremendously fruitful in electronics, hydrodynamics, and many other fields.

2 The inadequacy of this approach.

It was shown by D.K.C. MacDonald [5] that this approach is inconsistent when the phenomenological equation is nonlinear. It turned out to be no longer possible to include fluctuations without more detailed knowledge of their physical origin. His unwelcome message still often goes unheeded, either due to ignorance or for convenience [6].

In quantum mechanics the phenomenological approach meets an additional stumbling block: there exists no equation with damping to start from, because the Schrödinger equation by construction conserves energy. Instead one often starts from the analogy with the classical case [7,8], but this is a rather shaky basis and the results are controversial [9]. Hence in quantum mechanics one needs to take into account the physical origin not only of the fluctuations but also of the damping.

3 The bath.

One way of doing this consists in adding to the system S considered a second system B , with which S interacts. B is a heat bath, i.e., it has many degrees of freedom in order that the energy transferred from S gets lost in it, with negligible probability to ever return to S . A favorite choice for B is a large collection of harmonic oscillators, with Hamiltonian

$$H_B = \frac{1}{2} \sum_n (p_n^2 + k_n^2 q_n^2) = \sum_n k_n a_n^\dagger a_n + \text{const.}$$

The k_n are supposed to be spread out densely on the frequency scale. The idea is that the precise nature of the bath is immaterial and harmonic oscillators are easy to deal with. In addition it can be said that this is a realistic description of the normal modes of the electromagnetic field, or of the phonons in a crystal. More complicated nonlinear heat baths are rarely envisaged [10].

In principle one ought to solve the Schrödinger equation for the combined systems $S + B$ and extract from the total solution the required information about the behavior of S . The hope is that it can be described by an equation of motion for S alone, the Langevin equation. Our aim is to investigate the validity of such an equation by studying an explicitly solvable model. It is true that many authors have studied solvable models [9,11,12], but my aim is to reduce it to the simplest possible algebra and focus on the question of the validity of the Langevin equation.

4 Various models.

As systems S one often takes a one-dimensional particle in a potential field,

$$H_S = \frac{1}{2}P^2 + V(Q). \quad (3)$$

For the interaction H_I we list a few of the models that have been studied. The names are those in [8], the v_n are coupling constants.

(i) Ullersma model [11,13]: $H_I = Q \sum v_n q_n$.

(ii) Independent oscillator model [14]

$$H = \frac{1}{2}P^2 + V(Q) + \frac{1}{2} \sum [p_n^2 + k_n^2(q_n - v_n Q)^2].$$

(iii) The velocity coupling model [15]

$$H = \frac{1}{2}(P - \sum v_n q_n)^2 + V(Q) + \frac{1}{2} \sum (p_n^2 + k_n^2 q_n^2).$$

These Hamiltonians all have a bilinear coupling and they can be transformed into each other by canonical transformations. The last one is a simplified form of a charged particle in an electromagnetic field. Nonlinear interactions have also been considered [10,16].

If the potential in (3) is harmonic, $V(Q) = \frac{1}{2}\Omega^2 Q^2$, the Hamiltonians can be diagonalized and the models can be solved explicitly. In that case yet another model presents itself, which is more readily formulated in terms of creation and annihilation operators:

(iv) Rotating wave model

$$H = \Omega a_o^+ a_o + \sum k_n a_n^+ a_n + \sum v_n (a_o^+ a_n + a_n^+ a_o). \quad (4)$$

This is the one we shall employ here as a test for the various aspects of the Langevin equation, bearing in mind that it is rather special.

5 The Langevin equation model (4).

We first reproduce the standard way of obtaining the Langevin equation. The equations of motion for the Heisenberg operators of (4) are

$$\dot{a}_o(t) = -i\Omega a_o(t) - i \sum v_n a_n(t) \quad (5a)$$

$$\dot{a}_n(t) = -ik_n a_n(t) - i v_n a_o(t). \quad (5b)$$

Solve the second line so as to obtain variables $a_n(t)$ in terms of the yet unknown system operator $a_o(t)$. This step is essential in all derivations but can be done explicitly only for a harmonic bath.

$$a_n(t) = a_n(0)e^{-ik_n t} - iv_n \int_0^t e^{-ik_n(t-t')} a_o(t') dt'.$$

Substitute this in (5a) to get

$$\dot{a}_o(t) = -i\Omega a_o(t) - \sum v_n^2 \int_0^t e^{-ik_n(t-t')} a_n(t') dt' + L(t). \quad (6)$$

$$L(t) = -i \sum v_n e^{-ik_n t} a_n(0).$$

This has been called the “generalized Langevin equation”. However, it is *not* a true Langevin equation, as will be seen presently.

The justification for regarding $L(t)$ as a Langevin force is that it is independent of S . It is an operator in the Hilbert space of B , obeying the commutation relation

$$[L(t), L^+(t')] = \sum v_n^2 e^{-ik_n(t-t')}. \quad (7)$$

As the bath oscillators are densely distributed over the frequencies, this may be written

$$[L(t), L^+(t')] = \int_0^\infty g(k) dk e^{-ik(t-t')}, \quad (8)$$

with obvious definition of the “strength function” g .

$L(t)$ depends on the initial state of B , for which one traditionally takes thermal equilibrium with $\beta = 1/\kappa T$. One then gets

$$\langle L(t)L^+(t') \rangle = \int_0^\infty \frac{g(k)dk}{1 - e^{-\beta k}} e^{-ik(t-t')}, \quad (9a)$$

$$\langle L^+(t')L(t) \rangle = \int_0^\infty \frac{g(k)dk}{e^{\beta k} - 1} e^{-ik(t-t')}, \quad (9b)$$

where $\langle \dots \rangle$ denotes the average over the initial bath.

In spite of its name equation (6) is *not* a Langevin equation. It is still an exact consequence of the original equations (5) and therefore equally hard to solve. One therefore makes a “Markov approximation”, for instance by *assuming* that the integral extends virtually over only a short time interval, so that $a_o(t')$ may be identified with $a_o(t)$.

$$\dot{a}_o(t) = -i\Omega a_o(t) - \Gamma_o a_o(t) + L(t) \quad (10)$$

$$\Gamma_o = \int_0^\infty \sum v_n^2 e^{-ik_n \tau} d\tau = \int_0^\infty d\tau \int_0^\infty g(k) e^{-ik\tau} dk. \quad (11)$$

An “improved Markov approximation” consists in taking for $a_o(t')$ the value that is related to $a_o(t)$ by the *unperturbed* equation of motion of S ,

$$a_o(t') \approx e^{-i\Omega(t'-t)} a_o(t).$$

This leads to the same Langevin equation (10) but with Γ_o replaced with

$$\begin{aligned}\Gamma_1 &= \int_o^\infty d\tau \int_o^\infty g(k) e^{-i(k-\Omega)\tau} dk \\ &= -i \int_o^\infty \frac{g(k) dk}{k - \Omega} + \pi g(\Omega).\end{aligned}\quad (12)$$

The first term is a principal-value integral. When inserted in (8) it amounts to a shift $\Delta\Omega$ of the frequency Ω . The second term is real damping; we set $\pi g(\Omega) = \Gamma$.

We now proceed to test this result on the exact solution.

6 The exact solution.

The exact treatment of model (4) is given in ref. [2], ch. XVII, sec. 2. We here give an outline.

Consider the Heisenberg equations (5). They are linear and hence their solution has the form

$$a_o(t) = U(t)a_o(0) + \sum_n V_n(t)a_n(0) \quad (13a)$$

$$a_n(t) = W_n(t)a_o(0) + \sum_m S_{nm}(t)a_m(0). \quad (13b)$$

The coefficients U, V_n, W_n, S_{nm} are scalar functions of time and form a unitary matrix. Differentiate (13a) and express the result in terms of $a_o(t)$ and $a_n(0)$:

$$\begin{aligned}\dot{a}_o(t) &= \dot{U}a_o(0) + \sum_n \dot{V}_n a_n(0) \\ &= \dot{U}U^{-1}a_o(t) + \sum_n (\dot{V}_n - \dot{U}U^{-1}V_n)a_n(0).\end{aligned}\quad (14)$$

This looks like a Langevin equation but is still exact.

The quantities U, V_n can be written explicitly by means of an auxiliary function of $z = x + iy$,

$$G(z) = z - \Omega - \sum_n \frac{v_n^2}{z - k_n} = z - \Omega - \int_o^\infty \frac{g(k) dk}{z - k}.$$

This function is analytic in the z -plane without the positive real axis. One then has

$$U(t) = -\frac{1}{2\pi i} \int_{-\infty}^{\infty} \frac{e^{-ixt}}{G(x + i\epsilon)} dx \quad (\epsilon > 0)$$

Take the limit $\epsilon \rightarrow 0$,

$$G(x + i\epsilon) = x - \Omega - \oint \frac{g(k) dk}{x - k} + i\pi g(x). \quad (15)$$

Now comes the approximation.

The essential approximation is that g is small. Then one may argue that for $x - \Omega \gg g$ the two small terms in (15) are immaterial. On the other hand, for $x \sim \Omega$ they do matter but may be simplified by identifying the x in them with Ω , so that they become constants.

$$G(x + i\epsilon) \approx x - \Omega - \int \frac{g(k) dk}{\Omega - k} + i\pi g(\Omega) = x - \Omega - \Delta\Omega + i\Gamma. \quad (16)$$

Substitution in (15) yields

$$U(t) = e^{-i\Omega't - \Gamma t}, \quad \Omega' = \Omega + \Delta\Omega, \quad (17)$$

Hence (14) reduces to

$$\dot{a}_o(t) = (-i\Omega' - \Gamma)a_o(t) + L(t). \quad (18)$$

This is precisely the Langevin equation found previously by means of the “improved Markov approximation”, which had been obtained from the “generalized Langevin equation” by replacing the unknown $a_o(t')$ with the unperturbed $a_o(t')$. Thus the assumption of small g is indispensable for the Langevin equation.

For future use I give the value of V_n with the same approximation as used in (16)

$$V_n = W_n = \frac{v_n}{\Omega - k_n - i\Gamma} (e^{-i\Omega't - \Gamma t} - e^{-ik_n t}). \quad (19)$$

7 The damping.

We verify that (18) gives rise to damping. The energy of S , averaged over the initial state of B , is

$$E(t) = \Omega \left(\langle a_o^+(t)a_o(t) \rangle + \frac{1}{2} \right).$$

According to (18)

$$\frac{d}{dt} \langle a_o^+(t)a_o(t) \rangle = -2\Gamma \langle a_o^+(t)a_o(t) \rangle + \langle L^+(t)a_o(t) \rangle + \langle a_o^+(t)L(t) \rangle. \quad (20)$$

For the second term on the right one finds using (7), (13a) and (19)

$$\begin{aligned} & i \sum_n v_n e^{ik_n t} \sum_n V_m(t) \langle a_n^+(0)a_m(0) \rangle \\ &= i \sum_n v_n e^{ik_n t} V_n(t) (e^{\beta k_n} - 1)^{-1} \\ &= i \sum_n \frac{v_n^2}{\Omega' - k_n - i\Gamma} (e^{-i(\Omega' - k_n)t - \Gamma t} - 1) \frac{1}{e^{\beta k_n} - 1} \\ &= -i \int_0^\infty \frac{g(k)dk}{\Omega' - k - i\Gamma} \frac{1}{e^{\beta k} - 1} \quad \text{for} \quad t \ll \Gamma^{-1}. \end{aligned}$$

Since higher orders of g are neglected anyway this is

$$\frac{\pi g(\Omega)}{e^{\beta\Omega} - 1} - i \oint \frac{g(k)dk}{\Omega - k} \frac{1}{e^{\beta k} - 1}. \quad (21)$$

The last term of (20) is the complex conjugate of (21), so that we have found

$$\frac{d}{dt} \langle a_o^+(t)a_o(t) \rangle = -2\Gamma \langle a_o^+(t)a_o(t) \rangle + \frac{2\pi g(\Omega)}{e^{\beta\Omega} - 1}.$$

This shows that $\langle a_o^+(t)a_o(t) \rangle$ approaches the limiting value $(e^{\beta\Omega} - 1)^{-1}$ exponentially at the rate 2Γ . That is,

$$E(t) \longrightarrow \frac{1}{2}\Omega + \Omega(e^{\beta\Omega} - 1)^{-1} = \frac{1}{2} \coth(\frac{1}{2}\beta\Omega). \quad (22)$$

In spite of the damping the commutator $[a_o, a_o^+]$ must remain constant. This miracle is achieved by the Langevin term. Of course it is an exact consequence of (13a) because of the unitarity of the matrix, but is it still true for the solution of the *approximate* equation (18)? To verify this assume that the commutation relations are valid at t and take the derivative

$$\frac{d}{dt} [a_o(t), a_o^+(t)] = -2\Gamma [a_o(t), a_o^+(t)] + [L(t), a_o^+(t)] + [a_o(t), L^+(t)]. \quad (23)$$

Using (7) one has

$$\begin{aligned} [L(t), a_o^+(t)] &= -i \sum v_n e^{-ik_n t} [a_n(0), a_o^+(t)] \\ &= -i \sum v_n e^{-ik_n t} V_n^*(t) \\ &= -i \int_0^\infty \frac{g(k) dk}{\Omega - k + i\Gamma} (e^{i(\Omega-k)t - \Gamma t} - 1) \\ &= i \int_0^\infty \frac{g(k) dk}{\Omega - k + i\Gamma} \quad \text{for} \quad t \gg \Gamma^{-1}. \end{aligned}$$

Adding the hermitian conjugate one finds for the last two terms of (23) together $2\pi g(\Omega) = 2\Gamma$. This cancels the first term. In the same way one can verify that the other commutation relations are upheld.

8 Conclusions.

Three important lessons emerge from this model. First, the results are true only to first order in g , that is second order in the couplings v_n . Higher orders spoil the validity of (16) and hence of the entire idea of exponential damping. As a matter of fact, only when the interaction is small can one talk of energy dissipation of S , inasmuch as the energies of S and B cannot be clearly distinguished except in the limit of zero interaction.

Secondly, the term $\dot{U}U^{-1}a_o(t)$ in (14), which is responsible for the damping, involves a frequency shift $\Delta\Omega$ as well. This shift must accompany the damping because they are real and imaginary parts of the boundary values of $G(z)$, which is analytic in the upper half plane of z [8,17].

Thirdly, the expression $\Gamma = \pi g(\Omega)$ for the damping constant shows that *the damping is caused by those bath oscillators that are in resonance with S* . It follows that it is incorrect to argue that the bath frequencies are fast compared to the motion of the system S , as is done in the “singular coupling approximation” [18,3].

Another consequence of this remark is the following. If S is *not* a harmonic oscillator, but nonlinear as in (3), then the motion contains many Fourier components with different frequencies. Each of these components is damped by the strength function g taken at its personal frequency. The resulting damping is then not just a term $-\Gamma a_o(t)$, but can be represented only by a time integral with a memory kernel. In frequency language that can be represented by a damping coefficient which is a function of the frequency. The simple proportionality holds only in two cases: the harmonic oscillator (which has just one frequency); and in case $g(k)$ is constant, so that all Fourier components are damped

at the same rate (“Ohmic case”). It is true that the latter case cannot be strictly realized because for constant $g(k)$ the frequency shift in (16) diverges.

Finally it should be mentioned that an entirely different approach exists, in which an equation for the density matrix of S is derived, in analogy with the Fokker-Planck equation in classical theory. Unfortunately the relationship between this density matrix and the Heisenberg operators used in the Langevin approach is by no means simple [19].

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