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Analysis of Two Types of the Master and the Langevin Equations

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§ 1. Introduction.

As to the master and the Langevin equations, two types of equations for each of them are known ; the one contains a term with time-convolution[1] and the other does not[2),3),4)].

We consider two simple typical example models to examine which type of equations is more suitable for each model when we make approximations. As the models, we treat a harmonic oscillator with an external perturabtion causing the frequency modulation (adiabatic transitions)[2] in the case of the master equation, and that with external perturbations causing non-adiabatic transitions[5),6)] in the case of the Langevin equation.

In § 2, two types of basic equations are derived for each model, and in § 3 their solutions are discussed. We compare solutions of the exact and the approximate equations numerically, and show the results in figures.

In conclusion, we find that for our first model with adiabatic transitions the time-convolutionless type of equations gives exact behaviour of the system in the lowest "Born approximation", whereas the time-convolution type gives only approximate behaviour which coincides with the exact one only in the narrowing limit. For our second model with non-adiabatic transitions, however, we find the opposite situation, in which the time-convolution type gives exact behaviour in the "Born approximation". Thus the better choice between the two types of formulae depends on the structure of systems, and hence we should be careful in discussing the high-frequency or the short-time behaviour of a system by making use of one type of the master or the Langevin equation in its approximate form.

§ 2. Two Types of the Master and the Langevin Equations

Let us consider a system perturbed by a random force. We assume a stochastic Hamiltonian of the form

$$\mathscr{H}(t)=\mathscr{H}_0+\mathscr{H}_1(t), \tag{2. 1}$$

where $\mathscr{H}_0$ denotes the Hamiltonian of the system alone and $\mathscr{H}_1(t)$ an external perturbation which is a random function of time t. The motion of this system is governed by the stochastic Liouville equation for the density matrix of the system

$$\dot{W}(t) = -iLW(t), \tag{2.2}$$

where $L=L_0+L_1(t)$ is the stochastic Liouvillian corresponding to the Hamiltonian (2. 1). We are interested in the averaged behaviour of the system described by the density matrix $\rho(t)$ obtained by averaging $W(t)$ over the random process $\mathscr{H}_1(t)$. Two types of equations of motion for $\rho(t)$ have been derived:

$$\dot{\rho}(t) = -i(L_0+\langle L_1(t)\rangle_B)\,\rho(t) - \int_0^t d\tau X(\tau)\rho(t-\tau), \tag{2.3}$$

which we call the time-convolution type, and

$$\dot{\rho}(t) = -i(L_0+\langle L_1(t)\rangle_B)\rho(t) - \psi(t)\rho(t), \tag{2.4}$$

which we call the time-convolutionless type.

Similar discussion has been done in the Heisenberg picture too. However, in place of a stochastic system, let us now take explicitly into account the origin of a stochastic force, a heat bath; that is, let us consider a system in contact with a heat bath. The total composite system is assumed to have a Hamiltonian

$$\mathscr{H} = \mathscr{H}_S + \mathscr{H}_B + \mathscr{H}_{SB}, \tag{2.5}$$

where $\mathscr{H}_S$ is a Hamiltonian of the system, $\mathscr{H}_B$ the bath Hamiltonian, and $\mathscr{H}_{SB}$ the interaction between them. Two types of Langevin equations for an arbitrary dynamical variable A have been derived:

$$\dot{A}(t) = e^{iLt}\langle iL\rangle_B A(0) + \int_0^t d\tau\; e^{iL(t-\tau)}\;\phi_m(\tau)A(0) + K_m(t), \tag{2.6}$$

which we call the time-convolution type, and

$$\dot{A}(t) = e^{iLt}\,\langle iL\rangle_B\, A(0) - e^{iLt}\,\psi(t)A(0) + K(t), \tag{2.7}$$

which we call the time-covolutionless type.

Eqs. (2. 3) and (2. 4) are both exact, and they are equivalent with each other. But, if we make any approximation, this equivalence will be broken down. We shall find that which of Eqs. (2. 3) and (2. 4) will give the better approximation depends on a detailed structure of the random external force. With respect to the pair of Eqs. (2. 6) and (2. 7), the situation is the same.

To see the situation in detail, let us confine ourselves to simple models and to the "Born approximation", in which we retain terms up to the second order with respect to the stochastic force or the interaction. Eqs. (2. 3) and

(2. 4) will be applied to Kubo's model of the random frequency modulation[8], and Eqs. (2. 6) and (2. 7) to the problem of a harmonic oscillator with an interaction which causes non-adiabatic transitions.

Let us consider Kubo's oscillator model first. The complex coordinate $x(t)$ of this classical oscillator is assumed to obey the stochastic equation of motion

$$\frac{d}{dt} x(t)=i(\omega_0+g\omega_1(t))\, x(t), \tag{2. 8}$$

where we have introduced a coupling constant g explicitly. ω_0 is a fixed characteristic frequency, while $\omega_1(t)$ is assumed to be a stationary Gaussian process with vanishing average. This equation of motion is not the Liouville equation, but has the same structure as the latter: $x(t)$ corresponds to $W(t)$ of Eq. (2. 3), ω_0 to $-L_0$, and $g\omega_1(t)$ to $-L_1(t)$.

We are interested in the averaged coordinate $\langle x(t)\rangle_B$, which obeys the equation of motion

$$\frac{d}{dt} \langle x(t)\rangle_B=\{i\omega_0-g^2\int_0^t \Phi(\tau)\, d\tau\}\langle x(t)\rangle_B, \tag{2. 9}$$

where we have introduced the correlation function

$$\Phi(\tau_1-\tau_2)=\langle\omega_1(\tau_1)\,\omega_1(\tau_2)\rangle_B. \tag{2. 10}$$

The exact solusion of this equation is

$$\langle x(t)\rangle_B=\exp\{i\omega_0 t-g^2\int_0^t (t-\tau)\,\Phi(\tau)d\tau\}\; x(0). \tag{2. 11}$$

In the "Born approximation" for this model, the convolution type equation (2. 3) reduces to

$$\frac{d}{dt} \langle x(t)\rangle_B=i\omega_0\langle x(t)\rangle_B-\int_0^t d\tau\, X_2(t-\tau)\langle x(\tau)\rangle_B, \tag{2. 12}$$

where the kernel is given by

$$X_2(t-\tau)=\Phi(t-\tau)\, e^{i\omega_0(t-\tau)}. \tag{2. 13}$$

The exact equation (2. 9) is not reached within this approximation.

On the other hand, the convolutionless type equation (2. 4) gives in the "Born approximation"[2].

$$\frac{d}{dt} \langle x(t)\rangle_B=i\omega_0\,\langle x(t)\rangle_B-g^2\psi_2(t)\,\langle x(t)\rangle_B, \tag{2. 14}$$

where

$$\psi_2(t)=\int_0^t d\tau\,\Phi(\tau). \tag{2. 15}$$

We find that this approximation gives already the exact one (2. 9): the higher order terms in $\psi(t)$ should all vanish[2] owing to our assumption of Gaussian process.

Next, we consider a quantal harmonic oscillator interacting with the heat bath. We take the Hamiltonian (2. 5) composed of the forms

$$\mathscr{H}_S=\omega_0 a^+ a, \tag{2. 16a}$$

$$\mathscr{H}_B=\sum_k \omega_k b_k^+ b_k, \tag{2. 16b}$$

and

$$\mathscr{H}_{SB}=\sum_k (\kappa_k^* b_k^+ a+\kappa_k b_k a^+), \tag{2. 16c}$$

where a and a^+ represent the annihilation and the creation operators for the harmonic oscillator, while b_k and b_k^+ those for the bath; κ_k and κ_k^* are coupling constants. Making use of the expressions (2. 16) in Eqs. (2. 6) and (2. 7) in the "Born approximation" with respect to L_{SB}, we obtain the time-convolution type and the time-convolutionless type of Langevin equations for $a(t)$

$$\left(\frac{d}{dt}+i\omega_0\right)a(t)+\sum_k|\kappa_k|^2\int_0^t d\tau\, e^{-i\omega_k\tau}\, a(t-\tau)=-i\sum_k \kappa_k\, e^{-i\omega_k t}\, b_k, \tag{2. 17}$$

and

$$\left(\frac{d}{dt}+i\omega_0\right)a(t)+\sum_k|\kappa_k|^2\int_0^t d\tau\, e^{-i(\omega_0-\omega_k)\tau}\, a(t)=-i\sum_k\kappa_k\, e^{-i\omega_k t}\, b_k, \tag{2. 18}$$

respectively.

Eq. (2. 17) of the time-convolution type coincides with the exact result obtained by Scully and Whitney[6]: we can prove that the higher order terms with respect to L_{SB} in the perturbational expansion of $\psi_m(t)$ in Eq. (2. 6) vanish.[5]

§3. Numerical Calculations and Discussions

Two types of equations have been derived for the two special models in § 2. In this section, we shall compare two solutions of these equations for each model.

Let us first discuss Kubo's model, and for simplicity let us further assume the process $\omega_1(t)$ to be Markoffian, i.e.[9].

$$\Phi(\tau)=\Delta^2\, e^{-|\tau|/\tau_c}, \tag{3. 1}$$

where we have defined the amplitude and the correlation time of modulation frequency :

$$\Delta=\langle\omega_1^2\rangle_B^{1/2} \quad\text{and}\quad \tau_c=\frac{1}{\Delta^2}\int_0^\infty d\tau\, \Phi(\tau). \tag{3. 2}$$

Then, the second order equation obtained from the convolution type equation (2. 2) reads as

$$\frac{d}{dt}\langle x(t)\rangle_B = i\omega_0\langle x(t)\rangle_B - (g\Delta)^2\int_0^t d\tau \, \exp\left\{\left(i\omega_0 - \frac{1}{\tau_c}\right)(t-\tau)\right\}\langle x(t)\rangle_B, \tag{3. 3}$$

and has the solution[2)], which we call the "truncated solution" for this model,

$$\langle x(t)\rangle_B = \frac{e^{i\omega_0 t}}{2(1-4\alpha^2)^{1/2}}\Big[\{1+(1-4\alpha^2)^{1/2}\}\, e^{-\{1+(1+4\alpha^2)1/2\}\,t/2\tau_c} - \{1-(1-4\alpha^2)^{1/2}\}\, e^{-\{1+(1-4\alpha^2)1/2\}\,t/2\tau_c}\Big]\, x(0), \tag{3. 4}$$

where we have introduced the parameter

$$\alpha = g\Delta\tau_c. \tag{3. 5}$$

On the other hand, the exact equation (2. 9) and its exact solution (2. 11), which are in accord with those in the "Born approximation" for the convolution type, become, respectively[2)],

$$\frac{d}{dt}\langle x(t)\rangle_B = \left\{i\omega_0 - \frac{1}{\tau_c}(1-e^{-t/\tau_c})\right\}\langle x(t)\rangle_B, \tag{3. 6}$$

and

$$\langle x(t)\rangle_B = \exp\left\{i\omega_0 t - \alpha^2\left(\frac{t}{\tau_c} + e^{-t/\tau_c} - 1\right)\right\} x(0). \tag{3. 7}$$

We show in Figs. 1∼3 the curves of $\langle x(t)\rangle\, e^{-i\omega_0 t}/x(0)$ given by the exact and the truncated solution, Eqs. (3. 7) and (3. 4), for a set of values of α. The case $\alpha \ll 1$ corresponds to the narrowing limit, at which both solutions coincide.

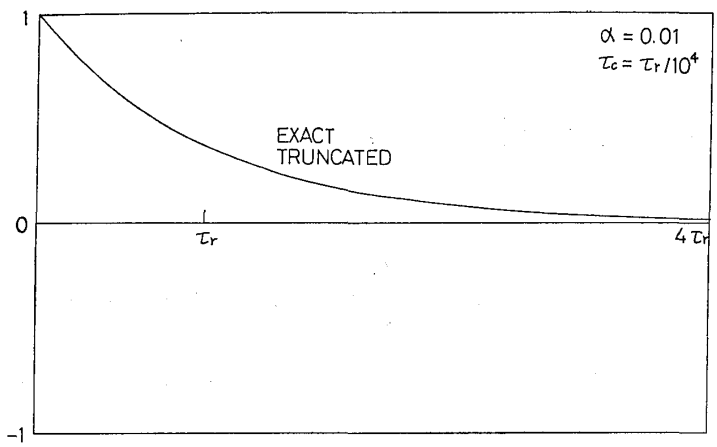

Fig. 1. $\alpha=0.01$. Two curves are almost exponentially decaying and coincide very well with each other for any time t. This case corresponds to the narrowing limit. τ_c is not shown as it is very small. The relaxation time τ_r is given by $\tau_r = 1/g^2\Delta^2\tau_c$ in Figs. 1∼3.

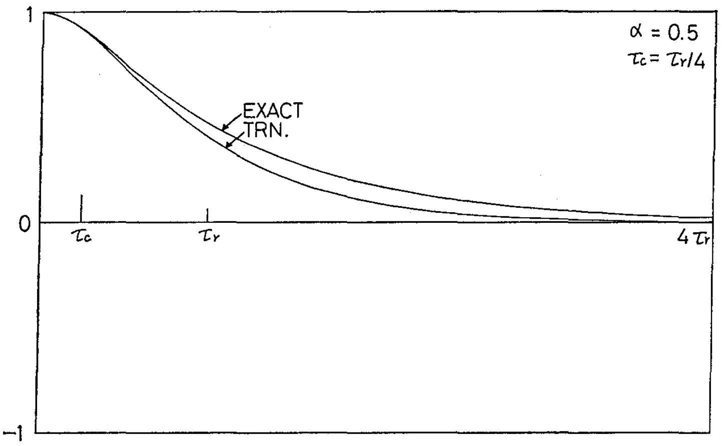

Fig. 2. $\alpha=0.5$. The exact curve decays monotonously, whereas the truncated one begins to oscillate at this value of α. Two curves coincide for $t\leq\tau_c$.

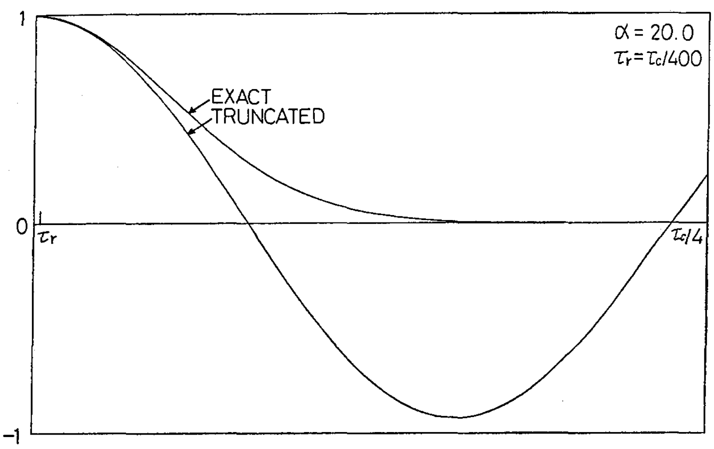

Fig. 3. $\alpha=20.0$. The exact curve is nearly Gaussian. The truncated one oscillates slowly and decays slowly. Two curves coincide only for $t\leq\tau_c/50$.

Now let us proceed to the case of harmonic oscillator. We compare the exact equation of time-convolution type (2. 17) and the truncated equation of time-convolutionless type (2. 18). Putting

$$\varphi(\tau)=\sum_k |\kappa_k|^2\, e^{-i\omega_k\tau}, \tag{3. 8}$$

we rewrite Eq. (2. 17) as

$$\dot{a}(t)=-i\omega_0 a(t)-\int_0^t dt\, \varphi(\tau)\, a(t-\tau)+K(t). \tag{3. 9}$$

In order to obtain explicitly a solution of Eq. (3. 9), we assume a Lorentzian density of states:

$$\sum_k |\kappa_k|^2\, \delta(\omega-\omega_k)=\frac{D}{\pi}\,\frac{\Delta^2}{\omega^2+D^2}. \tag{3. 10}$$

Then, we have the kernel

$$\varphi(\tau)\equiv\int_{-\infty}^{\infty}\frac{D}{\pi}\frac{\Delta^2}{\omega^2+D^2}e^{-i\omega\tau}\,d\tau=\Delta^2 e^{-D\tau}. \tag{3.11}$$

The correlation time τ_c of the heat bath is given by

$$\tau_c=\frac{1}{\varphi(0)}\int_0^{\infty}d\tau\,\varphi(\tau)=\frac{1}{D}. \tag{3.12}$$

If we change the variable $a(t)$ into

$$A(t)\equiv e^{-i\omega_0 t}\,a(t)\,; \tag{3.13}$$

then Eq. (3.9) is transformed into

$$\dot{A}(t)=-\int_0^t \Delta^2 e^{(i\omega_0-D)\tau}A(t-\tau)\,d\tau+K(t). \tag{3.14}$$

The solution of Eq. (3.14) is given by

$$\langle A(t)\rangle_B=\frac{1}{\nu-\mu}\{(\nu+D-i\omega_0)\,e^{\nu t}-(\mu+D-i\omega_0)e^{\mu t}\}\,A(0), \tag{3.15}$$

where ν and μ are the two roots of the equation

$$S^2+(D-i\omega_0)\,S+\Delta^2=0. \tag{3.16}$$

Similarly, we can calculate the solution of the truncated equation (2.18). In this case, we have

$$\dot{A}(t)=-\int_0^t d\tau\,\Delta^2 e^{(i\omega_0-D)\tau}A(t)+K(t), \tag{3.17}$$

and obtain the "truncated solution"

$$\langle A(t)\rangle=\exp\left[\frac{\Delta^2}{i\omega_0-D}\left(\frac{1-e^{(i\omega_0-D)t}}{D-i\omega_0}-t\right)\right]A(0). \tag{3.18}$$

We plot in Figs. 4~7 the curves of $\mathrm{Re}\langle A(t)\rangle/A(0)$ for the exact and the truncated solution, Eqs. (3.15) and (2.18) and for a set of dimensionless parameters

$$\Omega=\frac{\omega_0}{D}\ \text{ and }\ \hat{\alpha}=\frac{\alpha^2}{1+\Omega^2}\quad(\alpha=\Delta\,\tau_c). \tag{3.19}$$

In this model the narrowing condition is given by $\hat{\alpha}\ll 1$, and in this limit both the solutions (3.15) and (3.18) behave like

$$\langle A(t)\rangle\sim e^{-\hat{\alpha}t/\tau_c}.$$

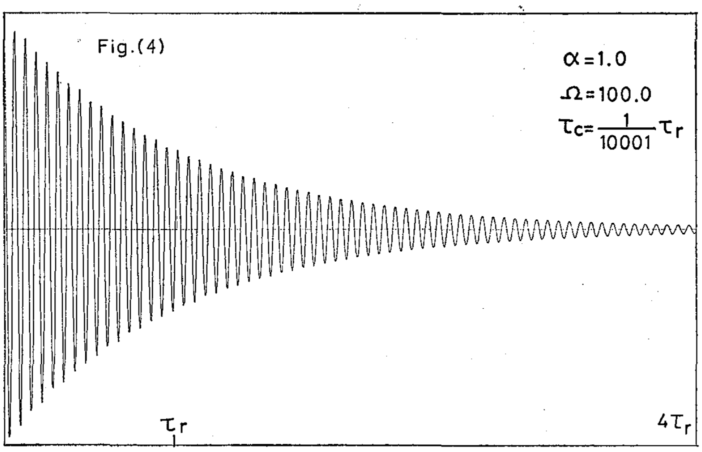

Fig. 4. $\hat{\alpha}=1.0\times10^{-5}$. Two curves are of the damped oscillation type and coincide with each other for any time t. This corresponds to the narrowing limit. τ_c is not shown as it is almost zero. τ_r is given by $\tau_r=(1+\Omega^2)\tau_c/\alpha^2$ in Figs. 4~7.

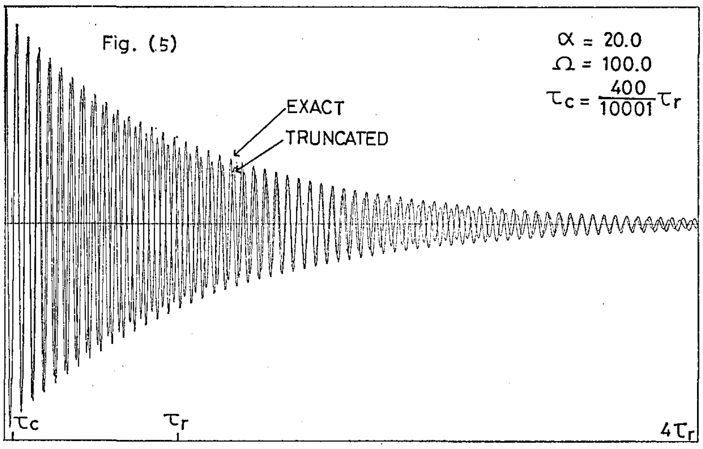

Fig. 5. $\hat{\alpha}=4.0\times10^{-4}$. Two curves begin to have different periods and decay constants. They coincide for $t\leq3\tau_c$.

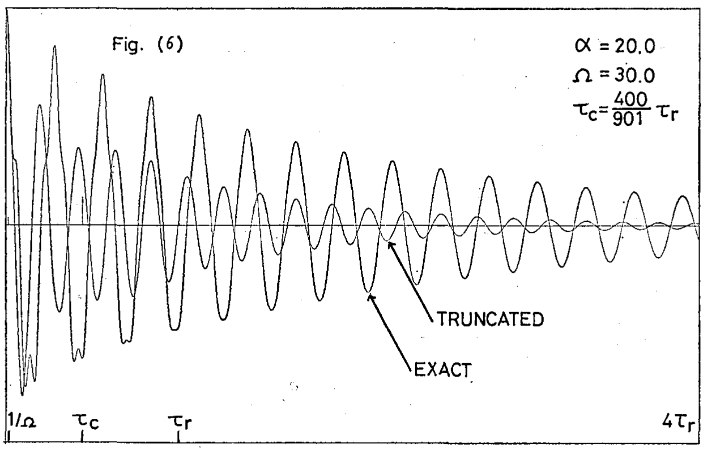

Fig. 6. $\hat{\alpha}=3.7\times10^{-2}$. Note the depressions at the lower peaks of oscillation of the exact curve. Two curves coincide for $t\leq2\Omega$.

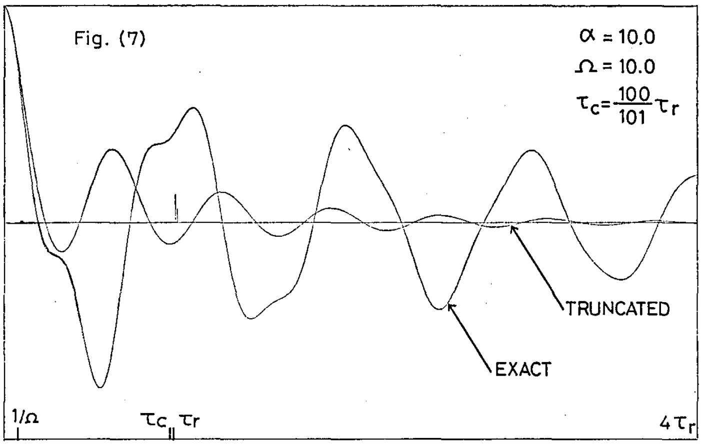

Fig. 7. $\hat{\alpha}=0.99$. The difference of the exact curve from the simple damping oscillation type is very evident, whereas the truncated one may be regarded as the simple damped oscillation. Two curves coincide for $t \leq 1/\Omega$.

In view of the results given above we should note that for a system with the interaction causing adiabatic transitions, such as Kubo's model, the time-convolutionless type of equations is expected to give a better solution even in the "Born approximation", whereas the time-convolution type gives only a poor one in that aprroximation. Unless the narrowing condition is satisfied the "truncated solution" behaves differently from the exact one and is valid only for a very short time. For the other model with the interaction causing non-adiabatic trasitions, however, we shall find the opposite situation. Therefore, we should appropriately choose one of the two types of equations case by case. However, it is an open question which type of equations, the time-convolution or the time-convolutionless type, we should apply to the system having simultaneously both types of the interactions discussed above.

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