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Brownian Motion of Nonlinear Oscillators: The Projection Operator Method and Its Application to a Double-Well-Potential Oscillator

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A projection operator method is presented, which provides the most efficient way for calculating the stationary behavior of nonlinear Brownian motion. A continued-fraction expansion of the Fourier–Laplace transform of the displacement correlation function or the spectral density is used. This method utilizes a successive optimization procedure on the nonlinear terms and includes the method of "statistical linearization" as the lowest order approximation. A systematic way to calculate the continued fraction numerically up to sufficient order for convergence is developed, which enables us to obtain the spectral density of a system previously uncomputable.

Numerical computations of the spectral density of a nonlinear oscillator with a double-well potential are presented and compared with the results obtained by statistical linearization.

KEY WORDS: Brownian motion; nonlinear; oscillator; double-well potential; projection operator method; continued fraction.

1. INTRODUCTION

The theory of Brownian motion has been and still is one of the most fruitful subjects in classical physics and related fields.[1–10] In the classical theory of Brownian motion we usually start from a phenomenological stochastic equation such as

$$\begin{aligned} \dot{x}_j(t) &= v_j(t) \\ \dot{v}_j(t) &= -\alpha_j v_j(t) + F_j(\mathbf{x}) + R_j(t), \qquad j = 1,\ldots, d \end{aligned} \tag{1}$$

which is a simple example of the Langevin equation for a Brownian particle

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with mass m $(=1)$ in a potential field $V(\mathbf{x})$ $[F_j(\mathbf{x}) = -\partial V/\partial x_j]$ in d-dimensional space. The random force $R_j(t)$ is assumed to be Gaussian and δ-correlated, i.e.,

$$\langle R_j(t)\rangle = 0, \qquad \langle R_j(t)R_k(t')\rangle = 2D_j\delta_{jk}\delta(t-t'), \qquad j,k = 1,\ldots,d \quad (2)$$

where $\langle\cdots\rangle$ denotes an average over an ensemble of the stochastic variables $R_j(t)$. The diffusion constant D_j is related to the friction constant α_j through the fructuation-dissipation theorem

$$D_j = \alpha_j kT \quad (3)$$

where k is the Boltzmann constant and T the temperature of the system.[5]

The Fokker–Planck equation for the probability distribution $f(\mathbf{x}, \mathbf{v}, t)$, corresponding to the Langevin equation (1), is given by

$$\frac{\partial}{\partial t} f(\mathbf{x}, \mathbf{v}, t) = \mathscr{D} f(\mathbf{x}, \mathbf{v}, t) \quad (4)$$

$$\mathscr{D} = \sum_{j=1}^{d} \left(\alpha_j \frac{\partial}{\partial v_j} v_j + D_j \frac{\partial^2}{\partial v_j^2} - v_j \frac{\partial}{\partial x_j} - F_j(\mathbf{x}) \frac{\partial}{\partial v_j} \right) \quad (5)$$

The stationary solution of this equation is expressed by the canonical distribution, i.e.,

$$f_{\mathrm{st}}(\mathbf{x}, \mathbf{v}) = \mathscr{N} \exp\left\{ -\frac{1}{kT} \left[\sum_j \frac{v_j^2}{2} + V(\mathbf{x}) \right] \right\} \quad (6)$$

There are two different kinds of dynamic behavior of the system. One is a transient motion from an initial nonstationary distribution, and the other is a stationary motion. In a linear system those two types of behavior should be identical, which is the fundamental point of the Onsager's theory of irreversible processes.[6] In a nonlinear case, however, these are quite different from each other and should be considered separately, except in the case where the initial nonstationary distribution is close to the stationary one. We will exclusively focus our attention on the stationary behavior, particularly on the stationary correlation functions or the spectral densities.

Several methods have been used to obtain the spectral densities, such as the method of statistical or equivalent linearization, the (renormalized) perturbation method, eigenvalue and eigenfunction analysis, and the projection operator method. It is quite important to know when each method gives good results qualitatively and quantitatively and when it does not.

The method of statistical linearization is widely used in engineering fields and is a primitive approximation.[11,12] It used to be believed to provide qualitative information. Recently this method has been investigated extensively in connection with the correction terms obtained by the other methods.[13,14] The (renormalized) perturbation method is quite popular for obtaining quantitative results.[8,10] However, this method is not convenient

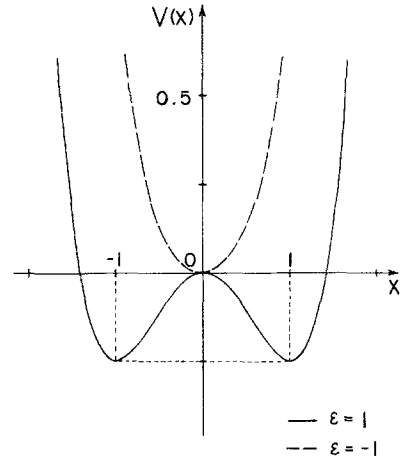

Fig. 1. Shape of the model potential $V(x)$.

for a system where some harmonic terms of $V(\mathbf{x})$ are, for example, negative. In order to get meaningful physical results for the system by this method, we have to carry out impractically high-order renormalization, due to the instability of the unperturbed parts. The eigenvalue and eigenfunction analysis cannot be applied to our case because it is quite difficult to obtain the eigenvalues and eigenfunctions of the operator (5), except in a few special cases.

The most useful and efficient way for the general cases will be shown to be the projection operator (Nakajima–Zwanzig) method[15] or the Mori method,[16] which can be shown to be equivalent. This method has been widely used for nonequilibrium statistical mechanics.[17–19] As for simple Brownian motion, Bixon and Zwanzig applied the method to a Duffing oscillator.[9] In spite of its usefulness, the projection operator method has hardly been used outside the field of nonequilibrium statistical mechanics. We will present the explicit calculation formulas for the spectral densities in the general cases, and demonstrate the power of the method for appropriate model systems in this paper.

We will choose model systems in order to illustrate the points discussed above. For simplicity we will consider the one-dimensional oscillator with a double-well potential, in which the potential field $V(x)$ is assumed as (Fig. 1)

$$V(x) = -\tfrac{1}{2}\epsilon x^2 + \tfrac{1}{4}x^4 \tag{7}$$

where $\epsilon = 1$. If $\epsilon = -1$, the model will be the Duffing oscillator. The nonlinear oscillator with a double-well potential has been investigated in various fields, especially with regard to ferroelectrics and structural phase

transitions.[21],[2] For these nonlinear oscillators we have not yet found the effects of various constants on the spectral density, such as narrowing, broadening, and shifts of resonant peaks. We will investigate these effects by calculating the exact spectral densities, and compare them with the corresponding quasiharmonic approximants.

In Section 2 we apply the projection operator method to the Fokker–Planck equation (4) and obtain a linear *non-Markovian* equation. Statistical linearization is discussed in the relation to the projection operator method. In Section 3 we find the expressions for the stationary correlation functions (or the spectral densities) and the linear response functions (or the dynamic polarizabilities). We show a formula to calculate the memory kernel and discuss its lower order approximations in Section 4. The nonlinear oscillator with a double-well potential (7) is analyzed in Section 5. For the purpose of comparison with previous work we also calculate the spectral density for the Duffing oscillator.

2. PROJECTION OPERATOR METHOD AND STATISTICAL LINEARIZATION

We introduce the projection operator $\mathscr{P}$, which projects a function onto a particular subspace of interest. The important properties in the study of Brownian motion are the motions of mean values of velocities and displacements, and their correlation functions. If we are concerned with these properties, the best choice of the projection operator is given by

$$\mathscr{P}h(\mathbf{x}, \mathbf{v}) = h_0 f_{\mathrm{st}} + \sum_{j=1}^{d} \left(\frac{x_j}{\langle x_j^2 \rangle_{\mathrm{st}}} h_{x_j} + \frac{v_j}{\langle v_j^2 \rangle_{\mathrm{st}}} h_{v_j} \right) f_{\mathrm{st}} \tag{8}$$

where

$$\begin{aligned} h_0 &= \int\int d\mathbf{x}\, d\mathbf{v}\, h(\mathbf{x}, \mathbf{v}), \qquad h_{x_j} = \int\int d\mathbf{x}\, d\mathbf{v}\, x_j h(\mathbf{x}, \mathbf{v}) \\ h_{v_j} &= \int\int d\mathbf{x}\, d\mathbf{v}\, v_j h(\mathbf{x}, \mathbf{v}) \end{aligned} \tag{9}$$

The average $\langle \cdots \rangle_{\mathrm{st}}$ is taken with the stationary distribution f_{st}, so the mean-squared velocities and the mean-squared displacements are given by

$$\langle v_i v_j \rangle_{\mathrm{st}} = kT\delta_{i,j}, \qquad \langle x_i x_j \rangle_{\mathrm{st}} = \langle x_i^2 \rangle_{\mathrm{st}} \delta_{i,j} \tag{10}$$

In order to obtain the equations of motion for the mean values, we operate with the projection operator $\mathscr{P}$, defined by Eq. (8), on the Fokker–

[2] Analytic calculations on a classical oscillator with the potential (7) were given by Onodera.[20] His model corresponds to the limiting case where the random force is infinitesimally small.

Planck equation (4). The projected probability distribution will obey the following equation:

$$\frac{\partial}{\partial t}\mathscr{P}f(\mathbf{x}, \mathbf{v}, t) = \mathscr{P}\mathscr{D}\mathscr{P}f(\mathbf{x}, \mathbf{v}, t) - \int_0^t ds\, k(s)\mathscr{P}f(\mathbf{x}, \mathbf{v}, t - s) + g(\mathbf{x}, \mathbf{v}, t) \tag{11}$$

where

$$k(s) = -\mathscr{P}\mathscr{D}(1 - \mathscr{P})e^{s(1-\mathscr{P})\mathscr{D}}(1 - \mathscr{P})\mathscr{D}\mathscr{P} \tag{12}$$

$$g(\mathbf{x}, \mathbf{v}, t) = \mathscr{P}\mathscr{D}(1 - \mathscr{P})e^{t(1-\mathscr{P})\mathscr{D}}(1 - \mathscr{P})f(\mathbf{x}, \mathbf{v}, 0) \tag{13}$$

The mean values of the velocities and the displacements defined by

$$\langle v_j; t\rangle = \int\int d\mathbf{x}\, d\mathbf{v}\, v_j f(\mathbf{x}, \mathbf{v}, t) \tag{14}$$

$$\langle x_j; t\rangle = \int\int d\mathbf{x}\, d\mathbf{v}\, x_j f(\mathbf{x}, \mathbf{v}, t), \qquad j = 1,..., d \tag{15}$$

are given by coefficients of the function $\mathscr{P}f(\mathbf{x}, \mathbf{v}, t)$. From Eqs. (5) and (9) the coefficients of $\mathscr{P}\mathscr{D}h(\mathbf{x}, \mathbf{v})$ obey the following relations:

$$[\mathscr{D}h]_0 = 0 \tag{16}$$

$$[\mathscr{D}h]_{x_j} = h_{v_j} \tag{17}$$

$$[\mathscr{D}h]_{v_j} = -\alpha_j h_{v_j} + \int\int d\mathbf{x}\, d\mathbf{v}\, F_j(\mathbf{x})h(\mathbf{x}, \mathbf{v}) \tag{18}$$

The equations of motion for the mean values will be obtained by the comparison of the coefficients of $\mathscr{P}f(\mathbf{x}, \mathbf{v}, t)$ on both sides of Eq. (11) with the above relations. The result is

$$\frac{d}{dt}\langle x_j; t\rangle = \langle v_j; t\rangle$$

$$\frac{d}{dt}\langle v_j; t\rangle = -\alpha_j\langle v_j; t\rangle - \Omega_j{}^2\langle x_j; t\rangle - \sum_{k=1}^{d}\int_0^t ds\, K_{jk}(s)\langle v_k; t - s\rangle + Y_j(t), \qquad j = 1,..., d \tag{19}$$

where

$$\Omega_j{}^2 = -\frac{\langle x_j F_j(\mathbf{x})\rangle_{\mathrm{st}}}{\langle x_j{}^2\rangle_{\mathrm{st}}} \tag{20}$$

$$K_{jk}(s) = \langle v_k{}^2\rangle_{\mathrm{st}}^{-1}\int\int d\mathbf{x}\, d\mathbf{v} \times [F_j(\mathbf{x}) + \Omega_j{}^2 x_j]e^{s(1-\mathscr{P})\mathscr{D}}[F_k(\mathbf{x}) + \Omega_k{}^2 x_k]f_{\mathrm{st}} \tag{21}$$

$$Y_j(t) = \int\int d\mathbf{x}\, d\mathbf{v}\, [F_j(\mathbf{x}) + \Omega_j{}^2 x_j]e^{t(1-\mathscr{P})\mathscr{D}}(1 - \mathscr{P})f(\mathbf{x}, \mathbf{v}, 0) \tag{22}$$

The functions $Y_j(t)$ are the terms that cannot be described by the quantities $\langle x_j; t\rangle$ and $\langle v_j; t\rangle$ $(j = 1,..., d)$, and come from the part of the initial distribution that does not belong to the subspace of the projection operator.

The equations of motion for the mean velocities and the mean displacements are not obtained in closed forms because of the existence of $Y_j(t)$. Only when the function $(1 - \mathscr{P})f(\mathbf{x}, \mathbf{v}, 0)$ vanishes or is vanishingly small do the equations become homogeneous. This is the case as far as the stationary correlation functions and the linear response functions are concerned (see the next section).

It is quite instructive to interpret Eq. (19) from a different point of view. We will take the average of the nonlinear Langevin equation (1) over the ensemble of the random forces, denoted by $\langle\cdots\rangle$. Then it is obvious from causality that

$$\begin{aligned} \langle R_j(t)x_j(t')\rangle &= 0 \qquad \text{if} \quad t_0 < t' < t \\ \langle R_j(t)x_j(t')\rangle &\neq 0 \qquad \text{if} \quad t_0 < t < t' \end{aligned} \tag{23}$$

where the initial time t_0 is taken to be zero. The initial displacements $x_j(0)$ are assumed to be statistically independent of $R_j(0)$. Now we consider the optimal linear approximation for the nonlinear force terms, using a variational procedure. We denote the linear approximation by $\sum_j \gamma_j x_j$ and determine the coefficients γ_j by the following condition:

$$\Psi(\boldsymbol{\gamma}) = \left\langle \sum_{j,k} [F_j(\mathbf{x}) - \gamma_j x_j][F_k(\mathbf{x}) - \gamma_k x_k] \right\rangle_{\text{st}} = \min \tag{24}$$

where the average is taken over the stationary distribution, because we are mostly interested in the stationary behavior. From Eq. (24) the function $\Psi(\boldsymbol{\gamma})$ satisfies the equation

$$\frac{\partial}{\partial \gamma_j} \Psi(\boldsymbol{\gamma}) = 0, \qquad j = 1,..., d \tag{25}$$

From the set of equations (25) we can obtain γ_j as

$$\gamma_j = \langle x_j{}^2\rangle_{\text{st}}^{-1} \sum_k \langle F_j(\mathbf{x})x_k\rangle_{\text{st}} = -\Omega_j{}^2 \tag{26}$$

The effective frequency Ω_j defined by Eq. (20) is shown to be identical with the one obtained by statistical linearization. The equations of motion averaged over the ensemble of the random forces are given by

$$\begin{aligned} &\frac{d}{dt}\langle x_j(t)\rangle - \langle v_j(t)\rangle = 0 \\ &\frac{d}{dt}\langle v_j(t)\rangle + \alpha_j\langle v_j(t)\rangle + \Omega_j{}^2\langle x_j(t)\rangle = \phi_j(t), \qquad j = 1,..., d \end{aligned} \tag{27}$$

where

$$\langle x_j(t)\rangle = [\exp(t\mathscr{D}^\dagger)]x_j, \qquad \langle v_j(t)\rangle = [\exp(t\mathscr{D}^\dagger)]v_j \tag{28}$$

$$\phi_j(t) = \langle F_j(\mathbf{x}) + \Omega_j{}^2 x_j(t)\rangle = [\exp(t\mathscr{D}^\dagger)][F_j(\mathbf{x}) + \Omega_j{}^2 x_j] \tag{29}$$

$$\mathscr{D}^\dagger = \sum_{j=1}^{d} \left[-\alpha_j v_j \frac{\partial}{\partial v_j} + \frac{1}{2} D_j \frac{\partial^2}{\partial v_j{}^2} + v_j \frac{\partial}{\partial x_j} + F_j(\mathbf{x}) \frac{\partial}{\partial v_j} \right] \tag{30}$$

Within the variational procedure it is not clear how to treat the nonlinear force terms $\phi_j(t)$ in Eq. (27). The simplest approximation is given by neglecting all effects of $\phi_j(t)$, which corresponds to statistical linearization. The resulting linear system is quite simple to analyze, but its usefulness as an approximation depends entirely on the property of the nonlinear forces $F_j(\mathbf{x})$. We will examine its adequacy for specific models in a later section.

If more accurate results are wanted than those obtained by statistical linearization, the nonlinear force terms $\phi_j(t)$ should be taken into consideration. In Eq. (27) the initial distribution, which is always Gaussian within statistical linearization, is not specified. In the general case, however, we have to know about the initial distribution $f(\mathbf{x}, \mathbf{v}, 0)$. We already know the exact expression for the equations of motion in Eq. (19). The two average expressions in Eqs. (19) and (27) are given by

$$\begin{aligned} \langle x_j; t\rangle &= \int\int d\mathbf{x}\, d\mathbf{v} f(\mathbf{x}, \mathbf{v}, 0)\langle x_j(t)\rangle \\ \langle v_j; t\rangle &= \int\int d\mathbf{x}\, d\mathbf{v} f(\mathbf{x}, \mathbf{v}, 0)\langle v_j(t)\rangle, \qquad j = 1,\ldots, d \end{aligned} \tag{31}$$

Comparing Eq. (27) with Eq. (19), we can see that the nonlinear force terms $\phi_j(t)$ can be separated into two different parts, a systematic part and a random part. The former causes friction with memory, because the nonlinear force terms are not δ-correlated, and the latter is the residual part, which cannot be described within the subspace given by the projection operator $\mathscr{P}$. The systematic part has the same dependence on the initial distribution as do $\langle \mathbf{x}(t)\rangle$ and $\langle \mathbf{v}(t)\rangle$.

3. CORRELATION FUNCTIONS AND RESPONSE FUNCTIONS

The principal dynamical quantities of interest are the correlation functions, especially the stationary ones. The stationary correlation function of the displacement $C_{jk}(t)$ is defined by

$$\begin{aligned} C_{jk}(t) &= \langle x_j(t)x_k(0)\rangle_{\mathrm{st}} \\ &= \int\int d\mathbf{x}\, d\mathbf{v}\, x_j e^{t\mathscr{D}} x_k f_{\mathrm{st}}(\mathbf{x}, \mathbf{v}) \\ &= \langle x_k\langle x_j(t)\rangle\rangle_{\mathrm{st}} \end{aligned} \tag{32}$$

where $\langle x_j(t)\rangle$ introduced in Eq. (28) is the average displacement over the ensemble of the random forces. The last part of Eq. (32) explicitly expresses the two different averages in the definition of $C_{jk}(t)$. From the definition we see that $C_{jk}(t)$ is mathematically the same as the average displacement $\langle x_j(t)\rangle$ for the initial distribution

$$f(\mathbf{x}, \mathbf{v}, 0) = x_k f_{\mathrm{st}}(\mathbf{x}, \mathbf{v}) \tag{33}$$

The function $Y_j(t)$ in Eq. (19) vanishes in this case, so the correlation function obeys the equation

$$\frac{d^2}{dt^2} C_{jk}(t) + \alpha_j \frac{d}{dt} C_{jk}(t) + \sum_l \int_0^t ds\, K_{jl}(s) \frac{d}{dt} C_{lk}(t - s) + \Omega_j^2 C_{jk}(t) = 0 \tag{34}$$

This equation is exact and all unknown factors are put into the memory kernels $K_{jl}(s)$.

The spectral density $S_{jk}(\omega)$ is given by the real part of the Fourier–Laplace transform $\hat{C}_{jk}(\omega)$ of $C_{jk}(t)$, i.e.,

$$S_{jk}(\omega) = \mathrm{Re}\, \hat{C}_{jk}(\omega) \tag{35}$$

$$\hat{C}_{jk}(\omega) = \int_0^\infty dt\, e^{i\omega t} C_{jk}(t) \tag{36}$$

From Eqs. (34) and (36) we can obtain

$$\sum_l \{(-\omega^2 + \Omega_j^2 - i\omega\alpha_j)\delta_{jl} - i\omega\hat{K}_{jl}(\omega)\}\hat{C}_{lk}(\omega) = \sum_l \{(-i\omega + \alpha_j)\delta_{jl} + \hat{K}_{jl}(\omega)\}\langle x_l^2\rangle_{\mathrm{st}} \tag{37}$$

where $\hat{K}_{jk}(\omega)$ is the Fourier–Laplace transform of $K_{jk}(t)$. Introducing the matrix representation, we can rewrite Eq. (37) as

$$\hat{\mathbf{C}}(\omega) = \boldsymbol{\Xi}(\omega)\boldsymbol{\Delta}(\omega)C(0) \tag{38}$$

where

$$\begin{aligned} (\hat{\mathbf{C}}(\omega))_{jk} &= \hat{C}_{jk}(\omega), \qquad (\mathbf{C}(0))_{jk} = \langle x_j^2\rangle_{\mathrm{st}}\delta_{jk} \\ (\boldsymbol{\Xi}^{-1}(\omega))_{jk} &= (-\omega^2 + \Omega_j^2 - i\omega\alpha_j)\delta_{jk} - i\omega\hat{K}_{jk}(\omega) \\ (\boldsymbol{\Delta}(\omega))_{jk} &= -(1/\omega)[(\boldsymbol{\Xi}^{-1}(\omega))_{jk} - \Omega_j^2\delta_{jk}] \end{aligned} \tag{39}$$

Using the relations between the matrix elements of $\boldsymbol{\Xi}$ and $\boldsymbol{\Delta}$, we obtain

$$\hat{\mathbf{C}}(\omega) = -(1/i\omega)\mathbf{C}(0) + (kT/i\omega)\boldsymbol{\Xi}(\omega) \tag{40}$$

$$S_{jk}(\omega) = (kT/\omega)\,\mathrm{Im}\,\Xi_{jk}(\omega) \tag{41}$$

The other correlations, such as the velocity–velocity and velocity–displacement correlations, can be obtained in the same manner.

Relation (41) is nothing but the fluctuation-dissipation theorem in the classical linear response theory.[22,5] We will show that the dynamic polarizability is given by $\Xi_{jk}(\omega)$.

Suppose an external electric field $\mathbf{E}(t)$ is put upon the system. The Fokker–Planck equation (4) is modified as

$$\frac{\partial}{\partial t} f(\mathbf{x}, \mathbf{v}, t) = [\mathscr{D} + \mathscr{D}_{\text{ext}}(t)] f(\mathbf{x}, \mathbf{v}, t) \tag{42}$$

where

$$\mathscr{D}_{\text{ext}}(t) = -\sum_j E_j(t) \frac{\partial}{\partial v_j} \tag{43}$$

At $t \leqslant 0$ the system is in a stationary state and at $t > 0$ the external field is applied. Then we can write the deviation of the mean displacements as

$$\langle x_j(t) \rangle = \langle x_j \rangle_{\text{st}} + \sum_k \int_0^t ds\, \chi_{jk}(t - s) E_k(s) \tag{44}$$

where the response function $\chi_{jk}(t)$ is defined by

$$\chi_{jk}(t) = \int\int d\mathbf{x}\, d\mathbf{v}\, x_j e^{t\mathscr{D}}(-\partial/\partial v_k) f_{\text{st}}(\mathbf{x}, \mathbf{v}) \tag{45}$$

From Eq. (6) the response functions are given by the velocity–displacement correlation

$$\chi_{jk}(t) = (1/kT)\langle x_j(t) v_k(0) \rangle_{\text{st}} \tag{46}$$

Using the same procedure for the displacement–displacement correlation functions we can find the following expression for the dynamic polarizability $\hat{\chi}_{jk}(\omega)$:

$$\hat{\chi}_{jk}(\omega) = \Xi_{jk}(\omega) \tag{47}$$

Therefore from Eq. (41) we obtain the relation

$$S_{jk}(\omega) = (kT/\omega)\, \text{Im}\, \hat{\chi}_{jk}(\omega) \tag{48}$$

which is the fluctuation-dissipation theorem in the classical limit.[5]

4. MEMORY KERNELS

We have shown in the previous sections how to calculate the correlation and response functions. All we have to know is the memory kernel $K_{jk}(t)$ or its Fourier–Laplace transform $\hat{K}_{jk}(\omega)$. The most efficient way to calculate

$\hat{K}_{jk}(\omega)$ is, I believe, the continued fraction representation formulated by Mori,[16] which is essentially a successive optimization procedure on the nonlinear terms.

The continued fraction representation for $\hat{K}_{jk}(\omega)$ is obtained as

$$\begin{aligned}\hat{K}_{jk}(\omega) &= \frac{1}{\langle v_k^2 \rangle_{\mathrm{st}}} \int\int d\mathbf{x}\, d\mathbf{v}\, [F_j(\mathbf{x}) + \Omega_j^2 x_j] \\ &\quad \times [-i\omega + (1 - \mathscr{P})\mathscr{D}]^{-1}[F_k(\mathbf{x}) + \Omega_k^2 x_k] f_{\mathrm{st}} \\ &= \cfrac{A_{jk}^{(0)}}{-i\omega + B_{jk}^{(1)} - \cfrac{A_{jk}^{(1)}}{-i\omega + B_{jk}^{(2)} - \cfrac{A_{jk}^{(2)}}{-i\omega + B_{jk}^{(3)} - \cdots}}}\end{aligned} \tag{49}$$

Here the constants $A_{jk}^{(l)}$ and $B_{jk}^{(l+1)}$ $(l = 0, 1, 2,...)$ are calculated by the corresponding optimization. Practically, however, we will use the relation between the continued fraction and the moment expansion, which is given, for example, in Ref. 23. The moment expansion of $\hat{K}_{jk}(\omega)$ is expressed by

$$\hat{K}_{jk}(\omega) = -\frac{1}{i\omega} \sum_{n=0}^{\infty} \left(\frac{1}{i\omega}\right)^m K_{jk}^{(m)} \tag{50}$$

where

$$K_{jk}^{(m)} = \frac{1}{\langle v_k^2 \rangle_{\mathrm{st}}} \int\int d\mathbf{x}\, d\mathbf{v}\, [F_j(\mathbf{x}) + \Omega_j^2 x_j][(1 - \mathscr{P})\mathscr{D}]^m [F_k(\mathbf{x}) + \Omega_k^2 x_k] f_{\mathrm{st}} \tag{51}$$

In order to obtain the values of the $K_{jk}^{(m)}$ in a systematic way, we introduce the functions $C_k^m(\mathbf{x}; n_1,..., n_d)$ such that

$$[(1 - \mathscr{P})\mathscr{D}]^m [F_k(\mathbf{x}) + \Omega_k^2 x_k] f_{\mathrm{st}} = \sum_{n_1 \cdots n_d} C_k^m(\mathbf{x}; n_1,..., n_d) v_1^{n_1} \cdots v_d^{n_d} f_{\mathrm{st}} \tag{52}$$

where we define

$$C_k^m(\mathbf{x}; n_1,..., n_d) = 0 \tag{53}$$

when at least one of the integers n_p $(p = 1,..., d)$ becomes negative. From the successive operation of $(1 - \mathscr{P})\mathscr{D}$ we have the following recursion formulas for $C_k^m(\mathbf{x}; n_1,..., n_d)$:

(I) For $m = 0$ and $k = 1,..., d$,

$$C_k^0(\mathbf{x}; n_1,..., n_d) = \begin{cases} F_k(\mathbf{x}) + \Omega_k^2 x_k & \text{if } (n_1,..., n_d) = (0,..., 0) \\ 0 & \text{if } (n_1,..., n_d) \neq (0,..., 0) \end{cases} \tag{54}$$

(II) For $m = 0, 1, 2, \ldots$ and $k = 1, \ldots, d$,

$$
\begin{aligned}
C_k^{m+1}(\mathbf{x}; n_1, \ldots, n_d) &= -\sum_p \Big\{ \frac{\partial}{\partial x_p} C_k^m(\mathbf{x}; n_1, \ldots, n_p - 1, \ldots, n_d) \\
&\quad + n_p \alpha_p C_k^m(\mathbf{x}; n_1, \ldots, n_p, \ldots, n_d) \\
&\quad + (n_p + 1) F_p(\mathbf{x}) C_k^m(\mathbf{x}; n_1, \ldots, n_p + 1, \ldots, n_d) \\
&\quad - \tfrac{1}{2}(n_p + 2)(n_p + 1) D_p C_k^m(\mathbf{x}; n_1, \ldots, n_p + 2, \ldots, n_d) \\
&\quad + \delta_{n_p,1} \prod_{q(\neq p)} \delta_{n_q,0} K_{pk}^{(m)} \Big\} \qquad (55)
\end{aligned}
$$

Using the Gaussian properties of the stationary velocity distribution, we can get an expression for $K_{jk}^{(m)}$:

$$
K_{jk}^{(m)} = -\sum_{n_1, \ldots, n_d} \left\langle \frac{\partial}{\partial x_j} C_k^m(\mathbf{x}; 2n_1, \ldots, 2n_d) \right\rangle \prod_{l=1}^{d} (2n_l - 1)!! \langle v_l^2 \rangle^{n_l} \qquad (56)
$$

Here and in the next section we denote the average over the stationary distribution $\langle \cdots \rangle_{\mathrm{st}}$, as $\langle \cdots \rangle$ without confusion. In order to derive Eqs. (55)–(56) we use the following two equalities, which can be easily proven:

$$
\sum_{n_1, \ldots, n_d} \left\langle C_k^m(\mathbf{x}; n_1, \ldots, n_d) v_p \prod_{l=1}^{d} v_l^{n_l} \right\rangle = 0 \qquad (57)
$$

$$
\sum_{n_1, \ldots, n_d} \left\langle x_p C_k^m(\mathbf{x}; n_1, \ldots, n_d) \prod_{l=1}^{d} v_l^{n_l} \right\rangle = 0, \qquad p = 1, \ldots, d \qquad (58)
$$

We can summarize the say to calculate $\hat{K}_{jk}(\omega)$ as follows:

(a) Obtain the functions $C_k^m(\mathbf{x}; n_1, \ldots, n_d)$ for the given force functions $F_k(\mathbf{x})$ or for the given potential field $V(\mathbf{x})$ by the recursion formulas (54) and (55).

(b) Calculate $K_{jk}^{(m)}$ by Eq. (56) with $C_k^m(x; n_1, \ldots, n_d)$ obtained in step (a).

(c) Derive the coefficients $A_{jk}^{(l)}$ and $B_{jk}^{(l+1)}$ in the continued fraction by the transformation formulas from the moment expansion.

(d) Calculate the $\hat{K}_{jk}(\omega)$ by Eq. (49) and then the $\hat{C}_{jk}(\omega)$ and $S_{jk}(\omega)$ by Eqs. (40) and (41).

There does not exist a general theory for convergence of the continued fraction. We do not consider such a problem in this paper, but leave it to the mathematicians. We will assume that the continued fraction converges almost everywhere on the real axis in the complex plane of ω. Therefore we will calculate the nth approximant of the continued fraction (or the $[n + 1, n]$ Padé approximant) and check the convergence of the successive approximants. These procedures will be carried out for specific examples in the next section.

It is of interest to consider the two lowest order approximations of the memory kernels. The lowest order approximant is given by neglecting the memory kernels, i.e.,

$$K_{jk}^{\mathrm{I}}(\omega) = 0 \tag{59}$$

The spectral density in this case $S_{jk}^{\mathrm{I}}(\omega)$ is expressed as

$$S_{jk}^{\mathrm{I}}(\omega) = \frac{\alpha_j kT}{(-\omega^2 + \Omega_j{}^2)^2 + \alpha_j{}^2\omega^2}\,\delta_{jk} \tag{60}$$

and it corresponds to the result of statistical linearization or the independent quasiharmonic model with effective frequencies Ω_j and friction constants α_j. The second lowest approximation is obtained by the first approximant of the continued fraction, which is given by

$$K_{jk}^{\mathrm{II}}(\omega) = \frac{A_{jk}^{(0)}}{-i\omega + B_{jk}^{(1)}} \tag{61}$$

From the coefficients of the moment expansion the $A_{jk}^{(0)}$ and $B_{jk}^{(1)}$ are

$$A_{jk}^{(0)} = \langle \partial^2 V/\partial x_j\, \partial x_k \rangle - \Omega_j{}^2\delta_{jk} \tag{62}$$

$$B_{jk}^{(1)} = 0 \tag{63}$$

Substituting Eqs. (61)–(63) into Eq. (41), we obtain the spectral density $S_{jk}^{\mathrm{II}}(\omega)$ as

$$S_{jk}^{\mathrm{II}}(\omega) = (kT/\omega)\,\mathrm{Im}\,\Xi_{jk}^{\mathrm{II}}(\omega) \tag{64}$$

where

$$[\Xi^{\mathrm{II}}(\omega)]^{-1} = [(-\omega^2 - i\omega\alpha_j)\delta_{jk} + \langle \partial^2 V/\partial x_j \partial x_k \rangle] \tag{65}$$

This approximant corresponds to the linearly coupled quasiharmonic model in which effective frequencies and friction constants are respectively $\langle \partial^2 V/\partial x_j{}^2 \rangle^{1/2}$ and α_j and the coupling constant between x_j and x_k is given by $\langle \partial^2 V/\partial x_j \partial x_k \rangle$. In the higher order approximation the memory effects appear because of nonlinear couplings and force terms.

5. ONE-DIMENSIONAL NONLINEAR OSCILLATOR WITH SINGLE- AND DOUBLE-WELL POTENTIALS

We have developed the general method for calculating the spectral density and the response functions for nonlinear Brownian motions in the previous sections. In this section we will consider as examples the Brownian motion of the nonlinear oscillators with single- and double-well potentials

in one-dimensional space ($d = 1$). For simplicity the potential is assumed to be expressed with a normalized variable x as [Eq. (7)]

$$V(x) = -\tfrac{1}{2}\epsilon x^2 + \tfrac{1}{4}x^4$$

where $\epsilon = \pm 1$. The Langevin equation is written as

$$\dot{x} = v, \qquad \dot{v} = -\alpha v + \epsilon x - x^3 + R(t) \tag{66}$$

where

$$\langle R(t)\rangle = 0, \qquad \langle R(t)R(t')\rangle = 2D\,\delta(t - t') \tag{67}$$

When $\epsilon = -1$, Eq. (66) represents a Duffing oscillator, i.e., a nonlinear oscillator with a single-well potential. A nonlinear oscillator with a double-well potential is obtained by taking $\epsilon = 1$. The former case is considered for the purpose of comparison with previous work.[8-10] Our main concern is with the latter case.

The spectral density $S(\omega)$, given by

$$S(\omega) = \frac{[\alpha + \gamma(\omega)]kT}{[-\omega^2 + \Omega^2 + \sum(\omega)]^2 + \omega^2[\alpha + \gamma(\omega)]^2} \tag{68}$$

will be calculated numerically by the method developed in the previous sections. Here the real and imaginary part of $\hat{K}(\omega)$ are denoted by

$$\gamma(\omega) = \mathrm{Re}\,\hat{K}(\omega), \qquad \Sigma(\omega) = (1/\omega)\,\mathrm{Im}\,\hat{K}(\omega) \tag{69}$$

Since the potential is expressed as a polynomial in x, the function $C^m(x; n)$ can be expanded in a power series in x, i.e.,

$$C^m(x; n) = \sum_{p=0}^{\infty} d_{n,p}^m x^p \tag{70}$$

Then from Eqs. (54) and (55) the recursion formula for $d_{n,p}^m$ is given as follows:

$$d_{n,p}^0 = \begin{cases} \epsilon + \Omega^2 & \text{if } (n, p) = (0, 1) \\ -1.0 & \text{if } (n, p) = (0, 3) \\ 0 & \text{if } (n, p) \neq (0, 1), (0, 3) \end{cases} \tag{71}$$

$$\begin{aligned} d_{n,p}^{m+1} = {} & -(p + 1)d_{n-1,p+1}^m - n\alpha d_{n,p}^m - \epsilon(n + 1)d_{n+1,p-1}^m \\ & + (n + 1)d_{n+1,p-3}^m + (n + 1)(n + 2)\alpha kT d_{n+2,p}^m - K^{(m)}\,\delta_{n,1}\,\delta_{p,0} \end{aligned} \tag{72}$$

where we again define $d_{n,p}^m = 0$ ($m = 0, 1, 2,\ldots$) for a negative integer n or p. From Eq. (57) the coefficients of the moment expansion of $\hat{K}(\omega)$ are expressed in terms of $d_{n,p}^m$ as

$$K^{(m)} = -\sum_{n,p} (2n - 1)!!\,\langle v^2\rangle^n (2p + 1)\langle x^{2p}\rangle d_{2n,2p+1}^m, \qquad m = 0, 1, 2,\ldots \tag{73}$$

The second moments of velocity and displacement are calculated using the stationary distribution (6), resulting in

$$\langle v^2 \rangle = kT, \qquad \langle x^2 \rangle = \frac{1}{2\epsilon q} \frac{d}{dq} \ln Z(q) \tag{74}$$

where q and $Z(q)$ are defined as

$$q = (kT)^{-1/2} \tag{75}$$

$$Z(q) = \int_{-\infty}^{\infty} dy \exp[2\epsilon q y^2 - y^4] \tag{76}$$

The function $Z(q)$ is expressed as

$$Z(q) = \Gamma(\tfrac{1}{4})\, {}_1F_1(\tfrac{1}{4}, \tfrac{1}{2}; q^2) + 2\epsilon\Gamma(\tfrac{3}{4}) q\, {}_1F_1(\tfrac{3}{4}, \tfrac{3}{2}; q^2) \tag{77}$$

in terms of the gamma function Γ and the confluent hypergeometric function

$${}_1F_1(\alpha, \gamma; z) = 1 + \frac{\alpha}{\gamma} \frac{z}{1!} + \frac{\alpha(\alpha + 1)}{\gamma(\gamma + 1)} \frac{z^2}{2!} + \cdots \tag{78}$$

Higher moments of displacement are given by the recursion formula

$$\langle x^{2n+2} \rangle = \langle x^{2n} \rangle + kT(2n - 1)\langle x^{2n-2} \rangle, \qquad n \geqslant 1 \tag{79}$$

$$\langle x^{2n-1} \rangle = 0 \tag{80}$$

The nth approximant of the continued fraction representation (49) is expressed as

$$\hat{K}_0(\omega) = 0 \tag{81}$$

$$\hat{K}_n(\omega) = \cfrac{A_0}{-i\omega + B_1 - \cfrac{A_1}{-i\omega + B_2 - \cdots - \cfrac{A_{n-1}}{-i\omega + B_n}}}, \qquad n \geqslant 1 \tag{82}$$

The approximate spectral density obtained from $\hat{K}_n(\omega)$ is denoted by $S_n(\omega)$. The spectral density $S_0(\omega)$ corresponds to the statistical linearization result and the exact one is given by

$$S(\omega) = \lim_{n \to \infty} S_n(\omega) \tag{83}$$

where the convergence is assumed.

Before doing more calculations for the spectral densities in the case of $\epsilon = 1$, we will consider the case of $\epsilon = -1$, i.e., the Duffing oscillator, in order to compare the results with previous calculations. It should be mentioned that our definition of the diffusion constant D is one-half that used in other papers (i.e., $D = 1/2$ in this case), and that our definition of the spectral density is the same as that used in Ref. 9 and differs by factor of two from that in other work. The coefficient of the nonlinear term denoted by β in other work is fixed at unity here. Table I gives the values of three

Table I. Calculated Values of $S(\omega)$ for $\alpha = 2$ and $kT = 0.25$

ω	$S(\omega)$	$S_0(\omega)$	$S^{(\omega)}_{\mathrm{KWII}}$
0	0.242945	0.238229	0.24432
0.5	0.205122	0.205175	0.20141
1.0	0.116792	0.119009	0.11278
1.5	0.051397	0.051856	0.05031
2.0	0.022312	0.022213	0.02219
2.5	0.010525	0.010405	0.01054
3.0	0.005447	0.005375	0.00546

spectral densities, the first of which is the limit of our method, the second the statistical linearization results, and the third the second Kraichnan–Wyld approximation (KWII) obtained by Morton and Corrsin.[8] The latter has been known as the best approximation, but our results are more accurate and more easily obtained than theirs.

The convergence of $\{S_n(\omega)\}$ occurs quite rapidly in the large-friction-constant case, where most approximation procedures yield good results. In the case shown in Table I, for instance, the first six digits of $S_9(0)$ are already correct. In the small-friction-constant case with strong nonlinearity, where the KWII results are not available because of a computation stability problem, the convergence is naturally slow. Typically

$$|S_{23}(0) - S_{22}(0)|/S_{23}(0) \simeq 0.05 \qquad \text{for} \quad \alpha = 0.5 \text{ and } kT = 1.0 \tag{84}$$

In spite of slow convergence, our method gives reliable results for cases that used to be uncomputable. Figures 2 and 3 show the spectral density in two

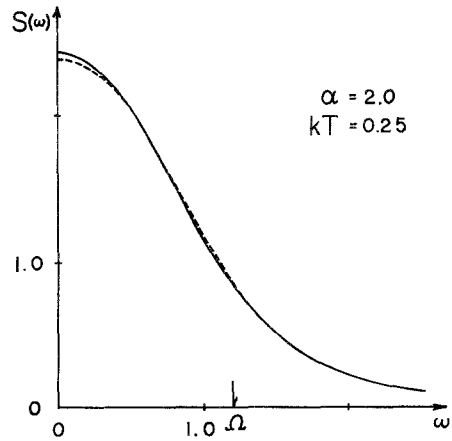

Fig. 2. Spectral density of the Duffing oscillator as a function of frequency in the case of $\alpha = 2.0$ and $kT = 0.25$. The zeroth approximation $S_0(\omega)$ and the limit function $S(\omega)$ are expressed by dashed and solid lines, respectively. Value of the effective frequency Ω is shown by the arrow.

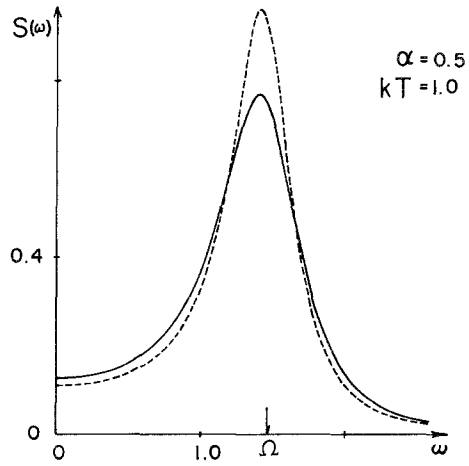

Fig. 3. Same as Fig. 2, except $\alpha = 0.5$ and $kT = 1.0$.

different cases. The first case ($\alpha = 2.0$, $kT = 0.25$) has been calculated by many authors and presents nothing new. The spectral density in the second case ($\alpha = 0.5$, $kT = 1.0$), however, is obtained here for the first time. In the Duffing oscillator case the statistical linearization or the quasiharmonic approximation shown by dashed lines is a qualitatively good approximation because the nonlinearity causes no drastic changes in the properties of the system. Quantitatively, however, this simple approximation does not yield good estimates, especially in the case of small friction constant and strong nonlinearity.

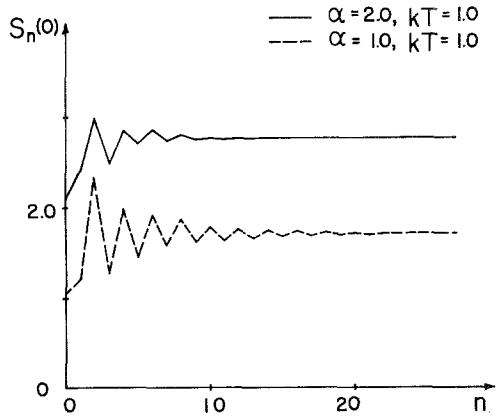

Fig. 4. Zero-frequency value of the normalized spectral density $S_n(\omega)$ as a function of n for the nonlinear oscillator with a double-well potential.

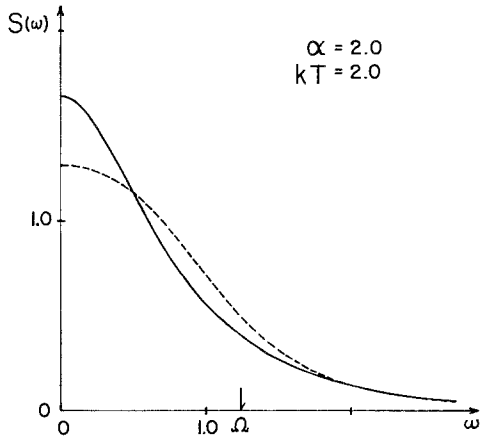

Fig. 5. Normalized spectral density of the nonlinear oscillator with a double-well potential in the case of $\alpha = 2.0$ and $kT = 2.0$. Dashed and solid lines as in Fig. 2.

As discussed above, our method is of great advantage in calculating the spectral density. Now we analyze, using our method, the Brownian motion of the nonlinear oscillator with a double-well potential, whose spectral density has not previously been calculated. In this case, as expected, the convergence of the continued fraction is slow, especially at small α. Figure 4 shows the converging pattern of $S_n(0)$ for two different cases. The zero-frequency values

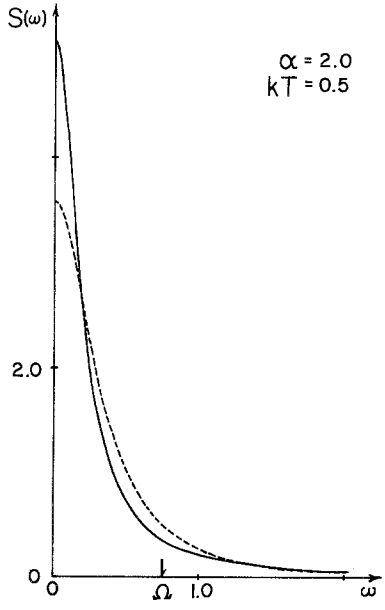

Fig. 6. Same as Fig. 5, except $kT = 0.5$.

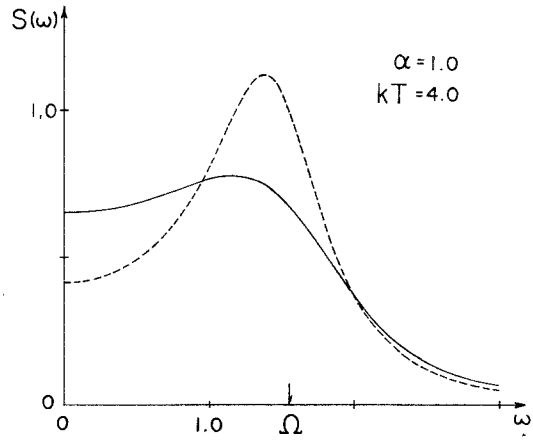

Fig. 7. Same as Fig. 5, except $\alpha = 1.0$ and $kT = 4.0$.

are used as a measure for our method for the following reason, as discussed by Bixon and Zwanzig.[9] The moment expansion (50) is a high-frequency expansion expected to converge only up to the farthest singularity from the origin in the complex frequency plane. The continued fraction is used for the analytic continuation of the high-frequency expansion to the entire frequency plane. Therefore the values of the continued fraction at the origin offer the best criterion for the adequacy of the procedure.

With $\alpha < 1$ the limit function $S(\omega)$ is hardly obtained, due to the slow convergence of $\{S_n(\omega)\}$. Typically

$$|S_{27}(0) - S_{26}(0)|/S_{27}(0) \simeq 0.12 \qquad \text{for} \quad \alpha = 0.5 \text{ and } kT = 1.0 \qquad (85)$$

In Figs. 5–10 the normalized spectral densities (solid line), given by

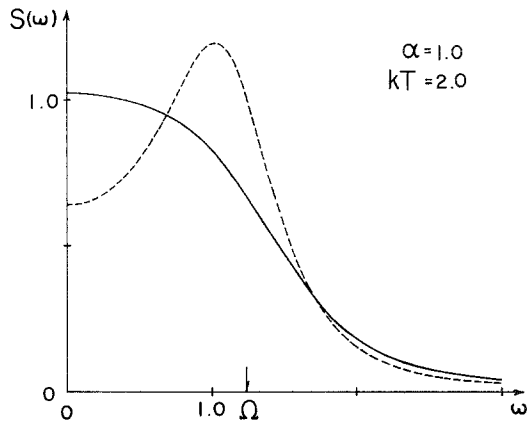

Fig. 8. Same as Fig. 7, except $kT = 2.0$.

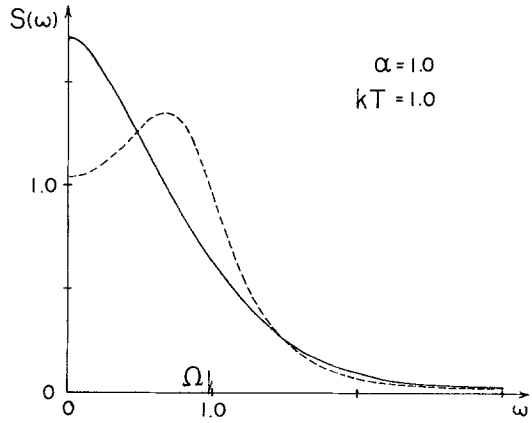

Fig. 9. Same as Fig. 7, except $kT = 1.0$.

$S(\omega)$ divided by $\langle x^2 \rangle$, and the normalized $S_0(\omega)$ (dashed line) are shown in several cases. The curves with $\alpha = 2.0$ are for $kT = 2.0$ and $kT = 0.5$ and they show a kind of overdamped behavior and narrowing effect. The sequence of curves with $\alpha = 1.0$ covers a wide range of temperature from $kT = 0.5$ to $kT = 4.0$. Although $S_0(\omega)$ clearly has resonant character for the case of $\alpha = 1.0$, the *resonant* peak in $S(\omega)$ tends to drop at high temperature and disappear at medium and low temperatures, while the *central* peak rises

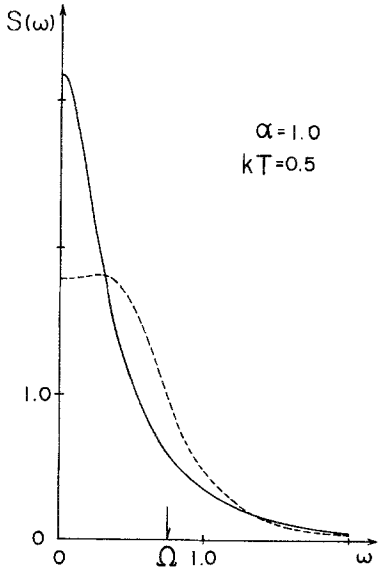

Fig. 10. Same as Fig. 7, except $kT = 0.5$.

in the latter cases. As the temperature decreases, the central peak dominates and its height becomes of order $\exp(\Delta/kT)$, where Δ is a positive constant related to the height of the potential barrier of $V(x)$. This behavior is to be expected, as one can see from the following simple argument: As the temperature decreases, the height of the barrier that the Brownian particle sees increases. This in turn increases the duration of the particle's stay on one side of the barrier. Even at high temperature these effects suppress the resonant behavior.

6. CONCLUDING REMARKS

There have been two main purposes of this paper: to present the general method for calculating the spectral density of nonlinear Brownian motion, and to present the results of the numerical calculations of the spectral density for the nonlinear oscillator with a double-well potential.

The projection operator method applied in this paper, using the continued fraction representation of the spectral density, is the most efficient method for calculating the stationary behavior of a nonlinear system. Statistical linearization is included in this procedure as the lowest order approximation. This method, developed in the field of nonequilibrium statistical mechanics, can be applied to widespread problems in engineering, which are described by the stochastic differential equations, because the method can be used for Brownian motion in an arbitrary potential field, provided the system is globally stable.

The efficiency of our method comes from the use of the exact static properties or the exact stationary moments of the quantities of interest. The requirement of the exact stationary moments causes no serious problems for finite-dimensional systems. In the infinite-dimensional case, or for the extension to field theory, however, this requirement is rarely satisfied in practice, so a kind of perturbational procedure may be necessary.

Numerical calculations of the displacement correlation function of the nonlinear oscillator with a double-well potential have been performed, using a continued-fraction expansion equivalent to exact specification of the first 56 frequency moments of the spectral density of the correlation function. The results of these calculations show fairly good convergence in most cases, except in the small-friction-constant case. Comparison between the exact and approximate results leads to the conclusion that the approximation of a quasiharmonic oscillator (or statistical linearization) does not always give even qualitatively good results if the potential field has a complex structure.

Recently Schneider and Strässler discussed the same model system as we do, as an example.[24] They also investigated Brownian motion in a

periodic potential in the large-friction-constant case and compared the results with experiments of ionic mobility.[25],[3]

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[3] Their papers were called to my attention by the referee.