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A Soluble Model for Quantum Mechanical Dissipation

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In order to derive the equations for dissipation and noise in a quantum mechanical system it is necessary to include the equations of motion of a suitably chosen bath interacting with the system. In this way the standard treatment arrives at an approximate master equation for the density matrix of the system, at the expense of a number of *ad hoc* assumptions. These assumptions are here scrutinized on the basis of an exactly soluble model. The conclusion is: the bath must obey certain specifications; the interaction must be weak; and the temperature must be so high that the interaction energy is within the classical domain rather than occurring in quanta. Some additional comments concerning dissipation in quantum mechanics are relegated to an appendix.

KEY WORDS: Dissipation; noise; quantum master equation.

1. INTRODUCTION AND MOTIVATION

Newton's classical equations of motion can readily be supplemented by a term to account for the friction. The concomitant noise may be taken into account by a Langevin term. For linear equations this gives a reasonable description. For nonlinear cases this short-cut is not uniquely defined and no reliable results can be obtained without a more detailed study of the actual noise source.(1) In quantum mechanics no short-cut is possible and it is necessary to include the cause of damping and noise explicitly, although the details of the mechanism may be immaterial. Thus, apart from the system of interest S, one has to include a bath B and an interaction between both. The total Hamiltonian is

$$H_{\mathrm{T}} = H_{\mathrm{S}} + H_{\mathrm{B}} + H_{\mathrm{T}} \tag{1}$$

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One now has to solve the Schrödinger equation for this combined system. The hope is that from this solution one may, at least in some approximation, deduce an equation for S alone.

The standard way to do this is as follows.(2) One takes as initial state of the total system a density matrix in the form of a product,

$$\rho_{\mathrm{T}}(0)=\rho_{\mathrm{S}}(0)\otimes\rho_{\mathrm{B}}^{\mathrm{e}} \tag{2}$$

where $\rho_{\mathrm{S}}(0)$ is the initial state of S, and $\rho_{\mathrm{B}}^{\mathrm{e}}$ the thermal equilibrium state of B. The total density matrix evolves according to

$$\rho_{\mathrm{T}}(t)=e^{-itH_{\mathrm{T}}}\rho_{\mathrm{T}}(0)\,e^{itH_{\mathrm{T}}} \tag{3}$$

The density matrix of S alone is obtained by averaging over B,

$$\rho_{\mathrm{S}}(t)=\mathrm{Tr}_{\mathrm{B}}\,e^{-itH_{\mathrm{T}}}\rho_{\mathrm{S}}(0)\otimes\rho_{\mathrm{B}}^{\mathrm{e}}e^{itH_{\mathrm{T}}} \tag{4}$$

This defines a linear map $\rho_{\mathrm{S}}(0)\to\rho_{\mathrm{S}}(t)$, which may be written symbolically

$$\rho_{\mathrm{S}}(t)=\mathscr{T}(t)\,\rho_{\mathrm{S}}(0) \tag{5}$$

where $\mathscr{T}$ is a superoperator, i.e., an operator acting in the space of matrices. This map can be computed explicitly for one well-known soluble model, namely a harmonic oscillator interacting with a bath of oscillators through a bilinear H_{I}.(3) In this paper we present a second soluble model.

In the absence of an exact solution, however, one has to resort to an expansion. For a short time Δt one may compute (3) to second order in the interaction and in this way one finds for (4)

$$\rho_{\mathrm{S}}(\Delta t)=\rho_{\mathrm{S}}(0)+\Delta t\,\mathscr{L}\rho_{\mathrm{S}}(0)+\cdots \tag{6}$$

where $\mathscr{L}$ is a time-independent superoperator. From this one concludes that $\rho_{\mathrm{S}}(t)$ obeys the differential equation

$$\dot{\rho}_{\mathrm{S}}(t)=\mathscr{L}\rho_{\mathrm{S}}(t) \tag{7}$$

However, this equation has been derived only at $t=0$, starting from the initial condition (2). The crucial assumption is that it holds at all times, with the implication that $\rho_{\mathrm{S}}(t)$ constitutes a semigroup whose infinitesimal generator is $\mathscr{L}$. The idea is that, although during the first time interval Δt correlations will build up between ρ_{S} and ρ_{B}, they will not affect the evolution during the subsequent interval Δt. This is the *repeated randomness assumption*, also called molecular chaos, random phase, or Stosszahlansatz.

It is essential for statistical mechanics of nonequilibrium processes, but it is little understood.

Thus the semigroup or Markov character is not derived but postulated. It is often argued that the bath variables vary rapidly, so that Δt can be taken long compared to the bath correlation times. Then the equilibrium distribution ρ_B^e is supposed to have time to be reestablished during Δt, and (6) may be used again. (This is the basis of the so-called "singular coupling method."[4]) Unfortunately, the harmonic oscillator model shows that the argument is incorrect: *friction and noise arise from those bath oscillators that are in resonance with the system.* The other oscillators give rise only to a modification of the frequency.

The purpose of the present work is to get a better understanding of the approximations needed to obtain a semigroup description in the form (7). A model is constructed of a quantum mechanical particle that moves along a lattice of sites while interacting with a bath. Starting from the exact equation, we shall find that (7) is approximately valid provided that (i) the bath is chosen suitably, (ii) the interaction with the bath is weak, and (iii) the temperature is so high that the quantized character of the interaction is immaterial.

A difference with the harmonic oscillator model is that our system S has a continuous spectrum, so that there is no resonance. Yet it will turn out again that the high-frequency bath oscillators merely modify the Hamiltonian, while the dissipation is caused by the oscillators in the low-frequency region.

2. THE MODEL AND ITS SOLUTION

The *system* S is a particle which may reside in any one of a number of sites ν, where ν runs over all integers from $-\infty$ to $+\infty$. The Hilbert space is spanned by the orthonormal states

$$|\nu), \qquad (\nu \mid \nu') = \delta_{\nu\nu'}$$

A step operator s is defined by

$$s\,|\nu) = |\nu+1), \qquad s^{-1}\,|\nu) = |\nu-1)$$

The operator $S = \frac{1}{2}(s + s^{-1})$ is hermitian. Its eigenfunctions, denoted by $|\eta)$, are

$$|\eta) = \frac{1}{(2\pi)^{1/2}} \sum_{-\infty}^{\infty} e^{i\eta\nu}\,|\nu) \qquad (0 \leqslant \eta < 2\pi)$$

The eigenvalues are $\cos \eta$. For the system Hamiltonian we take

$$H_S = \Omega S \qquad (\Omega = \text{const} \geqslant 0) \tag{8a}$$

Its matrix elements in the η-representation are

$$(\eta|\, H_S\, |\eta') = \Omega \cos \eta\; \delta(\eta - \eta')$$

The *bath* is taken to be an assembly of harmonic oscillators labeled n, frequencies k_n, step operators $a_n^\dagger$, a_n, excitation number N_n,

$$H_B = \sum_n k_n a_n^\dagger a_n, \qquad \text{eigenvalues} \quad \sum_n k_n N_n \tag{8b}$$

The k_n are positive, but so far not otherwise restricted.

For the *interaction* we take

$$H_I = S \sum_n v_n (a_n + a_n^\dagger) \equiv SB \tag{8c}$$

with coupling constants v_n. Here B is an abbreviated notation for an operator referring to the bath alone.

H_T commutes with S and is therefore diagonal in the η-representation:

$$\begin{aligned} (\eta|\, H_T\, |\eta') &= \delta(\eta - \eta')\{\Omega \cos \eta + H_\eta\} \\ H_\eta &= \sum_n k_n a_n^\dagger a_n + (\cos \eta) \sum_n v_n (a_n + a_n^\dagger) \\ &= \sum_n H_{\eta,n} \end{aligned} \tag{9}$$

The initial density matrix (2) is

$$\rho_T(0) = \rho_S(0) \prod_n (1 - e^{-\beta k_n})\, e^{-\beta k_n a_n^\dagger a_n} \tag{10}$$

β is the reciprocal temperature of the bath. Hence (3) reduces to

$$\begin{aligned} (\eta|\, \rho_T(t)\, |\eta') = (\eta|\, \rho_S(0)\, |\eta')\, e^{-i\Omega t(\cos\eta - \cos\eta')} \\ \times e^{-itH_\eta} \rho_B^e e^{itH_\eta} \end{aligned} \tag{11}$$

The second line is a product of independent factors,

$$\prod_n \{e^{-itH_{\eta,n}} (1 - e^{-\beta k_n})\, e^{-\beta k_n a_n^\dagger a_n} e^{itH_{\eta',n}}) \tag{12}$$

Taking the trace over the bath yields

$$(\eta|\, \rho_S(t)\, |\eta') = (\eta|\, \rho_S(0)\, |\eta')\, e^{-i\Omega t(\cos\eta - \cos\eta')} \\ \times \prod_n (1 - e^{-\beta k_n}) \sum_{N_n} \langle N_n|\, e^{-itH_{\eta,n}} e^{-\beta k_n a_n^\dagger a_n} e^{itH_{\eta',n}}\, |N_n\rangle \quad (13)$$

This expression is worked out in Appendix A, with the result

$$(\eta|\, \rho_S(t)\, |\eta') = (\eta|\, \rho_S(0)\, |\eta')\, e^{-i\Omega t(\cos\eta - \cos\eta')} \\ \times e^{iF(t)(\cos^2\eta - \cos^2\eta')} e^{-G(t)(\cos\eta - \cos\eta')^2} \quad (14)$$

where

$$F(t) = \sum_n \frac{v_n^2}{k_n}\left(t - \frac{\sin k_n t}{k_n}\right) \quad (15a)$$

$$G(t) = \sum_n \frac{v_n^2}{k_n^2}(1 - \cos k_n t) \coth \frac{\beta k_n}{2} \quad (15b)$$

This is the explicit form of (5).

3. THE COEFFICIENTS F AND G

Does the solution obey a differential equation (7)? Differentiating (14) and restoring the operator notation, one gets

$$\dot\rho_S(t) = -i\Omega[S, \rho_S(t)] + i\dot F(t)[S^2, \rho_S(t)] \\ - \dot G(t)\{S^2\rho_S(t) - 2S\rho_S(t)S + \rho_S(t)\, S^2\} \quad (16)$$

This differential equation is not, however, of the desired type (7) because $\dot F$ and $\dot G$ depend on time. The initial time has a special role owing to the initial condition (2), (10). We shall show that after an initial transient both $\dot F$ and $\dot G$ become constants.

At this point it is necessary to suppose that the k_n lie very dense on $(0, \infty)$. Define a strength function $g(k)$ by

$$g(k)\, \Delta k = \sum_{k < k_n < k + \Delta k} v_n^2$$

Then (15) may be written

$$F(t) = \int_0^\infty \frac{g(k)}{k}\left(t - \frac{\sin kt}{k}\right) dk \quad (17a)$$

$$G(t) = \int_0^\infty \frac{g(k)}{k^2}(1 - \cos kt) \coth \frac{\beta k}{2}\, dk \quad (17b)$$

It is clear that $g(k)/k$ must be integrable, to avoid infrared and ultraviolet divergences. This is a restriction on the bath. More specifically I suppose that $g(k)$ has a linear region, that is, there is a constant k_0 such that with sufficient approximation

$$g(k) = \gamma k \qquad (\gamma = \text{const}, k < k_0) \tag{18}$$

Consider $F(t)$ for t obeying

$$k_0 t \gg 2\pi \tag{19}$$

Then for $k > k_0$ one may omit $\sin kt$, so that

$$F(t) = t \int_0^\infty \frac{g(k)}{k}\, dk - \gamma \int_0^{k_0} \frac{\sin kt}{k}\, dk \tag{20a}$$

$$\equiv \Gamma t - \gamma \frac{\pi}{2} \tag{20b}$$

Hence $F(t)$ becomes proportional to t, apart from a constant, which is due to the transient and is called "initial slip." From (20) one sees that the slip is a small correction to $F(t)$ when t obeys (19).

Next consider $G(t)$ given by (17b):

$$G(t) = \gamma \int_0^{k_0} \frac{1 - \cos kt}{k} \coth \frac{\beta k}{2}\, dk + \int_{k_0}^\infty \frac{g(k)}{k^2} \coth \frac{\beta k}{2}\, dk$$

In addition to (19) we suppose

$$\beta k_0 \ll 1 \tag{21}$$

and may then write

$$\begin{aligned} G(t) &= \frac{2\gamma}{\beta} \int_0^{k_0} \frac{1 - \cos kt}{k^2}\, dk + \int_{k_0}^\infty \frac{g(k)}{k^2} \coth \frac{\beta k}{2}\, dk \\ &= \frac{2\gamma}{\beta} \left(\frac{\pi}{2} t - \frac{1}{k_0} \right) + \int_{k_0}^\infty \frac{g(k)}{k^2} \coth \frac{\beta k}{2}\, dk \\ &= \frac{\pi\gamma}{\beta} t + \Lambda \end{aligned} \tag{22}$$

Λ is a constant given by

$$\Lambda = \int_0^\infty \left\{ \frac{g(k)}{k^2} \coth \frac{\beta k}{2} - \frac{2\gamma}{\beta} \frac{1}{k^2} \right\} dk \tag{23}$$

It represents again an initial slip and is a small correction when (19) is obeyed.

The right-hand side of Eq. (16) consists of three terms. The first one represents the motion of the free system. The second term is also a commutator and corresponds therefore to a Hamiltonian evolution. From (20) one sees that it involves all bath oscillators: the high-frequency oscillators (beyond k_0) merely have the effect of modifying the Hamiltonian, just as in the harmonic oscillator model. In the third term the coefficient $\dot{G}(t) = \pi\gamma/\beta$ involves only the oscillators in the low-frequency region. This term represents damping, as can be seen from (14): it kills all off-diagonal elements of $(\eta|\, \rho_S \,|\eta')$. (The diagonal elements are strictly constant because $[H_T, S] = 0$.)

4. THE MARKOV CHARACTER

The conclusion is that, starting from the initial state (2), there is a transient time ϑ after which

$$\dot{\rho}_S = -i[H_S, \rho_S] + i\Gamma[S^2, \rho_S] + \frac{\pi\gamma}{\beta}\{2S\rho_S S - S^2\rho_S - \rho_S S^2\} \tag{24}$$

It follows from (19) that one must have $\vartheta > 2\pi/k_0$; that is, the transient is at least as large as the period at which the linear region (8) ends. In addition, the choice of k_0 is subject to (21), which implies

$$\vartheta > \hbar/\kappa T \tag{25}$$

that is, the transient cannot be less than the period at which quantum mechanics becomes noticeable. The former restriction is not fundamental as long as we are free to choose a suitable bath, but the restriction (25) is independent of the bath; it is a formulation of the general rule that quantum noise cannot be white.

The fact that $\rho_S(t)$ obeys (24) for $t > \vartheta$ does not prove the semigroup property. This property means that (supposing $0 < t_1 < t_2$), one can obtain $\rho_S(t_2)$ not only directly from $\rho_S(0)$, but also by first fnding $\rho_S(t_1)$ and then, starting from this as initial value, applying the evolution equation during $t_2 - t_1$. According to (14), that requires

$$F(t_2) = F(t_1) + F(t_2 - t_1), \qquad G(t_2) = G(t_1) + G(t_2 - t_1)$$

The expressions (20) and (22) do not obey this requirement. All one can say is that it is obeyed if not only t_1 and t_2 are large compared to ϑ, but one must also have $t_2 - t_1 \gg \vartheta$. Hence the semigroup property is approximately satisfied on a coarse-grained time scale.

More precisely, one should subdivide the time axis into intervals $\Delta t \gg \vartheta$ and then apply the linear approximation (6) successively to each interval. Of course, this discretization causes an error, which is large unless ρ_S varies relatively little during Δt. According to (24), this requires

$$\Omega\,\Delta t \ll 1, \qquad \Gamma\,\Delta t \ll 1, \qquad (\pi\gamma/\beta)\,\Delta t \ll 1 \tag{26}$$

The first inequality can be defused by going to the interaction representation. The second one gives, according to (19), $\gamma \ll 1$, if one utilizes the order-of-magnitude estimate $\Gamma \sim \gamma k_0$. The third one, according to (25), gives the same. The conclusion is that the interaction must be weak.

One way of obeying all these conditions is provided by the so-called $\lambda^2 t$ limit. One scales down the interaction coefficients v_n by a factor λ, extends the time considered,

$$v_n = \lambda v_n^*, \qquad g = \lambda^2 g^*, \qquad t = \lambda^{-2} t^*$$

and takes the limit $\lambda \to 0$ with fixed g^*, t^*. Applying this limiting procedure to (17), one finds painlessly

$$F(t) \to \Gamma t, \qquad G(t) \to (\pi\gamma/\beta)\,t$$

However, this device works so smoothly because it ignores the physical reality. It treats the interaction as infinitely weak and the long-time limit has the effect that only low-frequency oscillators of the bath matter. As a consequence one is always in the linear region (18) and all relevant oscillators are classical. The terms in (20) and (22) displaying the initial slip vanish in this limit, although of course in reality they are not zero.

5. THE STANDARD APPROXIMATION METHOD

In practical cases, of course, no exact solution is available and the master equation (7) can be obtained only by an approximation method, as described in Section 1. In order to test that method we apply it here to the present model. The necessary algebra has been performed in ref. 1, Section XVII.3. We outline the result.

Our Hamiltonian (1) is specified in (8). The operators B and S in the two subspaces have Heisenberg representations, which at time $-\tau$ are

$$B(-\tau) = e^{-i\tau H_B} B e^{i\tau H_B}, \qquad S(-\tau) = S$$

One then evaluates (3) to second order in the interaction, takes the trace, and differentiates, with the result

$$\begin{aligned}\dot{\rho}_S &= -i[H_I, \rho_S] \\ &\quad -\tfrac{1}{2}\int_0^\infty d\tau\, \langle [B, B(-\tau)]\rangle^e\, [S, [S, \rho_S]_+] \\ &\quad -\tfrac{1}{2}\int_0^\infty d\tau\, \langle [B, B(-\tau)]_+\rangle^e\, [S, [S, \rho_S]]\end{aligned} \tag{27}$$

The subscript + indicates the anticommutator, and $\langle \cdots \rangle^e$ denotes equilibrium average.

$$\langle \cdots \rangle^e = \mathrm{Tr}_B(\cdots \rho_B^e)$$

According to ref. 1, p. 449, one has

$$\langle [B, B(-\tau)]\rangle^e = -2i\int_0^\infty g(k)\sin k\tau\, dk$$

$$\langle [B, B(-\tau)]_+\rangle^e = 2\int_0^\infty g(k)\cos k\tau \coth(\tfrac{1}{2}\beta k)\, dk$$

Substitution in (27) yields

$$\begin{aligned}\dot{\rho}_S &= -i\Omega[S, \rho_S] \\ &\quad + i\left\{\int_0^\infty d\tau \int_0^\infty g(k)\sin k\tau\, dk\right\}(S^2\rho_S - \rho_S S^2) \\ &\quad - \left\{\int_0^\infty d\tau \int_0^\infty g(k)\cos k\tau \coth(\tfrac{1}{2}\beta k)\, dk\right\}(S^2\rho_S - 2S\rho_S S + \rho_S S^2) \\ &= -i\Omega[S, \rho_S] + i\left\{\int_0^\infty \frac{g(k)}{k}\, dk\right\}[S^2, \rho_S] \\ &\quad + \left\{\pi\int_0^\infty g(k)\coth(\tfrac{1}{2}\beta k)\,\delta(k)\, dk\right\}(2S\rho_S S - S^2\rho_S - \rho_S S^2)\end{aligned}$$

In terms of our previous notation this is (24).

Thus for the present model the standard approximation method yields the desired master equation. The transient has been eliminated by the bold step of extending in (27) the integrations over τ to infinity rather than to t. Moreover, the equation has been derived only for the special initial condition (2) and subsequently the semigroup property is enforced by means of the repeated randomness assumption. Finally, the fact that the approximation method produces the correct master equation is special for the present model; in more general cases the resulting master equation is unacceptable as it may lead to a $\rho_S(t)$ that is not positive definite; see Appendix B.

APPENDIX A. DERIVATION OF (14)

In order to work out (13) first note from (9) that

$$H_{\eta,n} = k_n(a_n^\dagger + u_n)(a_n + u_n) - k_n u_n^2$$

with $u_n = (v_n/k_n)\cos\eta$, $u_n = (v_n/k_n)\cos\eta'$. For the quantity $\{\cdots\}$ in (12) we may write (omitting the label n)

$$(1 - e^{-\beta k})\, e^{ikt(u^2 - u'^2)}\,\Xi$$

$$\Xi = \operatorname{Tr} e^{-ikt(a^\dagger + u)(a + u)} e^{-\beta k a^\dagger a} e^{ikt(a^\dagger + u')(a + u')}$$

Using a sequence of operator identities, the reader should be able to transform this into

$$\begin{aligned} \Xi = e^{-i(u^2 - u'^2)\sin kt} & \operatorname{Tr} e^{-\beta k a^\dagger a} \\ & \times \exp\{u'[a(e^{ikt} - 1) - a^\dagger(e^{-ikt} - 1)] \\ & + u[a(1 - e^{ikt}) - a^\dagger(1 - e^{-ikt})]\} \end{aligned}$$

On writing the trace as a sum over the eigenstates of $a^\dagger a$, one finds for it

$$[1 - \exp(-\beta k)] \exp\left[-(u - u')^2\,(1 - \cos kt)\coth\frac{\beta k}{2}\right]$$

Collecting results, one obtains (14), (15).

APPENDIX B. THE POSITIVITY CONDITION

The mapping $\mathscr{T}$ in (9) must conserve not only the trace and the hermiticity of the density matrix, but also the positive-definiteness. It has been proved[5] that a necessary and sufficient condition is that $\mathscr{T}$ has the form

$$\mathscr{T}\rho = \sum_\alpha A_\alpha \rho A_\alpha^\dagger \tag{B1a}$$

where the A_α are any set of operators obeying

$$\sum_\alpha A_\alpha^\dagger A_\alpha = 1 \tag{B1b}$$

Of course the exact operator $\mathscr{T}$ in (14) conserves positivity, but it is not manifest that it is actually of the form (B1). The first two factors are no problem: they may be combined into

$$(\eta|\, e^{-it\Omega tS + iFS^2} \rho_S(0)\, e^{i\Omega tS - iFS^2}\, |\eta')$$

Subsequently we may set

$$A_\alpha = B_\alpha e^{-i\Omega tS^2 + iFS^2}$$

and it remains to choose the operators B_α such that

$$(\eta| \sum_\alpha B_\alpha \rho B_\alpha^\dagger\, |\eta') = (\eta|\, \rho\, |\eta')\, e^{-G(\cos\eta - \cos\eta')^2} \tag{B2}$$

With the aid of the identity

$$e^{-G(\cos\eta - \cos\eta')^2} = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-\alpha^2}\, d\alpha\, e^{2i\alpha\sqrt{G}(\cos\eta - \cos\eta')}$$

it is clear that (B2) is obeyed on choosing

$$B_\alpha = \pi^{-1/2} e^{-\alpha^2/2} e^{i\alpha\sqrt{G}S}$$

and replacing the sum over α with an integral.

From the general condition (B1) it can be deduced that, *if a differential equation (7) exists*, it must have the form (first given by Kossakowski$^{(6)}$)

$$\mathscr{L}\rho_S = -i[K, \rho_S] + \sum_\alpha (V_\alpha \rho_S V_\alpha^\dagger - \tfrac{1}{2} V_\alpha^\dagger V_\alpha \rho_S - \tfrac{1}{2} \rho_S V_\alpha^\dagger V_\alpha)$$

K is a hermitian operator and determines the reversible Schrödinger-like evolution. The V_α are any set of operators and determine the irreversible, dissipative evolution.

The difficulty mentioned in Section 5 is that the usual result, based on standard second-order approximation in the strength of the coupling, does *not* have this form and is therefore unacceptable.$^{(1,7)}$ The reason why our present model does not suffer from this flaw is that our H_S and H_I commute. This model is therefore not able to shed any light on the problem of nonpositivity.

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