

Time Evolution of a Quantum System in Contact with a Nearly Gaussian-Markoffian Noise Bath

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A test system is assumed to interact with a heat bath consisting of harmonic oscillators or an equivalent bath with a proper frequency spectrum producing a Gaussian-Markoffian random perturbation. The effect of reaction of the test system to the bath is considered in the high temperature approximation. Elimination of the bath using the influence functional method of Feynman and Vernon yields a continuous fraction expression for the reduced density matrix of the test system. The result affords a basis to clarify the relationship between the stochastic and the dynamical approaches to treat the problem of partial destruction of quantum coherence of a system interacting with its environment.

§1. Introduction

Brownian motion of quantum systems or more generally quantum processes in dissipative systems have been a subject of great interest for many years. The interest has been renewed in recent years in connection with the work by Leggett *et al.* on the problem of quantum tunneling in macroscopic systems.^{1,2)} Recent progress in experimental techniques has made experiments feasible to test possible effects of dissipation on quantum phenomena.³⁾ It should be noticed, however, that the problem is not really new. One of the oldest examples is the radiation damping of an excited atom interacting the bath of radiation field.⁴⁾ There exist a great number of literatures on the various aspects and methods on this subject.⁵⁻⁷⁾

Dissipation is due to the interaction between the system, which we call the test system **A**, and the bath **B**. When the bath variables are eliminated from the basic equation of motion of the whole system, the test system is regarded to follow a dissipative dynamics. At the crudest stage, the dynamics is deterministic with proper parameters characterizing dissipation. In a more detailed description one considers fluctuations so that the dynamics has to bear a stochastic character. The classical example is the Langevin equation

describing the Brownian motion. The equation contains a friction term and a random force, which is assumed to be a Gaussian white noise with the intensity related to the friction by the fluctuation-dissipation theorem. A given sample of the random force determines a path of the particle. When the paths are integrated over all possible realizations, we are lead to the transition probability function of the Brownian particle from an initial to final states. Because of the Gaussian-white assumption, this follows a Fokker-Planck equation.

In many realistic cases, the system-bath interaction may be assumed in a good approximation to have a Gaussian nature. This is obviously true if the bath is regarded to consist of harmonic oscillators and should also be true if the interaction is a cumulative effect of a great number of weak interactions, when some sort of central limit theorem comes into play. A simple example is a spin precessing in a local random field which is a resultant of dipolar interactions of many other spins in the environment. Generalizing this simple example, we model the system of our interest by an effective Hamiltonian which is regarded as stochastic variable. Namely we introduce a stochastic variable or such variables representing the states of the bath and assume a certain law of stochastic evolution. We then consider

the interaction Hamiltonian as a function of such variables. We call this kind of models a *stochastic approach*⁸⁻¹¹⁾ in contrast to the *dynamical approach* in which one explicitly assumes a dynamical model for the bath and carries out usually some sort of perturbative calculations.

A stochastic approach is by its nature a phenomenological one. The underlying stochastic process is merely a model appropriate for the problem rather than something to be derived from microscopic considerations. This is regarded as an advantage since it can cover a wide category of physical cases from a unified point of view. Furthermore the calculations may be carried out by non-perturbative methods.

The most important and sufficiently realistic model among such stochastic models of bath-system interaction is the Gaussian noise which is further assumed to be Markoffian. Such a model has been used repeatedly to treat dynamical systems under the influence of its environment, for instance, nuclear spins, atoms or molecules in varying local environments.⁸⁾ The key question was the effect of non-white character, namely the effect of finiteness of the correlation time of the noise in comparison with the magnitudes of the noise. When the correlation time is very short, namely when the noise is regarded as white, we may have the motionally-narrowed limit, where simple perturbational calculation works well yielding exponential decays and the quantum coherence of the system is completely destroyed. This corresponds to the classical ideal Brownian motion. On the other hand, if the noise varies very slowly, the system maintains its quantum coherence. The reality may be found to lie between the two extremes, namely in intermediate situations. A very general method has been developed for a Gaussian-Markoffian noise to cover the whole range of its correlation time. The formal solutions can be written down in terms of a continued fraction expression.

One drawback of the stochastic approach is that it ignores the reaction of the test system to the bath.⁸⁻¹¹⁾ The effect of the bath is considered merely as an external force disregarding its dynamic degrees of freedom. This cor-

responds to assuming an infinite temperature for the bath. This makes no harm in many examples such as those of nuclear resonance problems. Nevertheless it is interesting to consider how we could remedy the drawback and to see how the stochastic model is related to a dynamic model.

In order to clarify a few points about the above mentioned problem, we use here the Feynman-Vernon formalism¹²⁾ assuming a bath composed of harmonic oscillators. The evolution of the density matrix of the test system can be generally expressed in terms of coherent state representation. When the interaction of the bath is introduced through the influence functional into the path integral expression, we find two types of terms representing the effect of the bath. One of the terms corresponds to the stochastic interaction with a Gaussian noise and the other corresponds to the dynamical effect which was missing in the stochastic model. Both of them are Gaussian noises but with different correlation functions. By assuming an appropriate spectrum for the oscillator frequencies, we are able to secure the Markoffian character in a high temperature approximation. We then show that the Laplace transform of the reduced density matrix for the test system is expressed in terms of a continued fraction. This enables us to recover the evolution equation of the stochastic model in a generalized form.

This paper is organized in the following way. In §2, we give a brief review of the formalism of the stochastic approach with a Gaussian Markoffian noise. Section 3 is devoted to an account of the path integral expression to include the influence functional in the coherent state representation. This shows that our treatment can, in principle, be applied to general classes of test systems. In §4, we derive a set of equations to determine the evolution of the density matrix of the test system averaged over all possible paths of the bath oscillators. The continued fractional expression of its Laplace transform is obtained from the equations. This explicitly shows the relation of the present approach to the stochastic one.

In the last section, we add a few remarks including the cases where Markoffian properties

are not realized. In the lowest approximation which corresponds to the conventional Born approximation we recover the familiar master equation.

§2. Brief Summary of Stochastic Approach⁸⁾

We consider a test system **A** interacting with a bath **B**. The states of **B** is denoted by $\Omega = (\Omega_1, \Omega_2, \dots)$. We assume that the evolution of **B** is stochastic and is described by a Markoffian equation,

$$\begin{aligned} \frac{\partial}{\partial t} P(\Omega, t) &= -\Gamma_{\Omega} P(\Omega, t) \\ &\equiv -\sum_{\Omega'} (\Omega | \Gamma | \Omega') P(\Omega', t), \end{aligned} \quad (2.1)$$

where $P(\Omega, t)$ is the probability to find **B** in the state Ω at time t and $(\Omega | \Gamma | \Omega')$ is the transition rate from Ω' to Ω . The equilibrium state of **B** is denoted by $|0\rangle$ and its conjugate by $\langle 0|$. They satisfy the relations,

$$\begin{aligned} \Gamma |0\rangle &= 0, \quad \langle 0| \Gamma = 0, \\ \langle 0|0\rangle &= 1. \end{aligned} \quad (2.2)$$

The quantal evolution of **A** is assumed to be governed by the Hamiltonian

$$H(t) = H_A + H_I(\Omega(t)), \quad (2.3)$$

where H_A is the Hamiltonian of **A** itself and H_I is the interaction with **B**. Because of the stochastic motion of **B**, the effective Hamiltonian $H(t)$ is stochastic. The quantal Liouville equation for the test system **A**

$$\frac{\partial}{\partial t} \rho(t) = (i\hbar)^{-1} H^{\times}(t) \rho(t) \quad (2.4)$$

is regarded here as a stochastic equation containing the stochastic parameter $\Omega(t)$. The notation H^{\times} means a commutator operation, namely

$$H^{\times} \rho \equiv H\rho - \rho H. \quad (2.5)$$

The formal solution of eq. (2.4) for a given sample of $\Omega(t)$ is written as

$$\rho(t) = \exp\left[-(i\hbar)^{-1} \int_{t_i}^t H^{\times}(t') dt'\right] \rho(t_i), \quad (2.6)$$

where the exponential operator is ordered in time, $\rho(t_i)$ being the initial density matrix of the test system.

We define the matrix $(\Omega | \bar{\rho}(t) | \Omega')$ as the average of (2.6) over all possible paths of $\Omega(t)$ with a prescribed initial state Ω' and a final state Ω of **B**. Then the matrix element of $\bar{\rho}(t)$ is easily shown to be the solution of the modified evolution equation

$$\begin{aligned} \frac{\partial}{\partial t} \bar{\rho}(\Omega, t) &= (i\hbar)^{-1} (H_A^{\times} + H_I^{\times}(\Omega)) \bar{\rho}(\Omega, t) \\ &\quad - \Gamma_{\Omega} \bar{\rho}(\Omega, t), \end{aligned} \quad (2.7)$$

with the initial condition $\bar{\rho}(\Omega, t_i) \propto \delta(\Omega - \Omega')$.

We shall be mostly concerned with Gaussian-Markoffian evolution of $\Omega(t)$ for which we have

$$\Gamma_{\Omega} = -\gamma \frac{\partial}{\partial \Omega} \left(\Omega + \frac{\partial}{\partial \Omega} \right). \quad (2.8)$$

The equilibrium distribution of Ω is given by

$$P_0(\Omega) \equiv (\Omega | 0) = (2\pi)^{-1/2} \exp(-\Omega^2/2), \quad (2.9)$$

which satisfies the condition

$$\Gamma_{\Omega} P_0(\Omega) = 0, \quad (2.10)$$

and the correlation function of the noise is

$$\langle \Omega(t) \Omega(0) \rangle = e^{-\gamma t}, \quad (2.11)$$

which defines the correlation time

$$\tau_c = 1/\gamma. \quad (2.12)$$

We assume that the interaction is explicitly expressed by

$$H_I^{\times}(\Omega) = \hbar \Delta \cdot \Omega V^{\times}, \quad (2.13)$$

where $\hbar \Delta$ is the magnitude of the interaction and V is the operator of **A** conjugate to the interaction force. Then eq. (2.7) takes the form

$$\begin{aligned} \frac{\partial}{\partial t} \bar{\rho}(\Omega, t) &= \left\{ (i\hbar)^{-1} H_A^{\times} - i \Delta \cdot \Omega V^{\times} \right. \\ &\quad \left. + \gamma \frac{\partial}{\partial \Omega} \left(\Omega + \frac{\partial}{\partial \Omega} \right) \right\} \bar{\rho}(\Omega, t). \end{aligned} \quad (2.14)$$

We take the average of the solution over the initial equilibrium of the bath and sum over the final state to obtain

$$\langle 0 | \bar{\rho}(t) | 0 \rangle = \iint d\Omega (\Omega | \bar{\rho}(t) | \Omega') d\Omega' P_0(\Omega'), \quad (2.15)$$

and introduce the Laplace transform

$$(0|\bar{\rho}[s]|0) = \int_{t_i}^{\infty} e^{-s(t-t_i)} (0|\bar{\rho}(t)|0) dt, \quad (2.16)$$

with the initial condition $\rho(t_i)$. Then we easily obtain

$$(0|\bar{\rho}[s]|0) = \frac{1}{s - (i\hbar)^{-1}H_A^\times + V^\times} \frac{\Delta^2}{s + \gamma - (i\hbar)^{-1}H_A^\times + V^\times} \frac{2\Delta^2}{s + 2\gamma - (i\hbar)^{-1}H_A^\times + \dots} V^\times \rho(t_i), \quad (2.17)$$

where the fractional operators mean inverse operators. This continued fractional expression has been used in treating various line shape problems with Gaussian random perturbation.^{13,14)}

§3. Influence Functional Formulation in Coherent State Representation

In this section we consider a test system **A** in contact with a heat bath **B** consisting of harmonic oscillators. In order to formulate the problem in a general way we introduce the coherent state representation¹⁵⁾ for the system **A** composed of bosons or fermions which is described by a set of annihilation and creation operators $\{a_\alpha, a_\alpha^+\}$. A coherent state $|\phi\rangle$ is defined by

$$|\phi\rangle = \exp\left(\zeta \sum_\alpha \phi_\alpha a_\alpha^+\right) |0\rangle, \quad (3.1)$$

where ϕ_α denotes a complex number (c-number) for bosons and a Grassmann number (G-number) for fermions. The constant ζ is equal to 1 for bosons and is equal to -1 for fermions. The state $|0\rangle$ is vacuum. Then we have

$$a_\alpha |\phi\rangle = \phi_\alpha |\phi\rangle, \quad (3.2)$$

and

$$\langle\phi| a_\alpha^+ = \langle\phi| \phi_\alpha^*, \quad (3.3)$$

where ϕ_α^* denotes a c- or G-number conjugate to ϕ_α . Different coherent states have the inner product

$$\langle\phi|\phi'\rangle = \exp\left(\sum_\alpha \phi_\alpha^* \phi'_\alpha\right) \equiv \exp(\phi^* \phi). \quad (3.4)$$

We use hereafter the abbreviation $\phi^* \phi$ for $\sum \phi_\alpha^* \phi_\alpha$. The completeness relation is expressed as

$$\iint N^{-1} d\phi^* d\phi |\phi\rangle e^{-\phi^* \phi} \langle\phi| = 1, \quad (3.5)$$

where we use the abbreviation

$$\iint N^{-1} d\phi^* d\phi \equiv \prod_\alpha \iint N_\alpha^{-1} d\phi_\alpha^* d\phi_\alpha, \quad (3.6)$$

for the measure of integration, the normalization constant N_α being equal to $2\pi i$ for bosons and 1 for fermions.

Then any state $|\Psi\rangle$ can be expressed as

$$|\Psi\rangle = \iint N^{-1} d\phi^* d\phi |\phi\rangle e^{-\phi^* \phi} \Psi(\phi^*), \quad (3.7)$$

or as

$$|\Psi\rangle = \iint N^{-1} d\phi^* d\phi |\phi\rangle \Psi'(\phi^*), \quad (3.8)$$

by defining

$$\Psi(\phi^*) = \langle\phi|\Psi\rangle, \quad (3.9)$$

or

$$\Psi'(\phi^*) = e^{-\phi^* \phi} \Psi(\phi^*), \quad (3.10)$$

which may be called the coherent state representation of $|\Psi\rangle$. For convenience we adopt here the second one as the definition of the coherent state representation.

The Hamiltonian of **A** is denoted by a normal-ordered expression $H_A(a^+, a)$, where a^+ and a denote the set of a_α and a_α^+ . The system is initially in a coherent state $|\phi_i\rangle$ and evolves over a time interval from t_i to t_f by the Hamiltonian to the final state

$$\begin{aligned} |\Psi(t_f)\rangle &= \exp[(i\hbar)^{-1}H_A(t_f - t_i)] |\phi_i\rangle \\ &= \iint N^{-1} d\phi_f^* d\phi_f |\phi_f\rangle e^{-\phi_f^* \phi_f} \langle\phi_f|\Psi(t_f)\rangle, \end{aligned} \quad (3.11)$$

where

$$\langle \phi_f | \Psi(t_f) \rangle = \langle \phi_f | \exp [(i\hbar)^{-1} H_A(t_f - t_i)] | \phi_i \rangle \quad (3.12)$$

is the coherent state representation of the final

state. By dividing the time interval into M segments as $\varepsilon = (t_f - t_i)/M$ and by inserting the completeness relation (3.5) at each joint of segments, we obtain a path integral expression taking the limit $M \rightarrow \infty$,

$$\langle \phi_f | \Psi(t_f) \rangle = \int D_f[\phi^*(\tau)\phi(\tau)] \exp [\phi_f^* \phi_f + (i/\hbar) S_A(\phi^*, \phi; t_f, t_i)], \quad (3.13)$$

where

$$\begin{aligned} S_A(\phi^*, \phi; t_f, t_i) &= \lim_{M \rightarrow \infty} \sum_{k=1}^M \varepsilon [i\hbar \phi_k^* (\phi_k - \phi_{k-1}) / \varepsilon - H_A(\phi_k^*, \phi_{k-1})] \\ &\equiv \int_{t_i}^{t_f} d\tau [i\hbar \phi^*(\tau) \dot{\phi}(\tau) - H_A(\phi^*(\tau), \phi(\tau))] \end{aligned} \quad (3.14)$$

is the action of the Schrödinger Lagrangian and

$$\int D_f[\phi^*(\tau)\phi(\tau)] \equiv \lim_{M \rightarrow \infty} \prod_{k=1}^{M-1} \int N^{-1} d\phi_k^* d\phi_k \quad (3.15)$$

denotes integration over the measure of the paths of $\{\phi^*(\tau), \phi(\tau)\}$ over the time interval (t_i, t_f) for the fixed initial state $\phi(t_i) = \phi_i$ and the final state $\phi^*(t_f) = \phi_f^*$. Inserting eq. (3.13) into eq. (3.11), we get

$$|\Psi(t_f)\rangle = \int D[\phi^*(\tau)\phi(\tau)] |\phi_f\rangle \exp [(i/\hbar) S_A(\phi^*, \phi; t_f, t_i)], \quad (3.16)$$

where $D[\phi^*(\tau)\phi(\tau)]$ means to include integration over the final states $|\phi_f\rangle$.

Combining eq. (3.16) and its conjugate we have the density operator at t_f

$$\rho_A(t_f) = |\Psi(t_f)\rangle \langle \Psi'(t_f)| = \iint N^{-1} d\phi_f^* d\phi_f \iint N^{-1} d\phi_f'^* d\phi_f' |\phi_f\rangle \rho_A(\phi_f^*, \phi_f'; t_f, t_i) \langle \phi_f'|, \quad (3.17)$$

where

$$\begin{aligned} \rho_A(\phi_f^*, \phi_f'; t_f, t_i) &= \int D_f[\phi^*(\tau)\phi(\tau)] \int D_f[\phi'^*(\tau)\phi'(\tau)] \\ &\times \exp [(i/\hbar) S_A(\phi^*, \phi; t_f, t_i)] \exp [-(i/\hbar) S_A^*(\phi'^*, \phi'; t_f, t_i)] \end{aligned} \quad (3.18)$$

is the coherent state representation of the density matrix in accord with the definition eq. (3.10).

We now introduce the bath **B** with the Hamiltonian

$$H_B = \sum_j \left(\frac{p_j^2}{2m_j} + \frac{1}{2} m_j \omega_j^2 x_j^2 \right), \quad (3.19)$$

with obvious notations and assume the initial density matrix for the total system

$$\rho_{\text{tot}}(t_i) = \rho_A(t_i) \rho_B^e, \quad (3.20)$$

for which ρ_B^e is assumed to be the equilibrium density matrix at a temperature $T = 1/k_B \beta$. The interaction of **A** with **B** is assumed to be

$$H_I = -V(a^+, a)X, \quad (3.21)$$

where

$$X = \sum_j c_j x_j. \quad (3.22)$$

Then the effect of the bath is incorporated into eq. (3.17) by

$$\rho_A^*(\phi_i^*, \phi_i'; t_f, t_i) = T \left(\int D_i[Q(\tau)] \int D_i[Q'(\tau)] \exp [(i/\hbar)S_A(Q; t_f, t_i)] \right. \\ \left. \times F(Q, Q'; t_f, t_i) \exp [(-i/\hbar)S_A^*(Q'; t_f, t_i)] \right), \quad (3.23)$$

with the well known influence functional of Feynman and Vernon¹²⁾

$$F(Q, Q'; t_f, t_i) = \exp \left\{ (-i/\hbar)^2 \int_{t_i}^{t_f} d\tau' \int_{t_i}^{\tau'} d\tau V^\times(Q, Q'; \tau') \right. \\ \left. \times [L_2(\tau' - \tau)V^\times(Q, Q'; \tau) - iL_1(\tau' - \tau)V^\circ(Q, Q'; \tau)] \right\}. \quad (3.24)$$

Here we have introduced the following notations for abbreviation. First we simply write $Q(\tau)$ or $Q'(\tau)$ for $(\phi^*(\tau), \phi(\tau))$ or $(\phi'^*(\tau), \phi'(\tau))$. Secondly we define

$$V^\circ(Q, Q'; t) = V(Q(t)) + V(Q'(t)), \quad (3.25)$$

$$V^\times(Q, Q'; t) = V(Q(t)) - V(Q'(t)), \quad (3.26)$$

and

$$iL_1(t) = i \int_{-\infty}^{\infty} d\omega J(\omega) \sin(\omega t), \quad (3.27)$$

$$L_2(t) = \int_{-\infty}^{\infty} d\omega J(\omega) \coth(\beta\hbar\omega/2) \cos(\omega t), \quad (3.28)$$

with the spectral density for the bath oscillators

$$J(\omega) = \hbar\omega \sum_j (c_j^2/4m_j\omega_j^2) (\delta(\omega - \omega_j) \\ + \delta(\omega + \omega_j)), \quad (3.29)$$

which is odd in ω , namely

$$J(-\omega) = -J(\omega). \quad (3.30)$$

We could assume ω to take only positive values, but it is more natural to allow for negative ω 's and impose the condition (3.30) on $J(\omega)$. If the system **A** consists of fermions, the symbol T takes care of time ordering with respect to the G-numbers appearing in the expression. The functions $iL_1(t)$ and $L_2(t)$ eqs. (3.27) and (3.28) are combined to

$$L(t) \equiv L_2(t) + iL_1(t) = \int_{-\infty}^{\infty} d\omega J(\omega) \\ \times \left(\frac{e^{\beta\hbar\omega}}{e^{\beta\hbar\omega} - 1} e^{i\omega t} + \frac{1}{e^{\beta\hbar\omega} - 1} e^{-i\omega t} \right). \quad (3.31)$$

The two terms in the bracket of the above expression correspond to exchange of energy quanta $\hbar\omega$ between the system **A** and the bath **B** at temperature T . The ratio $\exp(\beta\hbar\omega)$ of the terms makes **A** to attain Boltzmann weights for its quantum states. When the unequal weights are not important, the unequal weight of the relevant terms can be ignored so that the imaginary part eq. (3.27) can be disregarded corresponding the infinite temperature of the bath.

As was shown by Feynman and Vernon, the functions $L_1(t)$ and $L_2(t)$ can be interpreted as response functions of the bath medium to an external force K conjugate to the bath variable X . Namely if the effect of K on **B** is represented by

$$H_{\text{ext}} = -KX, \quad (3.32)$$

then K induces polarization of X . For a periodic force the response is described by the complex susceptibility which is given by the general equation¹⁶⁾

$$\chi(\omega) = \chi_0 - i\omega\beta \int_0^{\infty} dt e^{-i\omega t} \Phi(t). \quad (3.33)$$

Here

$$\Phi(t) = \langle X; X(t) \rangle \\ \equiv \beta^{-1} \int_0^{\beta} d\lambda \text{Tr}_B \{ \rho_B^{\circ} \exp(\lambda H_B) X \\ \times \exp(-\lambda H_B) X(t) \}, \quad (3.34)$$

and

$$\chi_0 = \beta \langle X; X \rangle = \beta \Phi(0), \quad (3.35)$$

are the relaxation function and the static susceptibility of the induced polarization ex-

pressed in terms of the canonical correlation function of $X(t)$. The imaginary part of χ and the power spectrum $\Phi[\omega]$ of $\Phi(t)$ are related to each other by

$$\chi''(\omega) = \pi\beta\omega\Phi[\omega], \quad (3.36)$$

where

$$\Phi[\omega] = (2\pi)^{-1} \int_{-\infty}^{\infty} dt e^{-i\omega t} \Phi(t). \quad (3.37)$$

If the symmetrized correlation of X is defined by

$$\Psi(t) = \langle X(0)X(t) + X(t)X(0) \rangle / 2, \quad (3.38)$$

its power spectrum

$$\Psi[\omega] = (2\pi)^{-1} \int_{-\infty}^{\infty} dt e^{-i\omega t} \Psi(t), \quad (3.39)$$

is related to that of the canonical correlation by

$$\Psi[\omega] = \beta E_\beta(\omega) \Phi[\omega] \quad (3.40)$$

where $E_\beta(\omega) = (\hbar\omega/2) \coth(\beta\hbar\omega/2)$ is the average thermal energy of an oscillator with the proper frequency ω . The spectral density $J(\omega)$ appearing in eqs. (3.27) and (3.28) is given by

$$J(\omega) = \frac{\hbar}{2\pi} \chi''(\omega) = \frac{\beta\hbar\omega}{2} \Phi[\omega]. \quad (3.41)$$

For an oscillator bath, we find from eqs. (3.22) and (3.34) that

$$\beta\Phi(t) = \sum_j (c_j^2 / 2m_j\omega_j^2) (e^{i\omega_j t} + e^{-i\omega_j t}) \quad (3.42)$$

to obtain eq. (3.29).

More generally, for any sort of bath, as long as its effect is considered to cause a Gaussian noise for the test system, the influence functional eq. (3.24) keeps its form where we have the kernels

$$iL_1(t) = -\frac{\beta\hbar}{2} \dot{\Phi}(t) = \frac{\beta\hbar}{2} \int_{-\infty}^{\infty} d\omega (i\omega) e^{i\omega t} \Phi[\omega], \quad (3.43)$$

and

$$L_2(t) = \Psi(t) = \beta \int_{-\infty}^{\infty} d\omega e^{i\omega t} E_\beta(\omega) \Phi[\omega]. \quad (3.44)$$

Namely, $iL_1(t)$ is essentially equal to the response function of the bath to a pulsive force $K \sim \delta(t)$ and $L_2(t)$ is the symmetrized correlation function eq. (3.38). This is seen from eqs. (3.36) and (3.40).

§4. A Gaussian-Markoffian Interaction in High Temperature Approximation

Now we assume a simple exponential decay for the relaxation function (3.34),

$$\Phi(t) = \Phi(0) \exp(-\gamma|t|), \quad (4.1)$$

and introduce the parameter Δ by

$$\hbar^2 \Delta^2 = \Phi(0) = \langle X; X \rangle, \quad (4.2)$$

which gives the measure of the mean square amplitude of the system-bath interaction eq. (3.21) and is proportional to $1/\beta$. The interaction V in eq. (3.21) is made a dimensionless quantity by assigning the dimension of frequency to Δ in order to keep correspondence to the stochastic approach reviewed in §2.

The power spectrum of Φ is

$$\Phi[\omega] = \frac{1}{\pi} \frac{\gamma}{\gamma^2 + \omega^2} \Phi(0), \quad (4.3)$$

and eq. (3.33) yields

$$\chi(\omega) = \frac{\beta\gamma}{\gamma + i\omega} \Phi(0), \quad (4.4)$$

and

$$J(\omega) = \frac{\hbar^2 \Delta^2}{2\pi} \frac{\beta\hbar\gamma\omega}{\gamma^2 + \omega^2}. \quad (4.5)$$

The assumption eq. (4.1) is the Debye form, but the spectrum $J(\omega)$ eq. (4.5) was called by Leggett *et al.* as the Drude form.

As is seen from eq. (3.43) the kernel $L_1(t)$ is simply

$$L_1(t) = \hbar^2 \Delta^2 \cdot \frac{\beta\hbar\gamma}{2} \exp(-\gamma t). \quad (4.6)$$

In the high temperature approximation which assumes

$$\beta\hbar\gamma \ll 1, \quad (4.7)$$

we may put $\beta E_\beta(\omega) \sim 1$, so that we have

$$L_2(t) = \hbar^2 \Delta^2 \exp(-\gamma t). \quad (4.8)$$

Thus we have the influence functional eq. (3.24) in the form

$$F(Q, Q'; t) = \exp \left\{ (-i\Delta)^2 \int_{t_i}^{t_f} d\tau' \int_{t_i}^{\tau'} d\tau e^{-\gamma(\tau'-\tau)} V^\times(Q, Q'; \tau') \right. \\ \left. \times \left(V^\times(Q, Q'; \tau) - i \frac{\beta\hbar\gamma}{2} V^\circ(Q, Q'; \tau) \right) \right\}. \quad (4.9)$$

Hereafter we write t for the final time t_f and omit the initial time t_i unless the previous notations are preferred for clarity.

We now insert this into eq. (3.23) and then differentiate the expression with respect to the final time t . For this purpose, we observe that the expression eq. (3.23) yields for an increment ε

$$\rho'_A(\phi_f^*, \phi_f'; t + \varepsilon) = T \left(\int D_f[Q(\tau)] \int D_f[Q'(\tau)] \exp [(i/\hbar)S_A(Q; t + \varepsilon)] \right. \\ \left. \times F(Q, Q'; t + \varepsilon) \exp [-(i/\hbar)S_A^*(Q'; t + \varepsilon)] \right). \quad (4.10)$$

Here

$$\exp [(i/\hbar)S_A(Q; t + \varepsilon)] = \exp [-\phi_f^* \phi_f + \phi_f^* \phi] (1 - i(\varepsilon/\hbar)H_A(\phi_f^*, \phi)) \exp [(i/\hbar)S_A(Q; t)], \quad (4.11)$$

and

$$F(Q, Q'; t + \varepsilon) = F(Q, Q'; t) + \varepsilon (-i\Delta)^2 V^\times(Q, Q'; t) \int_{t_i}^{t_f} d\tau e^{-\gamma(t-\tau)} \\ \times \left(V^\times(Q, Q'; \tau) - i \frac{\beta\hbar\gamma}{2} V^\circ(Q, Q'; \tau) \right) F(Q, Q'; t), \quad (4.12)$$

where the boundary value of V^\times needs a precise definition

$$V^\times(Q, Q'; t) = V(\phi_f^*, \phi) - V(\phi_f'^*, \phi_f'). \quad (4.13)$$

By taking the limit $\varepsilon \rightarrow 0$, we thus obtain

$$\frac{\partial}{\partial t} \rho'_A(\phi_f^*, \phi_f'; t) = T \left(\iint N^{-1} d\phi^* d\phi \iint N^{-1} d\phi'^* d\phi' e^{-\phi_f^* \phi_f + \phi_f'^* \phi_f'} \right. \\ \times [(i/\hbar)(H_A(Q(t)) - H_A(Q'(t))) \rho'_A(\phi_f^*, \phi_f'; t) \\ \left. - i\Delta V^\times(Q, Q'; t) \rho'_A(\phi_f^*, \phi_f'; t)] e^{-\phi_f^* \phi_f + \phi_f'^* \phi_f'} \right). \quad (4.14)$$

Here we introduce the set $\{\rho'_n(\phi^*, \phi'; t)\}$ and the corresponding operators $\{\rho_n(t)\}$ by the definitions

$$\rho'_n(\phi^*, \phi'; t) = T \left(\int D[Q(t)] \int D[Q'(t)] \right. \\ \left. \times \left\{ -i\Delta \int_{t_i}^{t_f} d\tau e^{-\gamma(t-\tau)} \left[V^\times(Q, Q'; \tau) - i \frac{\beta\hbar\gamma}{2} V^\circ(Q, Q'; \tau) \right] \right\}^n \right. \\ \left. \times \exp [(i/\hbar)S_A(Q; t)] F(Q, Q'; t) \exp [-(i/\hbar)S_A^*(Q'; t)] \right), \quad (4.15)$$

of which the first member has appeared in eq. (4.14). For later convenience we define the operator

$$\Theta \equiv V^\times - i \frac{\beta\hbar\gamma}{2} V^\circ, \quad (4.16)$$

with the notation for an anticommutator operation,

$$V \circ G \equiv VG + GV. \quad (4.17)$$

Equation (4.14) yields the operator equation

$$\frac{\partial}{\partial t} \rho_0(t) = (i\hbar)^{-1} H_A^\times \rho_0(t) - i\Delta V^\times \rho_1(t), \quad (4.18)$$

where we write $\rho_0(t)$ for $\rho_A(t)$.

Now we repeat the process to differentiate the expression eq. (4.14) or eq. (4.18) to get

$$\frac{\partial}{\partial t} \rho_1(t) = ((i\hbar)^{-1} H_A^\times - \gamma) \rho_1(t) - i\Delta V^\times \rho_2(t) - i\Delta \Theta \rho_0(t), \quad (4.19)$$

and more generally the set of equations

$$\frac{\partial}{\partial t} \rho_n(t) = ((i\hbar)^{-1} H_A^\times - n\gamma) \rho_n(t) - i\Delta V^\times \rho_{n+1}(t) - ni\Delta \Theta \rho_{n-1}(t). \quad (4.20)$$

Equations of motion (4.18)–(4.20) are a non-perturbative extension of the master equation including finite correlation effects of the bath modulation. The important point is that a motion of the test system is now described by the set of equations.

Now we define the Laplace transforms of $\{\rho_n(t)\}$ by

$$\rho_n[s] = \int_{t_i}^{\infty} e^{-s(t-t_i)} \rho_n(t) dt, \quad (4.21)$$

with the initial condition

$$\rho_n(t_i) = 0, \quad (\text{for } n < 0 \text{ and } n \geq 1), \quad (4.22)$$

and

$$\rho_0(t_i) = \rho_A(t_i). \quad (4.23)$$

The recurrence formula is solved to yield $\rho_0[s]$ in a continued fractional expression as

$$\rho_0[s] = \frac{1}{s - (i\hbar)^{-1} H_A^\times + V^\times \frac{\Delta^2}{s + \gamma - (i\hbar)^{-1} H_A^\times + V^\times \frac{2\Delta^2}{s + 2\gamma - (i\hbar)^{-1} H_A^\times + \dots}} \rho(t_i), \quad (4.24)$$

where each fraction means the corresponding inverse operator. The method of derivation of this is given in Appendix A.

The above result is quite in parallel to eq. (2.17). The main difference is that the operator appearing on the right of each fraction is not the same as that on the left side. Corresponding to eq. (2.14) we can show that eq. (4.24) is equivalent to the evolution equation

$$\frac{\partial}{\partial t} \bar{\rho}(\Omega, t) = \left\{ (i\hbar)^{-1} H_A^\times - i\Delta \cdot \Omega V^\times - i\Delta \frac{\beta\hbar\gamma}{2} \left(\Omega + \frac{\partial}{\partial \Omega} \right) V^\circ + \gamma \frac{\partial}{\partial \Omega} \left(\Omega + \frac{\partial}{\partial \Omega} \right) \right\} \bar{\rho}(\Omega, t), \quad (4.25)$$

where $\bar{\rho}(\Omega, t)$ is like that in eq. (2.7) the average of $\rho_A(t)$ over all possible paths of the noise produced by the bath-state of which is designated by a random variable Ω . This equivalence is seen by noticing that the diffusion operator Γ_Ω eq. (2.8) is essentially the same as the operator of harmonic oscillator ex-

cept for a difference in the weight function and so by using expansions in the eigenfunctions of Γ_Ω . Integer multiples of γ appears in this way in the expressions in eq. (4.25). By this procedure, we recover the similar recurrence equation as eq. (4.20) from eq. (4.25). In fact in the same way we easily prove eq. (2.17)

from eq. (2.14).

The presence of the imaginary term in Θ eq. (4.16) is an effect of reaction of the test system to the bath which was ignored in the stochastic approach. In order to retain the Markoffian property, namely the simple exponential decay of the kernels, the high temperature approximation is needed. The condition eq. (4.7) means that the bath temperature is high in comparison with the magnitude of energy quanta exchanged between the bath and the test system, or the temperature is high in comparison with the inverse of the characteristic time constant γ of the system-bath interaction. The high-temperature approximation takes account of the unbalance of energy of exchange

to the first order of the smallness parameter $\beta\hbar\gamma$.

Within this limitation, eq. (4.24) or (4.25) can be used as the basis of a generalized stochastic approach to study quantum systems which are in contact with a heat bath and are accordingly susceptible to dissipative effect to destroy the dynamical coherence of their evolution. The effect is generally characterized by the parameters Δ , γ , and ν_A . The last one is a characteristic frequency, or quantum level difference of the test system. If the conditions

$$\Delta/\gamma \ll 1, \quad \nu_A \ll \gamma, \quad (4.26)$$

are satisfied, the effect of interaction is reduced so that eq. (4.24) is approximated by

$$\rho[s] = \frac{1}{s - (i\hbar)^{-1}H_A^\times + V^\times} \frac{\rho(t_i)}{\frac{\gamma'}{1 - V^\times \frac{2i\beta\hbar\gamma'/2}{2 - V^\times \frac{3i\beta\hbar\gamma'/2}{3 - \dots}} V^\circ} \Theta} \quad (4.27)$$

where we put

$$\gamma' = \Delta^2/\gamma. \quad (4.28)$$

The condition may be called motional narrowing limit after the well known example in nuclear resonance problem. More generally ν_A may not be small compared with γ , then eq. (4.24) is replaced by

$$\rho[s] = \frac{1}{s - (i\hbar)^{-1}H_A^\times + V^\times \frac{\Delta^2}{\gamma - (i\hbar)^{-1}H_A^\times} \Theta} \rho(t_i), \quad (4.29)$$

in the lowest approximation. Now the interaction is reduced to the order of $\Delta^2/(\gamma + i\nu_A)$. As will be remarked in the concluding section, the Gaussian assumption for the system-bath interaction is not really needed if one is satisfied with the approximation, which correspond to eq. (4.29) and essentially assumes weak and fast interaction.

On the other hand, if the parameter γ is small, namely if $\Delta/\gamma \gg 1$, the system-bath interaction is essentially static and so dynamical coherence is not destroyed. It is not easy to make analytical treatments for the intermediate cases. However, numerical analysis can be made in such problem with use of eq. (4.20) or (4.24).

§5. Remarks on Non-Markoffian Weak Interactions

If the relaxation function $\Phi(t)$ or the spectral function $J(\omega)$ is not as simple as eq. (4.1) or (4.5), or the high temperature condition eq. (4.7) is not satisfied, it is not possible to obtain a non-perturbative expression like eq. (4.24). Here are added a few remarks for such cases.

The influence functional (3.24) is written generally as

$$F(Q, Q'; t) = \exp \left\{ (-i/\hbar)^2 \int_{t_i}^t d\tau' \int_{t_i}^{\tau'} d\tau \int_{-\infty}^{\infty} d\omega e^{-i\omega(\tau' - \tau)} \right. \\ \left. \times V^\times(Q, Q'; \tau')(N(\omega)V^\times(Q, Q'; \tau) + J(\omega)V^\circ(Q, Q'; \tau)) \right\}, \quad (5.1)$$

where

$$N(\omega) = J(\omega) \coth \left(\frac{\beta \hbar \omega}{2} \right). \quad (5.2)$$

Corresponding to eq. (4.15) we introduce the set of density operators by

$$\rho'(\phi_i^*, \phi_i'; t, \omega_1, \omega_2, \dots, \omega_n) = T \left(\int D[Q(t)] \int D[Q'(t)] \right. \\ \left. \times \prod_{k=1}^n \left\{ (-i/\hbar) \int_{t_i}^t d\tau e^{-i\omega_k(t-\tau)} (N(\omega_k)V^\times(Q, Q'; \tau) \right. \right. \\ \left. \left. + J(\omega_k)V^\circ(Q, Q'; \tau)) \right\} \exp [(i/\hbar)S_A(Q; t)] F(Q, Q'; t) \right. \\ \left. \times \exp [-(i/\hbar)S_A^*(Q'; t)] \right). \quad (5.3)$$

Then we have the operator equation

$$\frac{\partial}{\partial t} \rho(t) = (i\hbar)^{-1} H_A^\times \rho(t) + (i\hbar)^{-1} \int_{-\infty}^{\infty} d\omega_1 V^\times \rho(t, \omega_1). \quad (5.4)$$

We repeat the same process to get

$$\frac{\partial}{\partial t} \rho(t, \omega_1) = ((i\hbar)^{-1} H_A^\times - i\omega_1) \rho(t, \omega_1) + (i\hbar)^{-1} \int_{-\infty}^{\infty} d\omega_2 V^\times \rho(t, \omega_1, \omega_2) + (i\hbar)^{-1} \Theta(\omega_1) \rho(t), \quad (5.5)$$

where we define

$$\Theta(\omega) = N(\omega)V^\times + J(\omega)V^\circ. \quad (5.6)$$

We could continue the same process to higher hierarchies but it does not lead us to useful results.

If we terminate this hierarchal equation by ignoring the operator $\rho(t, \omega_1, \omega_2)$ in eq. (5.5), then we obtain

$$\rho[s] \approx \frac{1}{s - (i\hbar)^{-1} H_A^\times + (\hbar)^{-2} \int d\omega_1 V^\times \frac{1}{s - (i\hbar)^{-1} H_A^\times + i\omega_1} \Theta(\omega_1)} \rho(t_i), \quad (5.7)$$

for the Laplace transform of $\rho(t)$. If the interaction is weak enough, the relaxation induced by the perturbation is slow. Then we consider $\rho(t)$ at long times so that the integral in the denominator of eq. (5.7) is evaluated by setting s equal to zero, yielding the master equation, or the Pauli equation

$$\frac{\partial}{\partial t} \rho(t) = (i\hbar)^{-1} H_A^\times \rho(t) - \Gamma' \rho(t), \quad (5.8)$$

where Γ' is defined by

$$\Gamma' = \hbar^{-2} \int_0^\infty d\tau \int_{-\infty}^\infty d\omega e^{-i\omega\tau} V^\times(0) (N(\omega)V^\times(-\tau) + J(\omega)V^\circ(-\tau)), \quad (5.9)$$

or by

$$\Gamma' \rho = \hbar^{-2} \int_0^\infty d\tau \int_{-\infty}^\infty d\omega e^{i\omega\tau} G(\omega) \{ V^\times(0)(V(-\tau)\rho) - e^{\beta\hbar\omega} V^\times(0)(\rho V(-\tau)) \}, \quad (5.10)$$

where $V(\tau)$ represents the Heisenberg operator and $G(\omega)$ is defined by

$$G(\omega) = \frac{2J(\omega)}{e^{\beta\hbar\omega} - 1}. \quad (5.11)$$

This is usually derived by applying the lowest order perturbative calculation. It should be noticed that the above equation describes evolution of the reduced density matrix including the *off-diagonal* elements with respect to the unperturbed Hamiltonian. This corresponds to eq. (4.29). As was already remarked, this does not necessarily require the Gaussian nature of the interaction but only its weakness in the sense that the magnitude of the interaction is small in comparison with the characteristic frequencies.

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Appendix A

The Laplace transform of eqs. (4.8)-(4.20), ..., may be expressed as

$$\begin{bmatrix} \rho_0[s] \\ \rho_1[s] \\ \rho_2[s] \\ \rho_3[s] \\ \vdots \end{bmatrix} = \begin{bmatrix} s + \frac{i}{\hbar} H_A^\times & i\Delta V^\times & 0 & 0 & \cdots \\ \hline i\Delta\Theta & s + \frac{i}{\hbar} H_A^\times + \gamma & i\Delta V^\times & 0 & \cdots \\ 0 & 2i\Delta\Theta & s + \frac{i}{\hbar} H_A^\times + 2\gamma & i\Delta V^\times & \cdots \\ 0 & 0 & 3i\Delta\Theta & \ddots & \ddots \\ \vdots & \vdots & \vdots & \ddots & \ddots \end{bmatrix}^{-1} \begin{bmatrix} \rho(t_i) \\ 0 \\ 0 \\ 0 \\ \vdots \end{bmatrix}. \quad (A.1)$$

For any operators or matrices **A**, **B**, **C** and **D** we have

$$\left[\begin{array}{c|c} \mathbf{A} & \mathbf{B} \\ \hline \mathbf{C} & \mathbf{D} \end{array} \right]_{11}^{-1} = \frac{1}{\mathbf{A} - \mathbf{B} \frac{1}{\mathbf{D}} \mathbf{C}}, \quad (A.2)$$

where fractional expressions mean inverse operators. Then, by successive applications of eq. (A.2) to eq. (A.1), we obtain

$$\rho_0[s] = \frac{1}{s - (i\hbar)^{-1} H_A^\times + V^\times} \frac{\Delta^2}{s + \gamma - (i\hbar)^{-1} H_A^\times + V^\times} \frac{2\Delta^2}{s + 2\gamma - (i\hbar)^{-1} H_A^\times + \cdots} \rho(t_i). \quad (A.3)$$

Appendix B

In order to illustrate the points more closely, we consider a simple two-level system with the energy separation ω_0 described by the Hamiltonian

$$H_A(a^+, a) = \hbar\omega_0 a^+ a. \quad (B.1)$$

The operator of eq. (3.21) is assumed to be

$$V(a^+, a) = a^+ a. \tag{B·2}$$

This interaction causes the frequency shift of energy level as $\omega_0 + \Omega(t)$, where $\Omega(t)$ is a similar modulation discussed in §2. The excited and ground states of two-level system are denoted by $|1\rangle$ and $|0\rangle$. Then the density operator of the system may be written as

$$\rho(t) = P_1(t)|1, 1\rangle\rangle + P_2(t)|0, 0\rangle\rangle + P_3(t)|1, 0\rangle\rangle + P_4(t)|0, 1\rangle\rangle, \tag{B·3}$$

where we have introduced the notation

$$|i, j\rangle\rangle = |i\rangle\langle j|. \tag{B·4}$$

From eq. (4.24), the Laplace transform of this elements may be expressed as

$$\begin{bmatrix} P_1[s] \\ P_2[s] \\ P_3[s] \\ P_4[s] \end{bmatrix} = \begin{bmatrix} 1/s & 0 & 0 & 0 \\ 0 & 1/s & 0 & 0 \\ 0 & 0 & G_+[s] & 0 \\ 0 & 0 & 0 & G_-[s] \end{bmatrix} \begin{bmatrix} P_1(t_i) \\ P_2(t_i) \\ P_3(t_i) \\ P_4(t_i) \end{bmatrix}, \tag{B·5}$$

where

$$G_{\pm}[s] = \frac{1}{s \pm i\omega_0 + \frac{(1 \mp i\beta\hbar\gamma/2)\Delta^2}{s + \gamma \pm i\omega_0 + \frac{2(1 \mp i\beta\hbar\gamma/2)\Delta^2}{s + 2\gamma \pm i\omega_0 + \frac{3(1 \mp i\beta\hbar\gamma/2)\Delta^2}{s + 3\gamma \pm i\omega_0 + \dots}}}}. \tag{B·6}$$

In the stochastic approach, the factor of continued fraction is given by Δ^2 , but now $(1 \mp i\beta\hbar\gamma/2)\Delta^2$. This difference makes a slight difference to the nature of resolvent $G_{\pm}[s]$.

When γ satisfies the condition eq. (4.26), eq. (B·6) is expressed in the Lorentzian form as

$$G_{\pm}[s] = \frac{1}{s \pm i\omega_0 + \eta_{\pm}}, \tag{B·7}$$

where

$$\eta_{\pm} = \frac{\gamma'(1 \mp i\beta\hbar\gamma/2)}{1 + \frac{\mp 2i\beta\hbar\gamma/2}{2 + \frac{\mp 3i\beta\hbar\gamma/2}{3 + \dots}}}, \tag{B·8}$$

with $\Delta^2/\gamma \rightarrow \gamma'$. The real part of eq. (B·8) works upon eq. (B·7) as the damping, whereas the imaginary part the frequency shift. Hence we see that not only does the reaction parts causes the frequency shift, but also changes the damping rate.

In the slow modulation limit with the condi-

tion $\gamma \ll s \pm i\omega_0$, eq. (B·6) is evaluated as

$$G_{\pm}[s] = \frac{\sqrt{2}}{\Delta} \exp [(s \pm i\omega_0)^2 / 2\Delta^2] \times \text{Erfc} [(s \pm i\omega_0) / \sqrt{2}\Delta], \tag{B·9}$$

where Erfc (x) is the error integral and, to derive eq. (B·9), we have used the Laplace-Jacobi formula

$$e^{1/x^2} \cdot \text{Erfc} (1/x) = \frac{x/2}{1 + \frac{x^2/2}{1 + \frac{2x^2/2}{1 + \frac{3x^2/2}{1 + \dots}}}}. \tag{B·10}$$

In the case $(s \pm i\omega_0) \ll \sqrt{2}\Delta$, the error integral gives $\sqrt{\pi}/2$ and eq. (B·9) becomes the Gaussian form. This result is well known in the stochastic theory concerning on the spectral distribution.

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