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Quantum Langevin Equation

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It is shown (by means of a perturbation series) that for a class of potentials $V(x)$ the stationary distribution of the solution $x(t)$ of the quantum Langevin equation approaches in the weak-coupling limit ($f\to 0$) the quantum mechanical canonical distribution of the displacement of the oscillator, subject to the potential $V(x)$, if and only if $E(t)$ is the operator version of the purely random Gaussian process so that, in particular, higher symmetrized averages $\langle E(t_1)\cdots E(t_n)\rangle_s$ are expressible in terms of pair correlations, in the usual way.

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It is well known that classically the action of a heat bath of absolute temperature T on a particle in the bath can, under appropriate circumstances, be described by the "Langevin force"[1]

$$-f\,dx/dt+E(t), \tag{1}$$

where f is a friction coefficient and $E(t)$ a purely random Gaussian process, i.e., a Gaussian random process with mean zero and covariance given by the formula

$$\langle E(t_1)E(t_2)\rangle = 2kTf\;\delta(t_2-t_1). \tag{2}$$

If the particle (of mass m) is subject to an outside force derivable from the potential $V(x)$, one is led to the Langevin equation

$$m\frac{d^2x}{dt^2}+f\frac{dx}{dt}+V'(x)=E(t), \tag{3}$$

which can be made a basis for studying the *approach* to equilibrium of the particle (it is, of course, assumed that the heat bath being in essence infinite in size remains for all times in equilibrium).

The simplest (and most fundamental) fact of the theory of the Langevin equation is embodied in the theorem that, in the limit as $t\to\infty$, $P(x_0,p_0\,|\,x,p;t)$, where $P(x_0,p_0\,|\,x,p;t)$ is the probability density of x and p at time t given that at time 0 the particle was at x_0 with initial momentum p_0, is the *canonical* (Maxwell-Boltzmann) density.

We shall assume from now on that $V(x)$ approaches $+\infty$ as $x\to\pm\infty$. In the simplest case of the harmonic oscillator $V'(x)=\kappa^2x$, the Langevin equation can be solved explicitly and the above statement verified directly. For more general (nonlinear) forces one has to use the fact that the process $\{x(t),p(t)\}$ is Markovian and that P satisfies the Kramers equation.[2] The Maxwell-Boltzmann density is the *unique* stationary solution of the Kramers equation.

Is there an analogous theory within the realm of quantum mechanics? This question has been the subject of a large number of papers and at least two reviews,[3] to which the reader is directed for further references. It appears that with one exception[4] all papers deal exclusively with the harmonic oscillator (which turns out to be somewhat misleading), and the quantum Langevin equation is introduced by more or less heuristic arguments. To avoid polemic, we shall adhere to the line of thought which motivated Ford, Kac, and Mazur[4] (FKM), and while in so doing we shall restrict the physical implications of our conclusions, we shall gain in clarity and sharpness. In FKM, a purely dynamical *model* of a heat bath was proposed which rigorously yielded (in an appropriate limit) (3) and (2). The model is rather special since the heat bath is an assembly of coupled oscillators harmonically coupled to a particle which in turn is acted upon by an outside force $-V'(x)$. The only statistical assumption was that the heat bath was canonically distributed. The quantum Langevin equation was then obtained by treating the dynamical system quantum mechanically and interpreting the canonical distribution of the heat bath also quantum mechanically. The quantum mechanical version is formally identical with (3) except that now x and its derivatives are operators and so is $E(t)$. $E(t)$ is, in fact, a limit of a linear combination of creation and annihilation operators (for details see FKM) where one can calculate easily the commutator $[E(t_1), E(t_2)]$,

$$[E(t_1), E(t_2)] = if\hbar(\partial/\partial t_1 - \partial/\partial t_2)\delta(t_1 - t_2), \tag{4}$$

and the average

$$\langle E(t_1)E(t_2)\rangle_s = \tfrac{1}{2}\langle E(t_1)E(t_2) + E(t_2)E(t_1)\rangle = (mf/\pi)\int_0^\infty d\omega\,\hbar\omega\coth(\hbar\omega/2kT)\cos[\omega(t_1 - t_2)]. \tag{5}$$

It is, of course, understood that the average $\langle\,\rangle$ (without the subscript s which signifies symmetrization) is taken with respect to the (quantum mechanical) canonical ensemble of the heat bath, i.e., with respect to $\exp(-\beta H)$, with the H being the Hamiltonian of the heat bath which in terms of creation and annihilation operators is $H = \sum_k \hbar\omega_k \times (a_k^* a_k + \frac{1}{2})$. It goes without saying that (5) is the result of the same limiting process which leads to (4). This limiting process, described in detail in FKM, consists of letting the numbers of bath oscillators, as well as a certain cutoff frequency, approach infinity. The higher symmetrized averages $\langle E(t_1)E(t_2)\cdots E(t_n)\rangle_s$ obey the usual Gaussian property and, of course, $\langle E(t)\rangle = 0$. In order to avoid certain divergence difficulties as well as the ever present difficulties stemming from the inherent noncommutativity of quantum mechanical operators, we shall forego the search for the most suitable analog of the approach to equilibrium in the classical case and confine our attention to the distribution of the position coordinate $x(t)$ only.

The position of a quantum mechanical particle subject to an external potential $V(x)$ and in equilibrium with a heat bath of absolute temperature T should be distributed according to the probability density

$$\frac{\sum_{n=1}^{\infty}\exp(-\beta E_n)\psi_n^2(x)}{\sum_{n=1}^{\infty}\exp(-\beta E_n)}, \quad \beta = \frac{1}{kT}, \tag{6}$$

where the E_n's and ψ_n's are respectively the eigenvalues and the normalized eigenfunctions of the Schrödinger equation with potential V. [Because of our assumption that $V(x)\to\infty$ as $x\to\pm\infty$, the spectrum is discrete.] One might thus suspect that as $t\to\infty$ the probability density of $x(t)$ should approach the canonical density (6). But this cannot be so for $f\neq 0$, because for nonvanishing friction one should expect shifting and broadening of spectral lines. What one should, therefore, expect is that only in the *additional* limit $f\to 0$, the limiting distribution of $x(t)$ as $t\to\infty$ should be (6).

The (somewhat imperfect) analog of the approach to equilibrium in the classical case stated for future reference in terms of the moment-generating function $\langle\exp[bx(t)]\rangle$ is thus

$$\lim_{f\to 0}\lim_{t\to\infty}\langle\exp[bx(t)]\rangle = \int_{-\infty}^{\infty} dx\exp(bx)\,\frac{\sum_n \exp(-\beta E_n)\psi_n^2(x)}{\sum_n\exp(-\beta E_n)}. \tag{7}$$

In the sequel we shall sketch a proof of (7) first for potentials of the form $V(x) = \frac{1}{2}\kappa^2x^2 + \epsilon\exp(ax)$, with $\epsilon > 0$ and a real (so as not to violate hermiticity), and then for potentials of the form

$$V(x) = \tfrac{1}{2}\kappa^2x^2 + \epsilon\int_{-\infty}^{\infty} W(k)\exp(ikx)\,dk, \tag{8}$$

with $W(k^*) = W^*(k)$ (so that V is real). Actually, we shall only prove (7) to *all orders* in perturbation, but in the case (8) with suitably restricted $W(k)$ the perturbation series will converge for sufficiently small $|\epsilon|$.

The calculation of the expansion of the right-hand side of (7) is relatively easy and is most effectively accomplished by the use of the Feynman-Kac formula.[5] If we choose units such that $m = 1$, $\hbar = \sqrt{2}$, and $\kappa^2 = \frac{1}{2}$, then with potential $V(x) = x^2/4 + \epsilon\exp(ax)$ the coefficients of the ϵ^0 and ϵ

terms in the expansion are $\exp[b^2 g_0(0)/2]$ and

$$-\exp[(a^2+b^2)g_0(0)/2]\int_0^\beta d\beta_1\{\exp[ab\Delta(\beta_1)]-1\}\,, \tag{9}$$

respectively, where $g_0(0)=\coth(\beta/2)$ and $\Delta(\gamma)=\cosh(\beta/2-\gamma)/\sinh(\beta/2)$, $0\leq\gamma\leq\beta$. The notation $g_0(0)$ will become clear in the sequel [see (14)]. Considerably more involved is the perturbative treatment of the Langevin equation. It turns out that instead of taking the limit $t\to\infty$ in (7) it is enough to set

$$x(t)=u(t)-\epsilon a\int_{-\infty}^{t}K(t-\zeta)\exp[ax(\zeta)]d\zeta\,,$$

where

$$u(t)=\int_{-\infty}^{t}K(t-\zeta)E(\zeta)\,d\zeta \quad\text{and}\quad K(s)=\exp(-fs)\sin(\nu s)/\nu\,,$$

with $s>0$ and $\nu^2=\kappa^2-\frac{1}{4}f^2$. It is therefore sufficient to calculate the limit, as $f\to 0$, of $\langle\exp[bx(t)]\rangle$ with $x(t)$ defined as above. We shall need in the sequel the commutator $[u(t_1),u(t_2)]$ and $\langle\exp[bu(t)]\rangle$. Both are easily computed and we record the results:

$$[u(t_1),u(t_2)]=i\frac{\hbar}{m}\exp\left(-f\frac{|t_2-t_1|}{2}\right)\frac{\sin\nu(t_2-t_1)}{\nu}\,, \tag{10}$$

$$\langle\exp[bu(t)]\rangle=\exp[b^2 g(0)/2]\,, \tag{11}$$

where

$$g(0)=\langle u^2(t)\rangle=\frac{2f}{\pi}\int_0^\infty\hbar\omega\coth\left(\frac{\hbar\omega}{2kT}\right)\frac{d\omega}{(\omega^2-\kappa^2)^2+\omega^2f^2}\,, \tag{12}$$

or more generally

$$g(\zeta)=\tfrac{1}{2}\langle u(t)u(t+\zeta)+u(t+\zeta)u(t)\rangle=\frac{2f}{\pi}\int_0^\infty\hbar\omega\coth\left(\frac{\hbar\omega}{2kT}\right)\frac{\cos(\omega\zeta)}{(\omega^2-\kappa^2)^2+\omega^2f^2}\,d\omega\,. \tag{13}$$

As $f\to 0$ we obtain

$$g_0(\zeta)=\lim_{f\to 0}g(\zeta)=\coth(\beta/2)\cos(\zeta/\sqrt{2}\,)\,, \tag{14}$$

in the units chosen above. Finally, we record a generalization of (11)

$$\langle\exp[\sum_{k=1}^{n}b_k u(t_k)]\rangle=\exp[\sum_{i,j=1}^{n}b_i b_j g(|t_i-t_j|)/2]\,, \tag{15}$$

which underscores the Gaussian nature of $u(t)$ and is *identical* in form with the corresponding classical formula (except, of course, for the difference in the expressions for g, the classical g being obtained from the quantum mechanical one by letting $\hbar\to 0$). The essential quantum mechanical features appear because in the perturbative calculation of $\langle\exp[bx(t)]\rangle$ one encounters symmetrized averages $\langle\prod_k\exp[b_k\times u(t_k)]\rangle_s$ which by repeated applications of the Baker-Campbell-Hausdorf formula and the formula (10) for the commutators $[u(t_i),u(t_j)]$ (fortunately, these are c-numbers!) turn out to be the "classical" (12) multiplied by products of terms generated by the commutators.

It remains to sketch how one goes about calculating (recursively!) the terms of the power series (in ϵ) for $\langle\exp[bx(t)]\rangle$ and checking that in the limit $f\to 0$ they are equal to the corresponding terms in the expansion of the right-hand side of (7). We start with the identity

$$h(b;t)=\exp[bu(t)]-\epsilon a\int_0^b db'\exp[(b-b')u(t)]\int_{-\infty}^{t}d\zeta K(t-\zeta)h(a;\zeta)h(b';t)\,, \tag{16}$$

where $h(b;t)=\exp[bx(t)]$. This can be easily verified by premultiplying both sides of (16) by $\exp[-bu(t)]$ and taking derivatives of both sides with respect to b. For the more general perturbation (8) the identity is

$$h(b;t)=\exp[bu(t)]-\epsilon a\int_{-\infty}^{\infty}dk\,W(k)\int_0^b db\,\exp[(b-b')u(t)]\int_{-\infty}^{t}d\zeta\,K(t-\zeta)h(ik;\zeta)h(b';t). \tag{17}$$

Expanding h in powers of ϵ, so that $h(b;t)=\sum H_n(b;t)\epsilon^n$, we get from (16)

$$H_{n+1}(b;t)=-a\int_0^b db'\exp[(b-b')u(t)]\int_{-\infty}^t d\xi K(t-\xi)\sum_{i+j=n} H_i(a;\xi)H_j(b';t), \quad (18)$$

and it should be clear that $H_0(b;t)=\exp[bu(t)]$. A simple straightforward calculation gives, in the units chosen above,

$$H_1(b;t)=-\sqrt{2}\int_{-\infty}^t d\xi \exp[au(\xi)+bu(t)]\sin[abK(t-\xi)/\sqrt{2}], \quad (19)$$

and, upon averaging and using (15),

$$\langle H_1(b;t)\rangle=-\sqrt{2}\exp[(a^2+b^2)g(0)/2]\int_0^\infty d\lambda \exp[abg(\lambda)]\sin[abK(\lambda)/\sqrt{2}]. \quad (20)$$

How does one see that, in the limit $f\to 0$, (20) is the same as (9), or equivalently how does one see that

$$\lim_{f\to 0}\sqrt{2}\int_0^\infty d\lambda \exp[abg(\lambda)]\sin[abK(\lambda)/\sqrt{2}]=\int_0^\beta d\beta_1\{\exp[ab\Delta(\beta_1)]-1\}? \quad (21)$$

This is a nice excercise in contour integration and it uses in an essential way the identity

$$\varphi_0^+(i\sqrt{2}\beta)=\Delta(\beta) \quad (22a)$$

and

$$\varphi_0^+(\lambda+i\sqrt{2}\beta)=\varphi_0^-(\beta), \quad (22b)$$

where $\varphi_0^\pm(\lambda)\equiv\lim_{f\to 0}[g(\lambda)\pm iK(\lambda)/\sqrt{2}]=\cos(\lambda/\sqrt{2}\mp i\beta/2)/\sinh(\beta/2)$. The symmetry (22b) is formally identical with the familiar KMS (Kubo-Martin-Schwinger) condition. Verification of equality of coefficients of higher powers of ϵ requires no new ideas but more care and patience. For the *coefficients* of ϵ^2 and ϵ^3 the verification has been explicitly performed and this suggested a general inductive procedure which is in the process of being worked out.

We are, of course, aware that there may be a number of (possibly subtle) questions of rigor having mainly to do with interchanges of limiting processes. There is, however, no doubt in our minds that the results as presented are correct.

We conclude with two remarks. (1) There should be a nonperturbative proof of the approach to the quantum mechanical canonical distribution. One cannot escape the feeling that our calculations merely constitute an elaborate verification of the inner consistency of quantum mechanics. (2) If one follows our calculations in detail it becomes clear that the properties of $E(t)$ as embodied in (4) and (5), as well as in $E(t)$ being Gaussian, are not only sufficient for (7) but also *necessary*.[6] It follows that either the Langevin equation studied here is a fluke of the special FKM model which led to it or that there is no generally valid quantum Langevin equation. The authors who, guided by the harmonic oscillator, proposed alternative forms of the Langevin equation might well ponder these inexorable alternatives.

Last, but not least, it is a pleasure to thank Professor G. W. Ford for helpful and stimulating discussions and especially for letting us have his notes on the quantum mechanical aspects of the fluctuation-dissipation theorem. It was his formalism that suggested (16) [and, by simple extension, (18)] which paved the path to an inductive treatment of the perturbation expansion of the solution of the Langevin equation.

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[1]For simplicity we consider the one-dimensional case only.

[2]M. C. Wang and G. E. Uhlenbeck, Rev. Mod. Phys. 17, 323 (1945).

[3]H. Haken, Rev. Mod. Phys. 47, 67 (1975); J. Messer, Acta Phys. Austriaca 50, 75 (1979).

[4]G. W. Ford, M. Kac, and P. Mazur, J. Math. Phys. 6, 504 (1965), henceforth referred to as FKM. For a more realistic model which leads to the same Langevin equation, see J. T. Lewis and L. C. Thomas, in *Functional Integration and its Applications*, edited by A. M. Arthur (Clarendon, Oxford, 1975), pp. 97–123.

[5]For the use of the Feynman-Kac formula in the perturbative treatment of an anharmonic oscillator, see, e.g., Barry Simon, *Functional Integration and Quantum Physics* (Academic, New York, 1979) (in particular Sect. 20). Although only the ground-state energy is considered, the extension to the case of interest to us is quite easy. It depends on the extension to the so-called oscillator (or Ornstein-Uhlenbeck) process of the formalism first proposed by M. Kac, in *Proceedings of the Second Berkeley Symposium on Mathematics, Statistics, and Probability* (University of California, Berkeley, 1950), p. 189, for the Wiener process.

[6]This is rigorously true if one assumes that the commutator $[E(t_1), E(t_2)]$ is a c-number.