Journal of Statistical Physics, Vol. 115, Nos. 3/4, May 2004 (© 2004)

A New Approach to Noise in Quantum Mechanics

N. G. van Kampen[1]

Received July 23, 2003; accepted November 13, 2003

The standard way of describing noise in a quantum system consists in attaching to the system a reservoir or bath, which is assumed to be in thermal equilibrium. Subsequently the combined equation of motion is solved to second order in the interaction and by averaging the result over the bath one gets the density matrix of the system itself. However, the differential equation obtained in this way has a serious flaw, which can be attributed to the inappropriate initial condition. For this reason we here take as starting point the thermal equilibrium of the combined system; the averages and correlation functions of quantities of interest provide us with the required information about the noise. This is explicitly demonstrated on the special model of a harmonic oscillator coupled to a bath of harmonic oscillators at temperature T. The result is compared with the standard calculation and it is shown that the latter is incorrect for time intervals smaller than $kT/\hbar$. As an example the energy fluctuations in equilibrium are computed.

KEY WORDS: Quantum noise; correlation functions; equilibrium.

1. THE STANDARD THEORY

Langevin[1] treated the classical theory of Brownian particles by describing the rapidly and uncontrollably varying force exerted by surrounding molecules as an additional term in the equations of motion. The instantaneous value of that force cannot be described in detail but its short-time averages have simple properties. Later the notion of a stochastic function made it possible to create an elegant description, at the expense of some convenient assumptions. In fact, it was so elegant that it was readily adopted, together with its corollary the Fokker–Planck equation, whenever noise was supposed to play a role, such as in electrical circuits.[2] The actual cause of the noise was ignored in favor of ''using stochastic assumptions whenever

[1] Institute for Theoretical Physics, Utrecht University, Leuvenlaan 4, 3584 CE Utrecht, The Netherlands; e-mail: NG.vanKampen@phys.uu.nl

0022-4715/04/0500-1057/0

necessary to obtain useful results."[3] These assumptions postulate that the stochastic noise term is Gaussian and delta-correlated in time. Even the raining of molecules onto a surface has been so described, although it is evidently a Poisson process.[4]

In 1954 it was pointed out by D. K. C. MacDonald that for nonlinear equations the addition of a Langevin force is inconsistent.[5] One cannot add indiscriminately a Langevin term to a macroscopic equation when that equation is not linear. This was forcefully expressed by the question: Does a diode rectify its own fluctuations? This situation gave rise to some discussion, involving the notorious Itô-Stratonovich dilemma; for literature see ref. 6. The conclusion was that it is necessary to start from a more fundamental level which includes the physical cause and the actual form of the noise. This episode, however, was soon forgotten in favor of the so convenient Langevin device. Langevin terms have even been used in equations purporting to describe neurons and economics.[7]

In quantum mechanics, however, attempts to write a Langevin equation for operators were not successful because of the need to formulate the required stochastic properties for an operator random force.[8] (Incidentally, to avoid confusion it should be remarked that it is possible to add a suitably chosen Langevin term to the Schrödinger equation, but that merely leads to the general formula of Kossakowski–Lindblad.)[6, 9] The conclusion is again that one cannot avoid to add explicitly a description of the mechanism that is the physical cause of the noise and the damping. In other words, one must attach to the system S considered a reservoir or bath B, consisting of many particles, which are the source of fluctuating perturbations in system S. The idea is that the many degrees of freedom of B keep the bath at all times practically in thermal equilibrium so as not to perturb S. Yet the influence of S produces a slight deviation from that equilibrium, and this deviation acts back on S. This is the cause of both damping and noise in S; evidently they are of second order in the coupling strength.

This second order perturbation calculation is standard since Zwanzig.[10] The *total system* T = S + B is subject to a *total* Schrödinger equation with total Hamiltonian

$$H_{\mathrm{T}} = H_{\mathrm{S}} + H_{\mathrm{B}} + \alpha H_{\mathrm{I}}, \tag{1.1}$$

which includes an interaction αH_{I} with coupling constant α. One then takes an initial condition at $t = 0$, in which S and B are uncorrelated:

$$\rho_{\mathrm{T}}(0) = \rho_{\mathrm{S}}(0) \otimes \rho_{\mathrm{B}}^{\mathrm{eq}}. \tag{1.2}$$

The Schrödinger equation (or rather von Neumann equation) for its density matrix ρ_{T} can be solved to second order in α to give $\rho_{\mathrm{T}}(t)$ and subsequently $\rho_{\mathrm{S}}(t) = \mathrm{Tr}_{\mathrm{B}}\, \rho_{\mathrm{T}}(t)$. In this way one obtains $\rho_{\mathrm{S}}(t)$ for given initial $\rho_{\mathrm{S}}(0)$. Explicit calculation for small time Δt gives[6]

$$\rho_{\mathrm{S}}(\Delta t) = \rho_{\mathrm{S}}(0) - i[H_{\mathrm{S}}, \rho_{\mathrm{S}}(0)]\, \Delta t + \Delta t\, \mathscr{K} \rho_{\mathrm{S}}(0). \tag{1.3}$$

Here $\mathscr{K}$ is a "superoperator," i.e., a linear operator acting on the space of density matrices. One concludes that $\rho(t)$ obeys the differential equation

$$\dot{\rho}_{\mathrm{S}}(t) = -i[H_{\mathrm{S}}, \rho_{\mathrm{S}}(t)] + \mathscr{K} \rho_{\mathrm{S}}(t). \tag{1.4}$$

I shall refer to this as "the standard result."

2. THE PROBLEM

This standard result cannot, however, be correct for the following reason. Any differential equation for a density matrix must have the property that the trace of the matrix is constant (equal to unity), that the matrix remains hermitian, and that it remains positive definite. The most general form for such a differential equation has been derived by Kossakowski and by Lindblad.[11] The result (1.4) does not have this required form and may lead to a ρ at $t > 0$ which is not positive definite, and therefore may give rise to negative probabilities. What went wrong in the derivation?

It was not permitted to go from (1.3) to (1.4). Equation (1.3) was obtained using the condition (1.2) for the initial state. After the time step Δt, however, some correlation between S and B has been built up so that it is not correct to apply the same argument for the next Δt, let alone for the infinite sequence of time steps described by (1.4). The conclusion from (1.3) to (1.4) involves the assumption that these unavoidable correlations will not affect the result and that it is permitted to ignore them at each new time step Δt. This is the "Repeated Randomness Assumption" or "molecular chaos,"[12] which is indispensable in all derivations of irreversible equations. It was used explicitly by Boltzmann and Lorentz,[13] but ignored or hidden in most later treatments.

3. THE ANSWER

Actually the system S and the bath B are never uncorrelated as they are constantly interacting. The glib excuse that the interaction is switched on at $t = 0$ is unrealistic; how does one turn on the interaction between a Brownian particle and its surrounding molecules? At any rate this excuse does nothing to alleviate the need for a repeated randomness assumption. Our answer to this difficulty is to consider *the equilibrium state of the total system* $\mathrm{T}=\mathrm{S}+\mathrm{B}$, including the interaction,

$$\rho_{\mathrm{T}}^{\mathrm{eq}}=\exp[-\beta H_{\mathrm{T}}]/Z=\exp[-\beta(H_{\mathrm{S}}+H_{\mathrm{B}}+\alpha H_{\mathrm{I}})]/Z, \tag{3.1}$$

$$Z=\operatorname{Tr}\exp[-\beta H_{\mathrm{T}}]. \tag{3.2}$$

For any observable A_{S} relating to the system one may now compute the average

$$\langle A_{\mathrm{S}}\rangle^{\mathrm{eq}}=\operatorname{Tr}_{\mathrm{S+B}}\, A_{\mathrm{S}}\rho_{\mathrm{T}}^{\mathrm{eq}}$$

and the correlation function between two variables A_{S} and B_{S}, which in case their averages vanish is given by

$$\langle A_{\mathrm{S}}(t_1)\, B_{\mathrm{S}}(t_2)\rangle^{\mathrm{eq}}=\operatorname{Tr}_{\mathrm{S+B}}\{A_{\mathrm{S}}(t_1)\, B_{\mathrm{S}}(t_2)\, \rho_{\mathrm{T}}^{\mathrm{eq}}\}.$$

From this one finds in particular $\langle A_{\mathrm{S}}^2\rangle^{\mathrm{eq}}$, which is the magnitude of the fluctuations in A_{S}, while the autocorrelation function $\langle A_{\mathrm{S}} A_{\mathrm{S}}(\tau)\rangle^{\mathrm{eq}}$ measures their rate of decay. The dependence on the time difference $\tau=t_2-t_1$ is the one determined by the total Hamiltonian H_{T}.

Henceforth we omit the subscript S as we are interested only in observables relating to S, and omit the superscript $^{\mathrm{eq}}$ for the averages as they will all refer to the equilibrium of the total system. I shall now compute these quantities explicitly in order to compare them with the standard results. A previous calculation[14] was based on the usual expansion to second order in the interaction, but here I take an exactly solvable model in order to display more clearly the benefit of considering correlation functions rather than the unrealistic initial condition (1.2).

4. EXPLICIT COMPUTATIONS

First we have to choose a bath. Originally Senitzky[15] did not specify the bath but ever since people have taken B to be a collection of harmonic oscillators.[16] This is easy to handle and is justified by the idea that the equations for the noise should not be sensitive to the specific form of the bath. The main requirement is that the frequencies k of the oscillators form a dense distribution and extends over a long range so as to mimick white noise. The electromagnetic field is a prime example. It is to be expected, however, that quantum mechanics cuts off high frequencies, so that a spectrum can only be approximately white, as we shall see.

Next we choose for the system S a harmonic oscillator as well, in order to make explicit calculations possible. For the same reason I take the interaction bilinear so that the total Hamiltonian is a quadratic form:

$$H_{\mathrm{T}} = \tfrac{1}{2}(P_0^2 + \Omega^2 Q_0^2) + \tfrac{1}{2}\sum_k (P_k^2 + k^2 Q_k^2) + Q_0 \sum_k \alpha_k Q_k. \tag{4.1}$$

The frequencies k serve also as subscripts and α_k are coupling constants. The subscript $_0$ indicates the oscillator S. This model can be solved exactly by transforming to principal axes.

The quadratic form in the variables Q_0, Q_k may be diagonalized (Appendix A) by means of an orthogonal matrix X

$$Q_0 = \Sigma_\nu X_{0\nu} q_\nu, \qquad Q_k = \Sigma_\nu X_{k\nu} q_\nu. \tag{4.2}$$

When P_0, P_k are similarly transformed into new momenta

$$P_0 = \Sigma_\nu X_{0\nu}\, p_\nu, \qquad P_k = \Sigma_\nu X_{k\nu}\, p_\nu \tag{4.3}$$

the Hamiltonian reduces to

$$H_{\mathrm{T}} = \tfrac{1}{2}\sum_\nu (p_\nu^2 + \omega_\nu^2 q_\nu^2). \tag{4.4}$$

The eigenfrequencies ω_ν are the zeros of the analytic function

$$G(\omega) = \omega^2 - \Omega^2 - \sum_k \frac{\alpha_k^2}{\omega^2 - k^2}. \tag{4.5}$$

It is now possible to compute averages. In the first place we need the partition function

$$\begin{aligned} Z &= \mathrm{Tr}_{\mathrm{T}} \exp\left[-\frac{1}{2}\beta \sum_\nu (p_\nu^2 + \omega_\nu^2 q_\nu^2) \right] \\ &= \prod_\nu \mathrm{Tr}_\nu \left[-\frac{1}{2}\beta (p_\nu^2 + \omega_\nu^2 q_\nu^2) \right] \\ &= \prod_\nu \frac{1}{2\sinh(\tfrac{1}{2}\beta\omega_\nu)}. \end{aligned} \tag{4.6}$$

Subsequently one finds for the fluctuations, for example in P_0,

$$\langle P_0^2 \rangle = \sum_\nu X_{0\nu}^2 \langle p_\nu^2 \rangle = \sum_\nu \tfrac{1}{2} X_{0\nu}^2 \omega_\nu \coth(\tfrac{1}{2}\beta\omega_\nu). \tag{4.7}$$

Note that for $\beta \to 0$ (high temperature) this reduces to $\langle P_0^2 \rangle = \Sigma_\nu X_{0\nu}^2 \beta = \beta$, which is the standard formula. It will appear presently that $X_{0\nu}^2$ peaks at $\omega_\nu \approx \Omega$, so that the condition for this limit amounts to $\hbar\Omega \ll kT$, which is the classical limit.

5. GENERAL TREATMENT

In order to compute averages of operators relating to S we introduce the Fourier transform

$$K(x, y) \equiv \langle e^{ixP_0 + iyQ_0} \rangle$$
$$= \mathrm{Tr}\{\exp[ixP_0 + iyQ_0] \exp[-\beta H_\mathrm{T}]\}/Z, \tag{5.1}$$

involving two real parameters $x, y \in \mathbb{R}$. This trace is equal to

$$\Pi_\nu \, \mathrm{Tr}_\nu \{\exp[ix_\nu p_\nu + iy_\nu q_\nu] \exp\left[-\tfrac{1}{2}\beta(p_\nu^2 + \omega_\nu^2 q_\nu^2)\right]\}/Z,$$

where $x_\nu = xX_{0\nu}$ and $y_\nu = yX_{0\nu}$. In Appendix B this is found to result in

$$\langle e^{ixP_0 + iyQ_0} \rangle = \exp\left[-\frac{1}{4}\sum_\nu X_{0\nu}^2 \coth\left(\frac{1}{2}\beta\omega_\nu\right)\left\{\omega_\nu x^2 + \frac{y^2}{\omega_\nu}\right\}\right]. \tag{5.2}$$

From this the average of any polynomial in P_0, Q_0 is obtained by expanding both members in x, y and comparing powers. One example is (4.7) and furthermore

$$\langle Q_0^2 \rangle = \frac{1}{2}\sum_\nu X_{0\nu}^2 \frac{\coth(\frac{1}{2}\beta\omega_\nu)}{\omega_\nu}, \tag{5.3}$$

$$\langle P_0 Q_0 + Q_0 P_0 \rangle = 0, \qquad \text{so that} \qquad \langle P_0 Q_0 \rangle = -\langle Q_0 P_0 \rangle = -\frac{i}{2}. \tag{5.4}$$

Hence the average energy of our system is, in contrast with the standard result,

$$\langle E \rangle = \frac{1}{2}\sum_\nu X_{0\nu}^2 \left(\omega_\nu + \frac{\Omega^2}{\omega_\nu}\right) \coth\frac{1}{2}\beta\omega_\nu. \tag{5.5}$$

Again the standard result $\langle E \rangle = 1/\beta$ is retrieved for $\beta \to 0$ assuming that $X_{0\nu}^2$ peaks at $\omega_\nu \approx \Omega$.

Vice versâ, when the transform $K(x, y)$ is given one may reconstruct the density matrix, see Appendix C.

6. TIME DEPENDENCE

Time correlations are found in the same way by inserting the time dependence of the normal mode oscillators.

$$P_0(t) = \Sigma_\nu X_{0\nu}\, p_\nu(t) = \Sigma_\nu X_{0\nu} \{p_\nu(0) \cos \omega_\nu t - \omega_\nu q_\nu(0) \sin \omega_\nu t\}. \tag{6.1}$$

From this

$$\begin{aligned}\langle P_0(0)\, P_0(t)\rangle &= \langle \Sigma_\mu X_{0\mu}\, p_\mu \times \Sigma_\nu X_{0\nu} \{p_\nu \cos \omega_\nu t - \omega_\nu q_\nu \sin \omega_\nu t\}\rangle \\ &= \Sigma_\nu X_{0\nu}^2 \{\langle p_\nu^2\rangle \cos \omega_\nu t - \langle p_\nu q_\nu\rangle\, \omega_\nu \sin \omega_\nu t\} \\ &= \sum_\nu \tfrac{1}{2} X_{0\nu}^2 (\omega_\nu \coth \tfrac{1}{2} \beta\omega_\nu \cos \omega_\nu t + i\omega_\nu \sin \omega_\nu t).\end{aligned} \tag{6.2}$$

Similarly one finds

$$\langle P_0(0)\, Q_0(t)\rangle = \sum_\nu \frac{1}{2} X_{0\nu}^2 \left(\coth \frac{1}{2} \beta\omega_\nu \sin \omega_\nu t - i \cos \omega_\nu t\right), \tag{6.3}$$

$$\langle Q_0(0)\, P_0(t)\rangle = \sum_\nu \frac{1}{2} X_{0\nu}^2 \left(-\coth \frac{1}{2} \beta\omega_\nu \sin \omega_\nu t + i \cos \omega_\nu t\right), \tag{6.4}$$

$$\langle Q_0(0)\, Q_0(t)\rangle = \sum_\nu \frac{1}{2} X_{0\nu}^2 \left(\frac{1}{\omega_\nu} \coth \frac{1}{2} \beta\omega_\nu \cos \omega_\nu t + i\, \frac{\sin \omega_\nu t}{\omega_\nu}\right). \tag{6.5}$$

The summation over the zeros ω_ν of (4.5) can be written as a path integral taking into account (A.2):

$$\langle P_0(0)\, P_0(t)\rangle = \frac{1}{2\pi i} \oint \frac{\omega^2\, d\omega}{G(\omega)} \left\{\coth \frac{1}{2} \beta\omega \cos \omega t + i \sin \omega t\right\}, \tag{6.6}$$

$$\langle P_0(0)\, Q_0(t)\rangle = \frac{1}{2\pi i} \oint \frac{\omega\, d\omega}{G(\omega)} \left\{\coth \frac{1}{2} \beta\omega \sin \omega t - i \cos \omega t\right\}, \tag{6.7}$$

$$\langle Q_0(0)\, P_0(t)\rangle = \frac{1}{2\pi i} \oint \frac{\omega\, d\omega}{G(\omega)} \left\{-\coth \frac{1}{2} \beta\omega \sin \omega t + i \cos \omega t\right\}, \tag{6.8}$$

$$\langle Q_0(0)\, Q_0(t)\rangle = \frac{1}{2\pi i} \oint \frac{d\omega}{G(\omega)} \left\{\coth \frac{1}{2} \beta\omega \cos \omega t + i \sin \omega t\right\}. \tag{6.9}$$

The integration path is a loop around the positive real axis in the complex ω-plane, consisting of the two branches $(\infty + i\epsilon, i\epsilon)$ and $(-i\epsilon, \infty - i\epsilon)$. Hence we may write for (6.6) (and similarly for the other three)

$$\langle P_0(0)\, P_0(t)\rangle = -\frac{1}{2\pi i}\int_0^\infty \frac{\omega^2\, d\omega}{G_+(\omega)}\left\{\coth\frac{1}{2}\,\beta\omega\,\cos\omega t + i\,\sin\omega t\right\}$$

$$+\frac{1}{2\pi i}\int_0^\infty \frac{\omega^2 d\omega}{G_-(\omega)}\left\{\coth\frac{1}{2}\,\beta\omega\,\cos\omega t + i\,\sin\omega t\right\}. \qquad (6.10)$$

7. REDUCTION TO THE STANDARD RESULT

First assumption: the poles on the real axis lie densely (i.e., with mutual distances negligible compared to ϵ). The number of them in any interval Δk, each multiplied with its contribution α_k^2, will be denoted by $g(k)\,\Delta k$. Then (for $\omega > 0$)

$$G(\omega \pm i\epsilon) = \omega^2 - \Omega^2 - \int_0^\infty \frac{g(k)\, dk}{\omega^2 - k^2} \pm i\pi\,\frac{g(\omega)}{2\omega}, \qquad (7.1)$$

where the integral is to be taken as a principal value.

Second assumption: $g(k)$ is small, $g(k)/k \ll \Omega^2$. The last two terms in (7.1) are of importance only when ω^2 is close to Ω^2, which justifies the approximation

$$G(\omega \pm i\epsilon) = \omega^2 - \Omega^2 - \int_0^\infty \frac{g(k)\, dk}{\Omega^2 - k^2} \pm i\pi\,\frac{g(\Omega)}{2\Omega}$$

$$= \omega^2 - \Omega'^2 \pm i\Gamma'. \qquad (7.2)$$

The renormalized frequency Ω' is given by the principal-value integral

$$\Omega'^2 = \Omega^2 + \int_0^\infty \frac{g(k)\, dk}{\Omega^2 - k^2},$$

and $\Gamma' = \pi g(\Omega)/2\Omega$ has the role of a damping. The approximate functions $G_\pm(\omega)$ in (7.2) are analytic functions with zeros $\sqrt{\Omega'^2 \mp \Gamma'}$, that is, $\Omega' - i\Gamma$ and $\Omega' + i\Gamma$ respectively, with $\Gamma = \Gamma'/2\Omega$.

Write for (6.10)

$$\langle P_0(0)\, P_0(t)\rangle$$

$$= -\frac{1}{4\pi i}\int_0^\infty \frac{\omega^2\, d\omega}{G_+(\omega)}\left\{e^{i\omega t}\left(\coth\frac{1}{2}\,\beta\omega + 1\right) + e^{-i\omega t}\left(\coth\frac{1}{2}\,\beta\omega - 1\right)\right\}$$

$$+\frac{1}{4\pi i}\int_0^\infty \frac{\omega^2\, d\omega}{G_-(\omega)}\left\{e^{i\omega t}\left(\coth\frac{1}{2}\,\beta\omega + 1\right) + e^{-i\omega t}\left(\coth\frac{1}{2}\,\beta\omega - 1\right)\right\}. \qquad (7.3)$$

The first term on the first line containing the factor $e^{i\omega t}$ is cancelled by shifting the path to the North and in the second term the path may be shifted to the South leaving the contribution of the pole $\Omega' - i\Gamma$

$$\tfrac{1}{4}\,\Omega' e^{-i\Omega' t} e^{-\Gamma t} (\coth \tfrac{1}{2}\,\beta\Omega' - 1).$$

Similarly the first term on the second line yields a contribution after shifting its path to the North. The final result is (for $t > 0$)

$$\langle P_0(0)\, P_0(t)\rangle = \tfrac{1}{2}\,\Omega' e^{-\Gamma t}\{\coth \tfrac{1}{2}\,\beta\Omega' \cos \Omega' t + i \sin \Omega' t\}. \tag{7.4}$$

In the same way

$$\langle P_0(0)\, Q_0(t)\rangle = \tfrac{1}{2}\, e^{-\Gamma t}\{\coth \tfrac{1}{2}\,\beta\Omega' \sin \Omega' t - i \cos \Omega' t\}, \tag{7.5}$$

$$\langle Q_0(0)\, P_0(t)\rangle = \tfrac{1}{2}\, e^{-\Gamma t}\{-\coth \tfrac{1}{2}\,\beta\Omega' \sin \Omega' t + i \cos \Omega' t\}, \tag{7.6}$$

$$\langle Q_0(0)\, Q_0(0)\rangle = (1/2\Omega')\, e^{-\Gamma t}\{\coth \tfrac{1}{2}\,\beta\Omega' \cos \Omega' t + i \sin \Omega' t\}. \tag{7.7}$$

Thus we have found the standard result with damping Γ and renormalized frequency Ω'. However, the shifting of the path can only be done until it meets the first pole $\omega = 2\pi i/\beta$, which corresponds to a time factor $\exp[-(2\pi/\beta)\, t]$. Consequently the standard results are limited to times long compared to β, or frequencies ω obeying $\hbar\omega < kT$. This expresses the fact that in quantum mechanics no white noise exists as the high frequencies are cut off at $kT/\hbar$. Thus the stochastic treatment of noise is not valid for short times and no differential equation for $\rho(t)$ exists. Incidentally, this inevitable lack of the required randomization at short times, see ref. 17, is also the cause of the so-called quantum Zeno effect.

8. ENERGY CORRELATION

One application is the calculation of the single-time energy correlation

$$\langle E^2\rangle = \tfrac{1}{4}\,\langle (P_0^2 + \Omega^2 Q_0^2)(P_0^2 + \Omega^2 Q_0^2)\rangle. \tag{8.1}$$

As a preliminary we note that for a bare harmonic oscillator with Hamiltonian $\frac{1}{2}\,(P^2 + \Omega^2 Q^2)$ in thermal equilibrium. The partition function is

$$Z = \operatorname{Tr} \exp\left[-\frac{1}{2}\,\beta(P^2 + \Omega^2 Q^2)\right] = \frac{1}{2 \sinh \beta\Omega/2}.$$

and the average energy is well known:

$$\langle E\rangle=\frac{1}{2}\langle P^2+\Omega^2Q^2\rangle=-\frac{\partial}{\partial\beta}\log Z=\frac{1}{2}\Omega\coth\beta\Omega/2.$$

Note that only for high temperature does it reduce to the classical $1/\beta$. The desired quantity (8.1) takes the form

$$\begin{aligned}\langle E^2\rangle&=\frac{1}{4}\langle(P^2+\Omega^2Q^2)^2\rangle=\frac{1}{Z}\frac{\partial^2 Z}{\partial\beta^2}\\&=-\frac{1}{4}\Omega^2+\frac{1}{2}\Omega^2\coth^2\beta\Omega/2=2\langle E\rangle^2-\frac{1}{4}\Omega^2\end{aligned}\tag{8.2}$$

or, alternatively

$$\begin{aligned}\langle(E-\langle E\rangle)^2\rangle&=\frac{1}{4}\Omega^2(\coth^2\beta\Omega/2-1)\\&=\frac{\Omega^2}{4\sinh^2\beta\Omega/2}=\Omega^2Z^2.\end{aligned}\tag{8.3}$$

After this preliminary note, take the oscillator in interaction with the bath. The expansion of (8.1) in the normal modes gives

$$\begin{aligned}\langle E^2\rangle&=\tfrac{1}{4}\sum_{\nu\mu\rho\sigma}X_{0\nu}X_{0\mu}X_{0\rho}X_{0\sigma}\langle(p_\nu p_\mu+\Omega^2q_\nu q_\mu)(p_\rho p_\sigma+\Omega^2q_\rho q_\sigma)\rangle\\&=\tfrac{1}{4}\sum_{\nu\mu\rho\sigma}X_{0\nu}X_{0\mu}X_{0\rho}X_{0\sigma}[\langle p_\nu p_\mu p_\rho p_\sigma\rangle+\Omega^2(\langle p_\nu p_\mu q_\rho q_\sigma\rangle\\&\quad+\langle q_\nu q_\mu p_\rho p_\sigma\rangle)+\Omega^4\langle q_\nu q_\mu q_\rho q_\sigma\rangle].\end{aligned}$$

The averages vanish unless the four indices are pairwise equal, or all four equal. The contribution of the latter case is

$$\mathrm{I}=\tfrac{1}{4}\sum_\nu X_{0\nu}^4[\langle p_\nu^4\rangle+\Omega^2(\langle p_\nu^2q_\nu^2\rangle+\langle q_\nu^2p_\nu^2\rangle)+\Omega^4\langle q_\nu^4\rangle].$$

We shall need some conclusions from (B.2):

$$\begin{aligned}&\langle p_\nu^2\rangle=\tfrac{1}{2}C_\nu\omega_\nu, &&\langle q_\nu^2\rangle=\tfrac{1}{2}C_\nu/\omega_\nu, &&\langle p_\nu q_\nu\rangle=-\langle q_\nu p_\nu\rangle=-\tfrac{1}{2}i\\&\langle p_\nu^4\rangle=\tfrac{3}{4}C_\nu^2\omega_\nu^2, &&\langle q_\nu^4\rangle=\tfrac{3}{4}C_\nu^2/\omega_\nu^2, &&\langle p_\nu^2q_\nu^2\rangle=\langle q_\nu^2p_\nu^2\rangle=\tfrac{1}{4}C_\nu^2-\tfrac{1}{2}.\end{aligned}\tag{8.4}$$

The contribution of the terms with $\nu = \mu \neq \rho = \sigma$ is

$$\mathrm{II} = \tfrac{1}{4} \sum_{\nu \neq \rho} X_{0\nu}^2 X_{0\rho}^2 [\langle p_\nu^2 \rangle \langle p_\rho^2 \rangle + \Omega^2 (\langle p_\nu^2 \rangle \langle q_\rho^2 \rangle + \langle q_\nu^2 \rangle \langle p_\rho^2 \rangle) + \Omega^4 \langle q_\nu^2 \rangle \langle q_\rho^2 \rangle]$$

$$= \tfrac{1}{4} [\langle P_0^2 \rangle^2 + 2\Omega^2 \langle P_0^2 \rangle \langle Q_0^2 \rangle + \Omega^4 \langle Q_0^2 \rangle^2]$$

$$-\tfrac{1}{4} \sum_{\nu} X_{0\nu}^4 [\langle p_\nu^2 \rangle^2 + 2\Omega^2 \langle p_\nu^2 \rangle \langle q_\nu^2 \rangle + \Omega^4 \langle q_\nu^2 \rangle^2]$$

$$= \langle E \rangle^2 - \tfrac{1}{4} \sum_{\nu} X_{0\nu}^4 [\langle p_\nu^2 \rangle^2 + \Omega^4 \langle q_\nu^2 \rangle^2] - \tfrac{1}{2} \Omega^2 \sum_{\nu} X_{0\nu}^4 \langle p_\nu^2 \rangle \langle q_\nu^2 \rangle.$$

Then there are the two equal contributions with $\nu = \rho \neq \mu = \sigma$, and $\nu = \sigma \neq \mu = \rho$, which are equal:

$$\mathrm{III} = \mathrm{IV} = \tfrac{1}{4} \sum_{\nu \neq \mu} X_{0\nu}^2 X_{0\mu}^2 [\langle p_\nu^2 \rangle \langle p_\mu^2 \rangle + \Omega^2 (\langle p_\nu q_\nu \rangle \langle p_\mu q_\mu \rangle$$

$$+ \langle q_\nu p_\nu \rangle \langle q_\mu p_\mu \rangle) + \Omega^4 \langle q_\nu^2 \rangle \langle q_\mu^2 \rangle]$$

$$= \tfrac{1}{4} \langle P_0^2 \rangle^2 + \tfrac{1}{4} \Omega^4 \langle Q_0^2 \rangle^2 - \tfrac{1}{4} \sum_{\nu} X_{0\nu}^4 [\langle p_\nu^2 \rangle^2 + \Omega^4 \langle q_\nu^2 \rangle^2]$$

$$+ \tfrac{1}{4} \Omega^2 [(-\tfrac{i}{2})^2 + (\tfrac{i}{2})^2] - \tfrac{1}{4} \Omega^2 \sum_{\nu} X_{0\nu}^4 [-\tfrac{1}{2}].$$

The final result is, taking into account (8.4),

$$\langle E^2 \rangle = \mathrm{I} + \mathrm{II} + 2 \times \mathrm{III}$$

$$= \langle E \rangle^2 + \frac{1}{2} \langle P_0^2 \rangle^2 + \frac{1}{2} \Omega^4 \langle Q_0^2 \rangle^2$$

$$+ \frac{1}{2} \Omega^2 \sum_{\nu} X_{0\nu}^4 [\langle p_\nu^2 q_\nu^2 \rangle - \langle p_\nu^2 \rangle \langle q_\nu^2 \rangle] - \frac{1}{4} \Omega^2 + \frac{1}{4} \Omega^2 \sum_{\nu} X_{0\nu}^4$$

$$= 2\langle E \rangle^2 + \frac{1}{4} \{\langle P_0^2 \rangle - \Omega^2 \langle Q_0^2 \rangle\}^2 - \frac{1}{4} \Omega^2$$

$$= 2\langle E \rangle^2 - \frac{1}{4} \Omega^2 + \frac{1}{4} \left\{ \frac{1}{2} \sum_{\nu} X_{0\nu}^2 \left(\omega_\nu - \frac{\Omega^2}{\omega_\nu} \right) \coth \frac{1}{2} \beta \omega_\nu \right\}^2.$$

The term in { } is the correction to (8.2) due to the corrected treatment of the interaction with the bath.

It should be borne in mind, however, that in any application one must decide whether one needs this bare energy E or perhaps a related quantity involving some of the interaction energy.

APPENDIX A

In order to diagonalize the quadratic form

$$\tfrac{1}{2}\,\Omega^2 Q_0^2 + \tfrac{1}{2}\sum_k k^2 Q_k^2 + Q_0 \sum_k v_k Q_k \tag{A1}$$

one has to find the eigenvectors from the equations

$$\Omega^2 Q_0 + \sum_k v_k Q_k = \omega^2 Q_0$$

$$k^2 Q_k + v_k Q_0 = \omega^2 Q_k.$$

Clearly

$$Q_k = \frac{v_k}{\omega^2 - k^2}\, Q_0$$

$$(\omega^2 - \Omega^2)\, Q_0 = \sum_k \frac{v_k^2}{\omega^2 - k^2}\, Q_0.$$

The eigenvalues ω_ν^2 are the zeros of the analytic function $G(\omega)$ given in (4.5). The normalization reads, for each separate eigenmode ν,

$$1 = Q_0^2 + \sum_k Q_k^2 = Q_0^2 \left\{ 1 + \sum_k \frac{v_k^2}{(\omega_\nu^2 - k^2)^2} \right\} = Q_0^2\, \frac{G'(\omega_\nu)}{2\omega_\nu}.$$

Thus the orthogonal transformation is

$$X_{0\nu} = \sqrt{\frac{2\omega_\nu}{G'(\omega_\nu)}} \qquad X_{k\nu} = \frac{v_k}{\omega_\nu^2 - k^2} \sqrt{\frac{2\omega_\nu}{G'(\omega_\nu)}}. \tag{A2}$$

That made it possible to replace the sums in (6.2)–(6.5) with the integrals (6.6)–(6.9).

Note. One often considers, rather than (4.1), the Hamiltonian

$$H_{\mathrm{T}} = \frac{1}{2}(P_0^2 + \Omega^2 Q_0^2) + \frac{1}{2}\sum_k \left\{ P_k^2 + k^2 \left(Q_k + \frac{\alpha_k}{k^2} Q_0 \right)^2 \right\},$$

which is positive definite by construction.[18] In the present work the simpler form (4.1) is preferred at the expense of stipulating explicitly the positivity condition

$$\Omega^2 > \sum_\nu \frac{\alpha_k^2}{k^2} = \int_0^\infty \frac{g(k)}{k^2}\, dk. \qquad \text{(A3)}$$

This condition ensures that (7.1) exists for $\omega = 0$.

In order to make the transition to the integrals in (6.6)–(6.9) more precise note that the function

$$G(z) = z - \Omega^2 - \sum_\nu \frac{\alpha_k^2}{z - k^2}$$

is analytic in the entire z-plane with the cut along the positive real axis. Thanks to (A3) it has no zeros outside this cut and it behaves asymptotically for large z as $|z|^2$. Hence the loop integrals in (6.6)–(6.9) do indeed reduce to the integrals along the two sides of the positive real axis. It is then to be assumed that $G(z)$ can be continued across the cut to produce the two zeros $\Omega' \mp i\Gamma$.

APPENDIX B

To compute the trace for each separate ν the index may be ignored and it is convenient to employ temporarily a further canonical transformation:

$$p_\nu = \sqrt{\omega_\nu}\, p', \quad q_\nu = q'/\sqrt{\omega_\nu}, \quad \beta\sqrt{\omega_\nu} = \beta', \quad x_\nu \sqrt{\omega_\nu} = x', \quad y_\nu / \sqrt{\omega_\nu} = y'.$$

Thus we have to compute

$$\Theta(x', y'; \beta') = \mathrm{Tr}(\exp[ix'p' + iy'q'] \exp[-\tfrac{1}{2}\beta'(p'^2 + q'^2)]), \qquad \text{(B1)}$$

which may be written in either alternative form

$$= \mathrm{e}^{-ix'y'/2}\, \mathrm{Tr}(\exp[ix'p'] \exp[iy'q'] \exp[-\tfrac{1}{2}\beta'(p'^2 + q'^2)])$$
$$= \mathrm{e}^{+ix'y'/2}\, \mathrm{Tr}(\exp[iy'q'] \exp[ix'p'] \exp[-\tfrac{1}{2}\beta'(p'^2 + q'^2)]).$$

Clearly for $x' = y' = 0$ this reduces to (4.6). In order to compute this trace first differentiate[18]

$$\frac{\partial \Theta}{\partial \beta'} = -\frac{1}{2}\,\mathrm{Tr}\left((p'^2+q'^2)\exp[ix'p'+iy'q']\exp\left[-\frac{1}{2}\beta'(p'^2+q'^2)\right]\right)$$
$$= \frac{1}{2}\left(\frac{\partial^2\Theta}{\partial x'^2}+\frac{\partial^2\Theta}{\partial y'^2}\right)+\frac{1}{2}i\left(y'\frac{\partial\Theta}{\partial x'}-x'\frac{\partial\Theta}{\partial y'}\right)-\frac{x'^2+y'^2}{8}\Theta.$$

A rotation in the (p, q)-plane does not affect the trace and therefore Θ depends on x', y' only through $r=\sqrt{x'^2+y'^2}$ so that the second term on the right vanishes. Subsequently the factors $e^{-\lambda\beta'}$ and $e^{-r^2/4}$ may be split off:

$$\Theta = \Xi\exp[-\lambda\beta'-r^2/4], \qquad \frac{d^2\Xi}{dr^2}+\left(\frac{1}{r}-r\right)\frac{d\Xi}{dr}+(2\lambda-1)\,\Xi=0.$$

The eigenvalues are found to be $\lambda = l+\frac{1}{2}$ with $l = 0, 1, 2, 3,\ldots$ and the corresponding solutions are, in terms of Laguerre polynomials, $e^{-r^2/4}L_l(r^2/2)$. For $x' = y' = 0$ the sum of these eigensolutions must reduce to (4.6), hence

$$\Theta \equiv \mathrm{Tr}\,(\exp[ix'p'+iy'q']\exp[-\tfrac{1}{2}\beta'(p'^2+q'^2])$$
$$= \exp[-r^2/4]\sum_{l=0}^{\infty}\exp\,[-(l+\tfrac{1}{2})\,\beta']\,L_l(r^2/2)/L_l(0).$$

With the use of the generating functional of the L_l this may be written

$$\Theta = \exp[-r^2/4]\,\frac{\exp[-\frac{1}{2}\beta']}{1-e^{-\beta'}}\exp\left[-\frac{r^2/2}{e^{\beta'}-1}\right] = \frac{\exp\,[-\frac{1}{4}r^2\coth\frac{1}{2}\beta']}{2\sinh\frac{1}{2}\beta'}.$$

The final result is

$$\left\langle \exp\sum_\nu (ix_\nu p_\nu + iy_\nu q_\nu)\right\rangle = \Theta/Z = \exp\left[-\sum_\nu \frac{\omega_\nu x_\nu^2 + y_\nu^2/\omega_\nu}{4}\coth\frac{1}{2}\beta\omega_\nu\right]. \tag{B2}$$

Remembering the definition of x_ν, y_ν one obtains (5.2).

APPENDIX C

Suppose for a system with variables P, Q and unknown density matrix ρ the function of two variables

$$K(x, y) = \mathrm{Tr}\, e^{ixP+iyQ}\rho$$

is given and I want to determine the density matrix. In the representation in which Q is diagonal

$$K(x, y) = \mathrm{e}^{-ixy/2}\,\mathrm{Tr}\,\mathrm{e}^{ixP}\mathrm{e}^{iyQ}\rho$$

$$= \mathrm{e}^{-ixy/2}\iint dq\,dq'(q\,|\mathrm{e}^{ixP}|\,q')\,\mathrm{e}^{iyq'}(q'\,|\rho|\,q)$$

$$= \mathrm{e}^{-ixy/2}\iint dq\,dq'\,\delta(q-q'+x)\,\mathrm{e}^{iyq'}(q'\,|\rho|\,q)$$

$$= \mathrm{e}^{-ixy/2}\int dq'\,\mathrm{e}^{iyq'}(q'\,|\rho|\,q'-x)$$

$$= \int d\bar{q}\,\mathrm{e}^{iy\bar{q}}(\bar{q}+\tfrac{1}{2}x\,|\rho|\,\bar{q}-\tfrac{1}{2}x).$$

Inverting the Fourier transform

$$\left(\bar{q}+\frac{1}{2}x\,|\rho|\,\bar{q}-\frac{1}{2}x\right) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dy\,\mathrm{e}^{-iy\bar{q}}K(x, y).$$

In a more customary notation $\bar{q}+\frac{1}{2}x = q_1$ and $\bar{q}-\frac{1}{2}x = q_2$,

$$(q_1\,|\rho|\,q_2) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dy\,\mathrm{e}^{-iy(q_2+q_1)/2}K(q_1-q_2, y).$$

The generalization to N variables $\{q_\nu\} = \mathrm{q}$ with corresponding p is trivial:

$$(\mathrm{q}_1\,|\rho|\,\mathrm{q}_2) = (2\pi)^{-N}\int d^N\mathrm{y}\,\mathrm{e}^{-i\mathrm{y}\cdot(\mathrm{q}_1+\mathrm{q}_2)/2}K(\mathrm{q}_1-\mathrm{q}_2, \mathrm{y}).$$

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