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A generalized Green-Kubo formula is derived for a quantum dissipative system of driven Brownian particle, in which the coupling between the system and the environment is linear. The structure is essentially the same as that for the generalized Green-Kubo formula for driven granular particles. It is demonstrated that the correction to the conventional Green-Kubo formula is zero for a free Brownian particle.

§1. Introduction

Green-Kubo formula¹⁾ is one of the most fundamental relations in nonequilibrium statistical physics. The original derivation is restricted to the linear nonequilibrium case, but a number of generalizations are proposed by many researchers,²⁾⁻⁶⁾ though the relationship among their formulations is not still well understood.

We believe that roles of dissipation in Green-Kubo formula should be clarified, though it is unclear in the original derivation. Indeed, the Green-Kubo formula defines the transport coefficient which represents the dissipation. Moreover, if there is no dissipation in a system, the time integral of current correlation function in the formula should diverge. Therefore, purely mechanical derivation of Green-Kubo formula might be misleading, but correct derivations should include the dissipation explicitly.

Recently, Chong et al.⁷⁾ have derived a new generalized Green-Kubo formula for driven dissipative and classical particles as a natural extension of that by Evans and Morriss.²⁾ Their derivation has several remarkable points; (i) the formulation can include the integral fluctuation theorem without microscopic time-reversal symmetry, (ii) the role of dissipation is clear in their derivation, and (iii) one can develop the nonequilibrium mode-coupling theory for sheared granular liquids or sheared glassy systems. Their derivation is so general that one can expect that their method can be used for quantum cases. In this paper we demonstrate how to apply such a formula to quantum systems.

In this paper, we focus on a nonequilibrium steady state of a quantum Brownian particle. This is because (i) it is the simplest system among open quantum systems,⁸⁾⁻¹²⁾ (ii) we know the origin of dissipation of quantum Brownian system as the energy flux between the system and the environment, and (iii) there is the quantum version of the violation of fluctuation-dissipation relation.¹³⁾

The organization of this paper is as follows. In the next section, we specify the basic equations to be analyzed in this paper. In §3, we will obtain an exact solution of our model. In §4, we will present the formal form of generalized Green-Kubo formula whose bilinear form is reduced to the conventional Green-Kubo formula. In §5, we will focus on the case that a Brownian particle in a harmonic potential, in

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which the integration involved in the generalized Green-Kubo formula can be carried out. In §6, we will discuss and conclude our results. We also involve two Appendices, where Appendix A is devoted to the derivation of generalized Kubo's identity, and Appendix B gives an explicit calculation of the time evolution of the momentum of the Brownian particle.

§2. Model

Let us begin with a quantum master equation for a Brownian particle⁸⁾ under an external field $F_{ex}(t)$, which is essentially the same as Caldeira-Leggett model.¹⁰⁾ Note that the generalization to N Brownian particles is straightforward from that presented here. For simplicity, we restrict our interest to a particle coupled with the heat bath.

Let us consider a Brownian particle of mass m with its coordinate x and momentum p in a potential V(x) under a steady external field $F_{\text{ex}}(t)$.^{*)} The particle is assumed to be coupled with a bath consisting of a large number of harmonic oscillators with masses m_n and frequencies ω_n . Thus, the total Hamiltonian might be written as

$$H(t) = H_S + H_C + H_B + H_I + H_{\text{ex}}(t)$$

= $\frac{p^2}{2m} + V(x) - xF_{\text{ex}}(t) + \sum_n \left\{ \frac{p_n^2}{2m_n} + \frac{1}{2}m_n\omega_n^2 \left(x_n - \kappa_n \frac{x}{m_n\omega_n^2} \right)^2 \right\}.(2.1)$

Here, the system Hamiltonian of the particle is given by

$$H_S = \frac{p^2}{2m} + V(x),$$
 (2.2)

where we do not specify the form of the potential in the formulation in the main part of our paper. The bath Hamiltonian is represented by

$$H_B = \sum_n \hbar \omega_n \left(b_n^{\dagger} b_n + \frac{1}{2} \right) = \sum_n \left(\frac{1}{2m_n} p_n^2 + \frac{1}{2} m_n \omega_n^2 x_n^2 \right).$$
(2.3)

Here, b_n^{\dagger} and b_n denote the Bosonic creation and the annihilation operators of the bath, respectively, while x_n and p_n are the corresponding coordinate and the momentum. Similarly, the interaction Hamiltonian is given by

$$H_I = -x \sum_n \kappa_n x_n = -xB, \qquad (2.4)$$

where κ_n is the coupling constant, and the bath operator is

$$B \equiv \sum_{n} \kappa_n x_n = \sum_{n} \kappa_n \sqrt{\frac{\hbar}{2m_n \omega_n}} (b_n + b_n^{\dagger}).$$
 (2.5)

^{*)} Of course, the external field can be involved in the potential, but we separate the contribution of the external field from the stationary potential V(x).

We introduce the external Hamiltonian coupled with the external force F_{ex} as

$$H_{\rm ex}(t) = -xF_{\rm ex}(t). \tag{2.6}$$

Note that H_{ex} can be absorbed in H_S but we separate its contribution to clarify the response to the external field. We also introduce the counter-term Hamiltonian:

$$H_C = \mathcal{K}x^2 \equiv x^2 \sum_n \frac{\kappa_n^2}{2m_n \omega_n^2}.$$
 (2.7)

This counter-term Hamiltonian can be absorbed in the potential term V(x) as $V_{\text{eff}}(x) = V(x) + H_C$. However, if we regard the unperturbed Hamiltonian as $H_S + H_B$ without coupling between the system and the bath at t = 0, the effect of H_C appears in later expressions. We also note that H_C must be treated as a term of second order in the coupling, while H_I is of the first order.

Caldeira and Leggett¹⁰⁾ were interested in the low frequency behavior of particles. Then they adopted a quasi-classical approximation

$$x_S(-\tau) \equiv e^{-iH_S\tau/\hbar} x e^{iH_S\tau/\hbar} \approx x - \frac{i}{\hbar} [H_S, x]\tau, \qquad (2.8)$$

where k and T are the Boltzmann constant and the temperature, respectively. Here, however, we do not have to use this quasi-classical expression (2.8) for our argument. Here, we have introduced the commutation relation $[A, B] \equiv AB - BA$.

The starting equation is the Born-Markov approximation for the reduced density matrix of the Brownian particle, which obeys⁸⁾

$$\frac{d}{dt}\rho_{S}(t) = -\frac{i}{\hbar}[H_{S} + H_{C}, \rho_{S}(t)] + \frac{iF_{\text{ex}}(t)}{\hbar}[x, \rho_{S}(t)] - \frac{1}{\hbar}\int_{0}^{\infty} d\tau \text{tr}_{B}[H_{I}, [H_{I}(-\tau), \rho_{S}(t) \otimes \rho_{B}]].$$
(2.9)

Hereafter, we adopt the interaction picture with the respect to the unperturbed Hamiltonian $H_0 = H_S + H_B$. We shall assume that the initial condition satisfies

$$\rho_S(0) = \rho_{\rm eq} \otimes \rho_B, \qquad (2.10)$$

where

$$\rho_{\rm eq} = \frac{\exp[-\beta H_S]}{\operatorname{tr}_S \exp[-\beta H_S]}, \qquad \rho_B = \frac{\exp[-\beta H_B]}{\operatorname{tr}_B \exp[-\beta H_B]} \tag{2.11}$$

with $\beta = 1/kT$. Note that the assumption on $\rho_S(0)$ might be removable. Indeed, the steady distribution $\rho_S(t \to \infty)$ of Caldeira-Leggett model with Eq. (2.8) is relaxed to $\rho_S(0)$,^{8),11)} if the particle is trapped in a potential.

For the discussion of quantum Brownian motion we introduce the spectral functions

$$D(\tau) \equiv i \langle [B, B_B(-\tau)] \rangle_B, \qquad D_1(\tau) \equiv \langle \{B, B_B(-\tau)\} \rangle_B, \qquad (2.12)$$

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where $B_B(t) \equiv e^{iH_Bt/\hbar}Be^{-iH_Bt/\hbar}$ and $\{A, B\} \equiv AB + BA$. Note that H_S and H_B are decoupled with each other in the unperturbed state, where $\langle \cdots \rangle_B$ represents the average in terms of the density matrix ρ_B . We also note that $D(\tau)$ and $D_1(\tau)$ are respectively referred to as the dissipation and the noise kernel. Making use of the spectral density

$$J(\omega) = \sum_{n} \frac{\kappa_n^2}{2m_n \omega_n} \delta(\omega - \omega_n), \qquad (2.13)$$

we can write the explicit representations for the correlation functions

$$D(\tau) = 2\hbar \int_0^\infty d\omega J(\omega) \sin \omega \tau, \qquad (2.14)$$

$$D_1(\tau) = 2\hbar \int_0^\infty d\omega J(\omega) \coth\left(\frac{\beta\hbar\omega}{2}\right) \cos\omega\tau.$$
 (2.15)

After straightforward calculation, Eq. (2.9) can be rewritten as⁸⁾

$$\frac{d}{dt}\rho_{S}(t) = -\frac{i}{\hbar}[H_{S} + H_{C}, \rho_{S}(t)] + \frac{iF_{\text{ex}}(t)}{\hbar}[x, \rho_{S}(t)] + \frac{1}{2\hbar^{2}}\int_{0}^{\infty} d\tau \left(iD(\tau)[x, \{x_{S}(-\tau), \rho_{S}(t)\}] - D_{1}(\tau)[x, [x_{S}(-\tau), \rho_{S}(t)]]\right), \quad (2.16)$$

which is the basic equation of this paper.

The properties of the second line of $(2 \cdot 16)$ strongly depend on the behavior of the dissipation and the noise which are determined by $J(\omega)$. We adopt a continuous distribution of the bath modes and replace the spectral density by a smooth function of ω for the explicit calculation.

§3. The solution of Liouville equation

Let us rewrite Eq. (2.16) as

$$\frac{d}{dt}\rho_S(t) = -i\mathcal{L}^{\dagger}(t)\rho_S(t), \qquad (3.1)$$

where the Liouville operator is given by

$$i\mathcal{L}^{\dagger}(t) \equiv \frac{i}{\hbar} [H_S + H_C,] - \frac{iF_{\text{ex}}(t)}{\hbar} [x,] - \frac{1}{2\hbar^2} \int_0^\infty d\tau (iD(\tau)[x, \{x_S(-\tau), \}] - D_1(\tau)[x, [x_S(-\tau),]]). \quad (3.2)$$

Since this Liouville operator $i\mathcal{L}^{\dagger}(t)$ is independent of time, we can use the identity

$$T_{\leftarrow} \exp\left[-i\int_0^t ds \mathcal{L}^{\dagger}(s)\right] = 1 + \int_0^t dt_1 T_{\leftarrow} \exp\left[-i\int_0^{t_1} dt_2 \mathcal{L}^{\dagger}(t_2)\right] (-i\mathcal{L}^{\dagger}(t_1)), \quad (3\cdot3)$$

where T_{\leftarrow} represents the time ordering operator defined by $T_{\leftarrow}A(t_1)A(t_2) = A(t_1)A(t_2)$ for $t_1 > t_2$ and $T_{\leftarrow}A(t_1)A(t_2) = A(t_2)A(t_1)$ for otherwise. Substituting Eq. (2.10)

into Eq. $(3\cdot3)$, we obtain

$$\rho_S(t) = \rho_{\rm eq} + \int_0^t dt_1 T_{\leftarrow} e^{-i\int_0^{t_1} dt_2 \mathcal{L}^{\dagger}(t_2)} (-i\mathcal{L}^{\dagger}(t_1))\rho_{\rm eq}.$$
(3.4)

Here, $-i\mathcal{L}^{\dagger}\rho_{eq}$ consists of four terms:

$$-i\mathcal{L}^{\dagger}(t)\rho_{\rm eq} = \frac{iF_{\rm ex}(t)}{\hbar}[x,\rho_{\rm eq}] - \frac{i}{\hbar}\mathcal{K}[x^2,\rho_{\rm eq}] + \frac{i}{2\hbar^2}\int_0^\infty d\tau D(\tau)[x,\{x_S(-\tau),\rho_{\rm eq}\}] - \frac{1}{2\hbar^2}\int_0^\infty d\tau D_1(\tau)[x,[x_S(-\tau),\rho_{\rm eq}]].$$
(3.5)

The first term on the right-hand side of Eq. (3.5) produces the conventional Green-Kubo formula. With the aid of Kubo's identity (A.1), we can rewrite

$$[x, \rho_{eq}] = \rho_{eq} \int_0^\beta d\lambda e^{\lambda H_S} [H_S, x] e^{-\lambda H_S}$$
$$= -\frac{i\hbar}{m} \rho_{eq} \int_0^\beta d\lambda p_S(-i\hbar\lambda), \qquad (3.6)$$

where we have used $[H_S, x] = -i\hbar p/m$. Thus, the first term on the right-hand side of (3.5) is reduced to

$$\frac{iF_{\rm ex}(t)}{\hbar}[x,\rho_{\rm eq}] = \frac{F_{\rm ex}(t)}{m}\rho_{\rm eq}\int_0^\beta d\lambda p_S(-i\hbar\lambda). \tag{3.7}$$

Similarly, the second term on the right-hand side of (3.5) which is the order of square of the coupling constant can be calculated. From (A.1) we readily obtain

$$[x^2, \rho_{\rm eq}] = -\frac{i\hbar\rho_{\rm eq}}{m} \int_0^\beta d\lambda \{ x_S(-i\hbar\lambda), p_S(-i\hbar\lambda) \}, \qquad (3.8)$$

where we have used $[H_S, x^2] = -i\hbar(xp + px)/m$. Thus, the second term on the right-hand side of (3.5) is reduced to

$$-\frac{i}{\hbar}\mathcal{K}[x^2,\rho_{\rm eq}] = -\frac{\mathcal{K}\rho_{\rm eq}}{m} \int_0^\beta d\lambda \{x_S(-i\hbar\lambda), p_S(-i\hbar\lambda)\}.$$
(3.9)

The contributions from the third term and the fourth term on the right-hand side of (3.5) are more complicated. From (A.1), (A.2) and (A.3) we obtain an identity

$$[x, \{x_S(-\tau), \rho_{eq}\}] = \rho_{eq} \left([x, x_S(-\tau)] + [x, x_S(-i\hbar\beta - \tau)] \right) -\frac{i\hbar}{m} \rho_{eq} \int_0^\beta d\lambda p_S(-i\hbar\lambda) (x_S(-\tau) + x_S(-i\hbar\beta - \tau)). \quad (3.10)$$

Similarly, thanks to $(A \cdot 1)$ we obtain

$$[x, [x_S(-\tau), \rho_{eq}]] = \rho_{eq} \left([x, x_S(-i\hbar\beta - \tau)] - [x, x_S(-\tau)] \right) -i\hbar \frac{\rho_{eq}}{m} \int_0^\beta d\lambda p_S(-i\hbar\lambda) (x_S(-i\hbar\beta - \tau) - x_S(-\tau)). \quad (3.11)$$

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Thus, the third term and the fourth term on the right-hand side of (3.5) are reduced to

$$\frac{i}{2\hbar^2} \int_0^\infty d\tau D_1(\tau) [x, \{x_S(-\tau), \rho_{\rm eq}\}] - \frac{1}{2\hbar^2} \int_0^\infty d\tau D(\tau) [x, [x_S(-\tau), \rho_{\rm eq}]]$$

$$= \frac{\rho_{\rm eq}}{2\hbar^2} \int_0^\infty d\tau \tilde{D}_+(\tau) \{ [x, x_S(-\tau)] - \frac{i\hbar}{m} \int_0^\beta d\lambda p_S(-i\hbar\lambda) x_S(-\tau) \}$$

$$- \frac{\rho_{\rm eq}}{2\hbar^2} \int_0^\infty d\tau \tilde{D}_-(\tau) \{ [x, x_S(-\tilde{\tau})] - \frac{i\hbar}{m} \int_0^\beta d\lambda p_S(-i\hbar\lambda) x_S(-\tilde{\tau}) \}, \qquad (3.12)$$

where $\tilde{\tau} = \tau + i\hbar\beta$ and

$$\tilde{D}_{\pm}(\tau) \equiv D_1(\tau) \pm iD(\tau). \tag{3.13}$$

Thus, we can write

$$T_{\leftarrow} \exp[-i \int_0^t ds \mathcal{L}^{\dagger}(s)] (-\mathcal{L}^{\dagger}(t)) \rho_{\text{eq}} = (-i \mathcal{L}^{\dagger}(t)) \rho_S(t) = \Omega(t) \rho_S(t)$$
(3.14)

and

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$$\rho_S(t) = \rho_{\rm eq} + \int_0^t dt_1 T_{\leftarrow} e^{-i \int_0^{t_1} dt_2 \mathcal{L}^{\dagger}(t_2)} [\Omega(t_1) \rho_{\rm eq}], \qquad (3.15)$$

where

$$\begin{split} \Omega(t) &\equiv \frac{F_{\rm ex}(t)}{m} \int_0^\beta d\lambda p_S(-i\hbar\lambda) - \frac{\mathcal{K}}{m} \int_0^\beta d\lambda \{x_S(-i\hbar\lambda), p_S(-i\hbar\lambda)\} \\ &+ \frac{i}{2\hbar m} \int_0^\infty d\tau \Big\{ \tilde{D}_-(\tau) \int_0^\beta d\lambda p_S(-i\hbar\lambda) x_S(-\tau - i\hbar\beta) \\ &- \tilde{D}_+(\tau) \int_0^\beta d\lambda p_S(-i\hbar\lambda) x_S(-\tau) \Big\} \\ &+ \frac{1}{2\hbar^2} \int_0^\infty d\tau \left(\tilde{D}_+(\tau)[x, x_S(-\tau)] - \tilde{D}_-(\tau)[x, x_S(-\tau - i\hbar\beta)] \right). \end{split}$$
(3.16)

Before closing this section, we should note an important property of Ω which satisfies

$$\langle \Omega(t) \rangle_{\rm eq} \equiv {\rm tr}_S \{ \rho_{\rm eq} \Omega(t) \} = 0.$$
 (3.17)

This relation is easily verified from Eq. (3.5) with the invariant property of the trace under a cyclic permutation.

§4. Generalized Green-Kubo formula

Let us derive the generalized Green-Kubo formula. For simplicity, we assume the external force $F_{\text{ex}}(t) = F_0 e^{i\omega_0 t}$, and only discuss the average behavior of the momentum p

$$\langle p \rangle_t \equiv \mathrm{tr}_S \{ \rho_S(t) p \}.$$
 (4.1)

Substituting $(4 \cdot 1)$ into $(3 \cdot 15)$, we obtain

$$\langle p \rangle_t = \mathrm{tr}_S \{ \rho_{\mathrm{eq}} p \} + \int_0^t dt_1 \mathrm{tr}_S \{ T_{\leftarrow} e^{-i \int_0^{t_1} dt_2 \mathcal{L}^{\dagger}(t_2)} [\rho_{\mathrm{eq}} \Omega(t_1)] p \}.$$
(4.2)

With the help of the property

$$\operatorname{tr}_{S}\left\{e^{-i\int_{0}^{t}ds\mathcal{L}^{\dagger}(s)}[\Omega(t)\rho_{\mathrm{eq}}]p\right\} = \operatorname{tr}_{S}\left\{\rho_{\mathrm{eq}}\Omega(t)p_{H}(t)\right\}$$
(4.3)

with $p_H(t) \equiv e^{i \int_0^t ds \mathcal{L}(s)} p = e^{i \int_0^t ds H(s)/\hbar} p e^{-i \int_0^t ds H(s)/\hbar}$, we can write the generalized Green-Kubo formula, where the Liouville operator $i\mathcal{L}(t)$ satisfies Heisenberg's equation of motion $\dot{A}_H(t) = i\mathcal{L}(t)A_H(t) = \frac{i}{\hbar}[H(t), A_H(t)]$. We note that the last equality for $p_H(t)$ holds because of our special set-up, where we adopt the basic model under the Born-Markovian approximation with the linear coupling between the system and the environment.

The explicit form of $i\mathcal{L}(t)$ is given by

$$i\mathcal{L}(t) = \frac{i}{\hbar}[H_S + H_C,] - \frac{iF_{\text{ex}}(t)}{\hbar}[x,] - \frac{1}{2\hbar^2} \int_0^\infty d\tau \left(iD(\tau)\{x_S(-\tau), [x,]\} + D_1(\tau)[x_S(-\tau), [x,]]\right), \quad (4.4)$$

where we have used the invariant property of the trace under a cyclic permutation.

We can introduce

$$\Lambda \equiv i\mathcal{L}^{\dagger}(t) - i\mathcal{L}(t), \qquad (4.5)$$

whose expectation value corresponds to the phase volume contraction in classical situations. The operator Λ is immediately obtained as

$$A = \frac{1}{2\hbar^2} \int_0^\infty d\tau D_1(\tau) \left([x, [x_S(-\tau),]] + [x_S(-\tau), [x,]] \right) - \frac{i}{2\hbar^2} \int_0^\infty d\tau D(\tau) \{ [x, x_S(-\tau)], \}.$$
(4.6)

Thus, we expect $\langle \Lambda \rangle_t$ represents the quantum counter-part of the phase volume contraction.

In the steady state limit, we should take the limit of $t \to \infty$ as

$$\langle p \rangle_{\rm SS} \equiv \lim_{t \to \infty} \langle p \rangle_t = \int_0^\infty dt {\rm tr}_S[\rho_{\rm eq} \Omega(t) p_H(t)].$$
 (4.7)

The contribution of the first term on the right-hand side of (3.16) is

$$\langle p \rangle_{\rm SS}^{(1)} = \frac{F_0}{m} \int_0^\infty dt \int_0^\beta d\lambda \langle p_S(-i\hbar\lambda)p_H(t) \rangle_{\rm eq} e^{i\omega_0 t}, \tag{4.8}$$

which is the conventional Green-Kubo formula. The contribution of the second term on the right-hand side of (3.16) is

$$\langle p \rangle_{\rm SS}^{(2)} = -\frac{\mathcal{K}}{m} \int_0^\infty dt \int_0^\beta d\lambda \langle \{ x_S(-i\hbar\lambda), p_S(-i\hbar\lambda) \} p_H(t) \rangle_{\rm eq}, \tag{4.9}$$

where we have used $\langle p(t) \rangle_{\text{eq}} = 0$. The contribution of the third term on the right-hand side of (3.16) is

$$\langle p \rangle_{\rm SS}^{(3)} = \frac{i}{2\hbar m} \int_0^\infty dt \int_0^\infty d\tau \Big\{ \tilde{D}_-(\tau) \int_0^\beta d\lambda \langle p_S(-i\hbar\lambda) x_S(-\tilde{\tau}) p_H(t) \rangle_{\rm eq} \Big\}$$

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$$-\tilde{D}_{+}(\tau)\int_{0}^{\beta}d\lambda \langle p_{S}(-i\hbar\lambda)x_{S}(-\tau)p_{H}(t)\rangle_{\rm eq}\Big\}.$$
(4.10)

The contribution of the fourth term on the right-hand side of (3.16) is

$$\langle p \rangle_{\rm SS}^{(4)} = \frac{1}{2\hbar^2} \int_0^\infty d\tau \int_0^\infty dt \left(\tilde{D}_+(\tau) \langle [x, x_S(-\tau)] p_H(t) \rangle_{\rm eq} - \tilde{D}_-(\tau) \langle [x, x_S(-\tilde{\tau})] p_H(t) \rangle_{\rm eq} \right).$$
(4.11)

Thus, we obtain the generalized Green formula

$$\langle p \rangle_{\rm SS} = \sum_{i=1}^{4} \langle p \rangle_{\rm SS}^{(i)}.$$
 (4.12)

It is obvious that three terms $\sum_{i=2}^{4} \langle p \rangle_{\rm SS}^{(i)}$ represent the nonlinear correction to the conventional Green-Kubo formula, in which the effect of the external force appears through the time evolution of $p_H(t)$. We also note that $\langle p \rangle_{\rm SS}^{(2)}$ and $\langle p \rangle_{\rm SS}^{(3)}$ essentially come from non-dissipative parts, though $p_H(t)$ should involve dissipative effects. So far, there is no approximation once we start from the basic equations presented in §2.

It should be noted that the current $p_H(t)$ in Eqs. (4.8)–(4.11) can be replaced by $\Delta p_H(t) \equiv p_H(t) - p_H(\infty)$ if $p_H(\infty)$ is finite because of Eq. (3.17).

§5. Simple example

In the previous section, we have presented formal representations of generalized Green-Kubo formulae, but such formal expressions might be insufficient to demonstrate its relevancy. In this section, we demonstrate what the result is in the case of V(x) = 0. It should be noted that the model is exactly solvable for the harmonic potential but in such a case there is no steady current of the particle because of the trap of the particle in the potential.

If we assume V(x) = 0 and $\omega_0 = 0$, $x_S(-\tau)$, $x_S(-i\hbar\lambda)$ and $p_S(-i\hbar\lambda)$ are respectively written as

$$x_S(-\tau) = x + \frac{p}{m}\tau,\tag{5.1}$$

$$x_S(-i\hbar\lambda) = x - i\hbar\lambda\frac{p}{m},\tag{5.2}$$

$$p_S(-i\hbar\lambda) = p. \tag{5.3}$$

From Eq. $(5\cdot3)$ we immediately obtain

$$\int_0^\beta d\lambda p_S(-i\hbar\lambda) = \beta p. \tag{5.4}$$

With the aid of Eqs. (4.8) and (B.11), thus, we obtain

$$\langle p \rangle_{\rm SS}^{(1)} = \frac{F_0}{m} \int_0^\infty dt \int_0^\beta d\lambda \langle p^2 \rangle_{\rm eq} e^{-2\gamma t} = \frac{F_0}{2\gamma},\tag{5.5}$$

where we have used $\langle p^2 \rangle_{eq} = mkT$. This is the result from the conventional Green-Kubo formula. We also need to stress that this result is identical to the exact solution of $p_H(t \to \infty)$ in Eq. (B·11) without any statistical average. Thus, we expect that the contributions from Eqs. (4·9)–(4·11) are zero in this simple example. Indeed, it is quite easy to prove the above statement.

Let us evaluate the contribution of Eq. (4.9). From (5.2) and (5.3), we obtain

$$\{x_S(-i\hbar\lambda), p_S(-i\hbar\lambda)\} = xp + px - 2\frac{i\hbar\lambda}{m}p^2.$$
(5.6)

Therefore, we immediately obtain

$$\langle \{ x_S(-i\hbar\lambda), p_S(-i\hbar\lambda) \} p_H(t) \rangle_{\text{eq}} = 0, \qquad (5.7)$$

where we have used $\langle \{x_S(-i\hbar\lambda), p_S(-i\hbar\lambda)\} \rangle_{eq} = 0$ and function containing odd powers of x or p becomes traceless. Here we note $p_H(t)$ is given by Eq. (B·11).

Let us evaluate the integral terms on the right-hand side of (2.16). By using (5.1) we can write

$$[x, \{x_S(-\tau), \rho_{\text{eq}}\}] = [x, \{x, \rho_{\text{eq}}\}] + \frac{\tau}{m} [x, \{p, \rho_{\text{eq}}\}].$$
(5.8)

Therefore, we directly obtain

$$\operatorname{tr}_{S}\{[x, \{x_{S}(-\tau), \rho_{\mathrm{eq}}\}]p_{H}(t)\} = 0, \qquad (5.9)$$

where we have used $\operatorname{tr}_{S}\{[x, \{x_{S}(-\tau), \rho_{\operatorname{eq}}\}] = 0 \text{ and Eq. (B.11)}.$

Similarly, from

$$[x, [x(-\tau), \rho_{\rm eq}]] = [x, [x, \rho_{\rm eq}]] + \frac{\tau}{m} [x, [p, \rho_{\rm eq}]]$$
(5.10)

we immediately obtain

$$\operatorname{tr}_{S}\{[x, [x_{S}(-\tau), \rho_{\mathrm{eq}}]]p_{H}(t)\} = 0, \qquad (5.11)$$

where we have used $\operatorname{tr}_{S}\{[x, [x_{S}(-\tau), \rho_{eq}]] = 0 \text{ and } Eq. (B.11).$

Therefore, the generalized Green-Kubo formula for the motion without potential is reduced to the result obtained by conventional Green-Kubo formula as

$$\langle p \rangle_{\rm SS} = \frac{F_0}{2\gamma}.\tag{5.12}$$

To know the nonlinear contributions in Eqs. (4.9)-(4.11) explicitly, we need to introduce nonlinear effects of potential or the interaction between particles.

§6. Discussion and conclusion

We have obtained the generalized Green-Kubo formula. The final expression should be nearly equal to (4.8)-(4.11). We also verify the validity of our formulation

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in the simplest case for a free Brownian particle under the external force F_{ex} , where the result is obtained from the conventional Green-Kubo formula.

There are a couple of unsolved questions to be answered. (i) The generalized Green-Kubo formula is not directly related to that we have obtained for classical systems,⁷⁾ where $\Omega(t)$ is sum of $\beta \langle \dot{H}_S \rangle_{eq} - \langle \Lambda \rangle_{eq}$, where $\langle \Lambda \rangle_{eq}$ is the classical phase volume contraction. (ii) Saito¹³⁾ found that $\langle \dot{H}_S \rangle$ (more precisely, quantum version of Rayleigh's dissipation function) is directly related to quantum version of Harada-Sasa relation.¹⁴⁾ However, the connection between my formulation and quantum Harada-Sasa relation is not clear. (iii) We believe that it is straightforward to derive the integral fluctuation theorem in this context without using time-reversed path. This is the next task. (iv) Closely related to the above, how to understand generalized Onsager-Casmir relation in this context?⁴⁾ (v) How to apply this formulation to the case of microscopic time irreversible quantum systems?¹⁵⁾ (vi) We have analyzed a case of steady external force, but we should extend the formulation for the case of time-dependent external field. This is indeed necessary to discuss fluctuation-dissipation relation and its violation. See also the argument by Utsumi and Saito.¹⁶⁾ (vii) We should analyze the case of nonlinear potentials to clarify the correction of conventional Green-Kubo formula. In this case, we cannot obtain the exact solution.

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Appendix A —— Generalized Kubo's Identity ——

Kubo used an important identity in his paper.¹⁾ This identity can be written as

$$[A, e^{-\beta H_S}] = e^{-\beta H_S} \int_0^\beta d\lambda e^{\lambda H_S} [H_S, A] e^{-\lambda H_S} = -i\hbar e^{-\beta H_S} \int_0^\beta d\lambda \dot{A}_S(-i\hbar\lambda), \quad (A\cdot 1)$$

where A is any observable. One can generalize this identity to Fermionic commutation relation or the case including double commutators as

$$\{A, e^{-\beta H_S}\} = 2e^{-\beta H_S}A + e^{-\beta H_S} \int_0^\beta d\lambda e^{\lambda H_S} [H_S, A] e^{-\lambda H_S}, \qquad (A.2)$$

$$[A, e^{-\beta H_S} B_S(-\tau)] = e^{-\beta H_S} [A, B_S(-\tau)] + e^{-\beta H_S} \int_0^\beta d\lambda e^{\lambda H_S} [H_S, A] e^{-\lambda H_S} B_S(-\tau)$$

$$= e^{-\beta H_S} [A, B_S(-\tau)] - i\hbar e^{-\beta H_S} \int_0^\beta d\lambda \dot{A}_S(-i\hbar\lambda) B_S(-\tau). \quad (A.3)$$

The derivation of these identities are straightforward. First, we derive Eq. $(A \cdot 2)$. It is easy to confirm

$$\frac{d}{d\beta}e^{\beta H_S}\{A, e^{-\beta H_S}\} = e^{\beta H_S}H_S\{A, e^{-\beta H_S}\} + e^{\beta H_S}\{A, \frac{d}{d\beta}e^{-\beta H_S}\} = e^{\beta H_S}[H_S, A]e^{-\beta H_S}$$
(A·4)

On the other hand, it is easy to confirm the identity

$$\frac{d}{d\beta} \int_0^\beta d\lambda e^{\lambda H_S} [H_S, A] e^{-\lambda H_S} = e^{\beta H_S} [H_S, A] e^{-\beta H_S}.$$
(A·5)

Thus, we readily obtain Eq. (A·2) where we have used $e^{\beta H_S} \{A, e^{-\beta H_S}\} \rightarrow 2A$ as $\beta \rightarrow 0$. The derivation of Eq. (A·3) is almost identical to the above. If we can use $(d/d\beta)e^{\beta H_S}[A, e^{-\beta H_S}B_S(-\tau)] = e^{\beta H_S}[H_S, A]e^{-\beta H_S}B_S(-\tau)$ and $e^{\beta H_S}[A, e^{-\beta H_S}B_S(-\tau)] \rightarrow [A, B_S(-\tau)]$ as $\beta \rightarrow 0$, we readily obtain Eq. (A·3).

$\begin{array}{c} \textbf{Appendix B} \\ ----- Explicit Calculation of p_H(t) ----- \end{array}$

It is possible to obtain the exact solution of $p_H(t)$ if the potential is absent and $\omega_0 = 0$. The formal solution $p_H(t)$ is written as

$$p_H(t) = e^{i\mathcal{L}t}p = \sum_{n=0}^{\infty} \frac{t^n}{n!} (i\mathcal{L})^n p, \qquad (B\cdot 1)$$

where $i\mathcal{L}$ is given by $i\mathcal{L}(t)$ with putting $\omega_0 = 0$ in Eq. (4.4). Thus, the most important process to obtain $p_H(t)$ is to obtain $i\mathcal{L}p$ which consists of the five terms as $i\mathcal{L} = \sum_{i=1}^{5} i\mathcal{L}_i$. The first of $i\mathcal{L}p$ is

$$i\mathcal{L}_1 p \equiv \frac{i}{\hbar} [H_S, p] = 0. \tag{B.2}$$

The second term of $i\mathcal{L}p$ is

$$i\mathcal{L}_2 p \equiv \frac{i}{\hbar}[H_c, p] = -2\mathcal{K}x.$$
 (B·3)

The third term is given by

$$i\mathcal{L}_3 p \equiv -\frac{iF_0}{\hbar}[x,p] = F_0. \tag{B.4}$$

The fourth term is the most complicated, which is given by

$$i\mathcal{L}_4 p \equiv -\frac{i}{2\hbar^2} \int_0^\infty d\tau D(\tau) \{x_S(-\tau), [x, p]\} = \frac{1}{\hbar} \int_0^\infty d\tau D(\tau) x_S(-\tau)$$
$$= \frac{x}{\hbar} \int_0^\infty d\tau D(\tau) - \frac{p}{m} \int_0^\infty d\tau D(\tau) \tau$$
$$= -2\gamma p + 2\mathcal{K} x, \tag{B.5}$$

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where we have used (5.1) for the second equality, and

$$\int_{0}^{\infty} d\tau D(\tau) = 2\hbar \lim_{\epsilon \to \infty} \int_{0}^{\infty} d\omega \int_{0}^{\infty} d\tau J(\omega) e^{-\epsilon\tau}$$
$$= 2\hbar \lim_{\epsilon \to 0} \int_{0}^{\infty} d\omega \frac{\omega J(\omega)}{\omega^{2} + \epsilon^{2}} = 2\hbar \mathcal{K}.$$
(B·6)

We should emphasize that the contribution of counter Hamiltonian (B·3) is cancelled from the contribution of Eq. (B·6). The five contribution to $i\mathcal{L}p$ is given by

$$i\mathcal{L}_5 p \equiv -\frac{1}{2\hbar^2} \int_0^\infty d\tau D_1(\tau) [x_S(-\tau), [x, p]] = 0.$$
 (B·7)

Thus, from Eqs. $(B\cdot 2)-(B\cdot 7)$ we obtain

$$i\mathcal{L}p = -2\gamma p + F_0, \tag{B.8}$$

or equivalently

$$i\mathcal{L}\Delta p = -2\gamma\Delta p,\tag{B.9}$$

where

$$\Delta p \equiv p - \frac{F_0}{2\gamma}.\tag{B.10}$$

Thus, we obtain $(i\mathcal{L})^n \Delta p = (-2\gamma)^n \Delta p$.

This leads to

$$p_H(t) = \sum_{n=0}^{\infty} \frac{t^n}{n!} (i\mathcal{L})^n p = \frac{F_0}{2\gamma} + \left(p - \frac{F_0}{2\gamma}\right) e^{-2\gamma t}.$$
 (B·11)

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