Linear response and modified fluctuation-dissipation relation in random potential

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In this work, a physical system described by the Hamiltonian $\mathbf{H}_\omega = \mathbf{H}_0 + \mathbf{V}_\omega(t)$ consisting of a solvable model $\mathbf{H}_0$ and external random and time-dependent potential $\mathbf{V}_\omega(t)$ is investigated. Under the conditions in which, for each realization, the potential changes smoothly so that the evolution of the system follows the Schrödinger dynamics, and that the average external potential with respect to all realizations is constant in time, an adjusted equilibrium state can be defined as a reference state and the mean dynamics can be derived from taking the average of the equation with respect to the configuration parameter ω. It provides extra contributions from the deviations of the Hamiltonian and evolves the state along the time by the Heisenberg and Liouville–von Neumann equations. Consequently, the Kubo formula and the fluctuation-dissipation relation (FDR) are modified in the sense that the contribution from the information of randomness and memory effects from the time dependence is also present. The modified Kubo formula now has a contribution from two terms. The first term is an antisymmetric cross correlation between two observables measured by a probe as expected, and the latter term is an accumulation of the propagation of the effects from the randomness. When the considered system is in the adjusted equilibrium state at the time the measurement probe interacts, the latter contribution vanishes, and the standard FDR is recovered.

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I. INTRODUCTION

The fluctuation-dissipation relation (FDR) is one of the most well-known formulas in statistical physics, especially in weakly perturbed systems around equilibria. The relation was first coined by Callen and Welton in 1951 [1] and was later developed by Kubo in 1957 [2]. It states that the rate of energy dissipation, which one can measure, can be described via a fluctuation of the system in terms of the correlation among the group of considered quantities [1–4]. The relation can be successfully applied to physical implementation, such as in a measurement process in experiment, since one can perturb the system to obtain a response function and infer its properties to understand the behaviors of the considered system.

However, reports over recent decades have indicated that the FDR does not hold appropriately in many situations, such as glassy or driven systems [3,5–22]. In a system with sufficiently slow change toward equilibrium, possibly due to the composition of many complicated effects concerning interactions, the FDR could be modified into a quasi-FDR in which the correlation and response functions are extended into more general forms [3,5]. Such extensions cover, both theoretically and experimentally, many cases of models that concern, for instance, long-time relaxation, structural glasses [6,7], spin glasses [8–13], the Ising model with dipolar interactions [14], the spin-boson model [15], and the Glauber-Ising chain [16]. A driven system is another type of Hamiltonian model that is separate from the standard FDR for a different reason, namely the time dependence of the Hamiltonian. Nonetheless, such a system provides similar characteristics to those of the glassy class, i.e., the significantly slow evolution toward equilibrium or steady state. In essence, the effects of the time-dependent Hamiltonian can arise from the memory content of the dynamics, which prevents the system from lying in or near the equilibrium component [17–22].

In the literature, the derivations of such deviations of the FDR and the Kubo formula can be obtained by modifying the linear-response formulation with perturbation from a bath [2]; interested readers can consult Refs. [4,23–26] and references therein for further information on various modifications. Almost all of those references presented similar modifications of the standard FDR, i.e., an extra term was added to the equation.

In this work, we introduce an alternative mechanism to obtain modification of the Kubo formula and the FDR by employing the role of random, time-dependent potential. We consider a family of nonautonomous, or driven, systems with random potential interacting with an external bath (e.g., a measuring probe), and we investigate how the FDR is modified in such systems. A crucial point of our work is the choice of the reference state, called the adjusted equilibrium state, which is defined as Gibbs' state obtained by averaging over all random realizations of the Hamiltonian. The contribution to the modification of the FDR arises in two terms. The first term comes from the system's interaction with the bath, which is expected from the cross correlations generated during the dynamics. The second term comes from the propagation of noisy terms at later times, which perturbs the aforementioned cross correlations. With the chosen reference state, the modified FDR is derived. In the limiting case in which the fluctuation is absent, the contribution from the second term diminishes, leaving only that from the first term, as commonly obtained in other approaches to modify the FDR.

This article is organized into four sections. In Sec. II, a framework of the random Schrödinger-type dynamics is formulated, the reference state is defined, and the equations for the mean dynamics are derived. In Sec. III, the derivations of the Kubo formula and the modified FDR are presented. In Secs. II and III, we focus on the mathematical arguments and

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relations, leaving the discussion of the physical interpretation and relevance to Sec. IV, where we also discuss our results as they pertain to the work of other authors available in the literature. Finally, the conclusions are summarized in Sec. V.

II. FORMULATION

To incorporate the effects from the noisy background into a quantum model, we employ the usual formalism of a random Hamiltonian that is constructed to be a random operator acting on Hilbert space, and it is also time-dependent to reflect the nonautonomy of the underlying physical implementation. In the following subsections, we propose a model of a system with random potential and practical conditions to define a new reference state of the dynamics, under the assumption that the mean Hamiltonian is time-constant. Thereafter, we introduce a mean dynamics, which is an average of all possible governing equations, leading to the nonhomogeneous governing equations of quantum states and operators. More importantly, the mean equation and the chosen reference state will be foundations for the analysis to obtain the modified Kubo formula and the FDR in the next section.

A. A Model

We consider a system described by a time-dependent Hamiltonian,

$$\mathbf{H}_\omega(t) = \mathbf{H}_0 + \mathbf{V}_\omega(t), \tag{1}$$

where $\mathbf{H}_0$ is a fixed Hamiltonian and $\mathbf{V}_\omega(t)$ is a random potential operator defined by $\mathbf{V}_\omega(t)\varphi = v_\omega(t)\varphi$ for each φ in Hilbert space $\mathcal{H}$, where $v_\omega(t)$ is a smooth function of t. For the sake of brevity, let $\mathbf{H}_\omega$ denote $\mathbf{H}_\omega(t)$, where the parameter ω indicates a configuration or realization in probability space (Ω,μ), with a measure μ. In this sense, the Hamiltonian $\mathbf{H}_0$ can be viewed as the background Hamiltonian of our system, e.g., a sample in an experiment, submerged in a noisy environment whose effects are reflected in the random potential $\mathbf{V}_\omega(t)$. Conceptually, we imagine a composite system S, which can be decomposed as $S = S_0 \cup S_\omega$, where S_0 is a considered system (e.g., a sample in an experiment) and S_ω is a (virtual) external system (e.g., the noisy environment in the experiment) connecting to S_0, with the effects from S_ω encoded in the potential $\mathbf{V}_\omega(t)$. This means that S_ω possesses random fluctuation, making it a reservoir that supplies or extracts energy by a random amount of $v_\omega(t)$ at time t. This causes the measured total energy of the composite system S to depend on time t. In our consideration, the composite system S is also in weak contact with a reservoir B (e.g., another measurement probe or a controlled environment) with a parameter $\beta = 1/k_B T$, where T is the bath temperature.

We assume that $\mathbf{H}_0$ is a solvable Hamiltonian of the considered system S_0, equipped with a set of eigenfunctions $\{\phi_k\}$ in Hilbert space $\mathcal{H}$ corresponding to eigenvalues $\{E_k\}$, where $k = 1,2,\ldots,d := \dim\mathcal{H}$. For such a system, one can obtain an equilibrium state or Gibbs state that maximizes the von Neumann entropy among all states with a given energy E_0 [27,28] as

$$\sigma_\beta := \frac{e^{-\beta\mathbf{H}_0}}{\mathrm{Tr}[e^{-\beta\mathbf{H}_0}]} = \sum_{k=1}^{d}\left(\frac{e^{-\beta E_k}}{\sum_{j=1}^{d} e^{-\beta E_j}}\right)|\phi_k\rangle\langle\phi_k|. \tag{2}$$

We note that σ_β is equilibrium only for the case $v_\omega(t) = 0$ at all time t. In this case, $E_0 = \langle\mathbf{H}_0\rangle_{\sigma_\beta} := \mathrm{Tr}[\sigma_\beta\mathbf{H}_0]$, where $\langle\mathbf{A}\rangle_\rho = \mathrm{Tr}(\rho\mathbf{A})$ is an average of the operator $\mathbf{A}$ over a state ρ. On the contrary, for the system governed by $\mathbf{H}_\omega$, it becomes more complicated to find an equilibrium state (if it exists) from a given energy because the Hamiltonian $\mathbf{H}_\omega$ is time-dependent; hence, the energy $\mathrm{Tr}[\sigma_\beta\mathbf{H}_\omega(t)]$ of the system in the state σ_β is no longer a constant of motion. In particular, for a realization ω, the state of the form $\frac{e^{-\beta\mathbf{H}_\omega}}{\mathrm{Tr}(e^{-\beta\mathbf{H}_\omega})}$ is not an equilibrium state for all time. Moreover, since $\mathbf{H}_\omega$ also depends on a configuration ω, one may not obtain the same result from different realizations or measurements. In this work, we impose additional assumptions to define an appropriate constant of motion to construct another version of an equilibrium state for the overall evolution, including the effects of the anomalous potential $\mathbf{V}_\omega(t)$.

B. Equilibrium state

We denote by $\mathbb{E}_\omega(X_\omega) := \int_\Omega X_\omega d\mu(\omega)$ the expectation or ω average of random variable X_ω with respect to the measure μ on the probability space (Ω,μ). In a physical sense, this corresponds to taking the average value of X over all possible realizations of noisy environments. To construct an appropriate equilibrium state, we assume that

$$\mathbf{V} := \mathbb{E}_\omega[\mathbf{V}_\omega(t)] \text{ is constant in time.} \tag{3}$$

From the condition (3), we find that $\mathbf{H}_0$ and $\mathbf{V}$ are time-independent and are also constants of motion. Thus, the equilibrium state in this case, called the *adjusted equilibrium state*, can be written as

$$\sigma'_\beta = \frac{e^{-\beta(\mathbf{H}_0+\nu\mathbf{V})}}{\mathrm{Tr}(e^{-\beta(\mathbf{H}_0+\nu\mathbf{V})})}, \tag{4}$$

where β and ν are Lagrange multipliers, as formulated in Ref. [27]. Without loss of generality, we set $\nu = 1$ by absorbing the scaling into the random part of the Hamiltonian. Note that the parameter β must be equal to the inverse temperature of the bath when $\mathbf{V}_\omega(t) = 0$ for all time t.

Moreover, by employing the equivalence between the Schrödinger and Heisenberg pictures, for an evolution of the operator $\mathbf{A} \mapsto \mathbf{A}(t)$ and its dual evolution for a state $\rho \mapsto \rho(t)$, one obtains

$$\langle\mathbf{A}\rangle_{\rho(t)} = \mathrm{Tr}[\rho(t)\mathbf{A}] = \mathrm{Tr}[\rho\mathbf{A}(t)] = \langle\mathbf{A}(t)\rangle_\rho. \tag{5}$$

Exact forms of the evolution maps will be discussed in the following subsection.

C. Dynamics of operators and states

For a fixed configuration ω, the dynamics of the system in this specific realization is well-defined formally since $v_\omega(t)$ is assumed to be a smooth function. The evolution of an observable operator $\mathbf{A}$ and its dual dynamics, respectively, are

$$\frac{d}{dt}\mathbf{A}_\omega(t) = i\mathcal{L}_\omega^t[\mathbf{A}_\omega(t)] := i[\mathbf{H}_\omega,\mathbf{A}_\omega(t)], \tag{6}$$

$$\frac{d}{dt}\rho_\omega(t) = -i\mathcal{L}_\omega^t[\rho_\omega(t)] = -i[\mathbf{H}_\omega,\rho_\omega(t)]. \tag{7}$$

Formally, the evolution can take the form

$$\mathbf{U}_\omega(t,t') = \mathcal{T}\exp\left(-i\int_{t'}^{t}\mathbf{H}_\omega(\tau)d\tau\right),$$

where $\mathcal{T}$ is a time-ordering operator, with its reverse time-ordering operator denoted by $\overline{\mathcal{T}}$ [29]; here, we set $\mathbf{U}_\omega(t,0) := \mathbf{U}_\omega(t)$ for simplicity. Similarly, we also define the dynamics generated by the *mean* Hamiltonian $\mathbf{H} = \mathbf{H}_0 + \mathbf{V}$. The mean dynamics of the operators $\mathbf{A}$ and ρ can be obtained by taking the averages of Eqs. (6) and (7) over all configurations. This yields

$$\frac{d}{dt}\mathbf{A}(t) = i[\mathbf{H},\mathbf{A}(t)] + i\mathcal{C}_t(\mathbf{H},\mathbf{A})^\dagger, \tag{8}$$

$$\frac{d}{dt}\rho(t) = -i[\mathbf{H},\rho(t)] - i\mathcal{C}_t(\mathbf{H},\rho), \tag{9}$$

where $\mathbf{A}(t)$ and $\rho(t)$ denote the ω average of the solutions $\mathbf{A}_\omega(t)$ and $\rho_\omega(t)$ in Eqs. (6) and (7), respectively, and

$$\mathcal{C}_t(\mathbf{H},\cdot) := \mathbb{E}_\omega([\delta\mathbf{H}_\omega(t),\mathbf{U}_\omega(t)\cdot\mathbf{U}_\omega^\dagger(t)]) \tag{10}$$

with $\delta\mathbf{H}_\omega(t) := \mathbf{H}_\omega(t) - \mathbf{H}$. Note that $\mathcal{C}_t(\mathbf{H},\cdot)$ is a nonhomogeneous contribution from the mean deviation of the configurations about the mean Hamiltonian $\mathbf{H}$. We remark that Eq. (9) has a formal solution,

$$\rho(t) = e^{-it\mathcal{L}}\rho(0) + \eta_\rho(t), \tag{11}$$

where

$$\eta_\rho(t) := i\int_0^t e^{-i(t-s)\mathcal{L}}\mathcal{C}_s(\mathbf{H},\rho)ds. \tag{12}$$

One can see that, from Eq. (10), $\mathcal{C}_t(\mathbf{H},\cdot)$ takes an argument as an initial observable operator in the Heisenberg picture or an initial state in the Schrödinger picture; see the discussion in Sec. IV A. Moreover, from Eq. (9), one can see that the term $\mathcal{C}_t(\mathbf{H},\rho) = \mathcal{C}_t(\mathbf{V},\rho)$ contains information on the dependence between the Hamiltonian and the density operator or the state. In particular, $\mathcal{C}_t(\mathbf{H},\cdot)$ vanishes when $\delta\mathbf{H}_\omega(t)$ commutes with $\mathbf{A}_\omega(t)$ and $\rho_\omega(t)$ at any time t.

III. MODIFIED KUBO FORMULA AND FLUCTUATION-DISSIPATION RELATION

After construction of the model and derivation of the mean dynamics, we consider a linear-response theory and apply the obtained mean dynamics to explore the effects of the randomness that is contained in the nonhomogeneous term in Eq. (9). Our analysis follows a similar procedure to that in Ref. [30] and the original linear-response formalism of Kubo [2]; see Sec. III A. Ultimately, we will show that the contribution from the randomness of the composite system, as an accumulation of the propagation of the nonhomogeneous (noisy) term in the mean dynamics, will result in the modified Kubo formula and the FDR in Sec. III B. Finally, a limiting condition to obtain the standard Kubo formula is given, and the same restriction will be applied in order to obtain the modified FDR, which is expressed in a frequency representation of the response function.

A. Effects from the bath

From Eq. (9), we obtain an ensemble average of a physical quantity corresponding to the operator $\mathbf{A}$. By employing the equivalence between the Heisenberg and Schrödinger pictures, we need to investigate only the dynamics of the state ρ. Henceforth, we will consider the linear-response formulation as defined in Ref. [2] to find the behaviors of the system when it is in weak contact with a bath. First, we define a small interaction term with the bath as

$$\mathcal{L}_I^t(\cdot) := [\mathbf{B},\cdot]h_{\mathbf{B}}(t), \tag{13}$$

where $\mathbf{B}$ is an operator representing the effects from the bath, and $h_{\mathbf{B}}$ is its corresponding c number. Adding this term to Eq. (9) leads to a perturbed dynamics,

$$\frac{d}{dt}\rho(t) = -i\big(\mathcal{L} - \mathcal{L}_I^t\big)\rho(t) - i\mathcal{C}_t(\mathbf{H},\rho), \tag{14}$$

where $\mathcal{L}$ is the Liouville operator corresponding to the mean Hamiltonian $\mathbf{H}$. Equation (14) admits a formal solution that can be written as

$$\rho(t) = e^{-it\mathcal{L}}\rho(0) + i\int_0^t e^{-i(t-s)\mathcal{L}}\mathcal{L}_I^s\rho(s)ds + \left[\eta_\rho(t) + i\int_0^t e^{-i(t-s)\mathcal{L}}\mathcal{L}_I^s\eta_\rho(s)ds\right] + O\big(h_{\mathbf{B}}^2\big). \tag{15}$$

In the case in which the initial state $\rho(0)$ is an adjusted equilibrium state σ'_β, it follows that $e^{-it\mathcal{L}}\sigma'_\beta = \sigma'_\beta$. Combining Eqs. (5) and (15) and performing an iteration to calculate the average of the observable $\mathbf{A}$, we obtain

$$\begin{aligned}\langle\mathbf{A}(t)\rangle_\rho &= \langle\mathbf{A}\rangle_{\sigma'_\beta} + i\int_0^t[\mathrm{Tr}(\sigma'_\beta[\mathbf{A}(t),\mathbf{B}(s)])h_{\mathbf{B}}(s)]ds\\ &\quad + \mathrm{Tr}\left[\eta_{\sigma'_\beta}(t)\mathbf{A} + i\int_0^t e^{-i(t-s)\mathcal{L}}\mathcal{L}_I^s\eta_{\sigma'_\beta}(s)\mathbf{A}ds\right]\\ &\quad + O\big(h_{\mathbf{B}}^2\big).\end{aligned} \tag{16}$$

From the expression above, one can see that an average value of a physical quantity is deviated not only by perturbation from a bath (the second term on the right-hand side), but also by the nonhomogeneous term $\eta_{\sigma'_\beta}(t)$ in the third term and coupling between the bath and random effects in the fourth term. In the sense that the bath is a measurement probe, a linear response that is related to a measured quantity will be deviated by those effects. We will discuss this interesting point in more detail in Sec. IV A.

B. Modified Kubo formula and fluctuation-dissipation relation

Now we consider a linear-response function, which is defined by

$$\chi_{\mathbf{AB}}(t,t') = \left.\frac{\partial\langle\mathbf{A}(t)\rangle_\rho}{\partial h_{\mathbf{B}}(t')}\right|_{h_{\mathbf{B}}=0}. \tag{17}$$

Then we obtain from Eq. (16), for $0 \leqslant t' \leqslant t$, that

$$\chi_{\mathbf{AB}}(t,t') = 2i\theta(t-t')[\mathrm{Tr}(\sigma'_\beta[\mathbf{A}(t),\mathbf{B}(t')]) + \Delta_{\mathbf{AB}}(t,t')], \tag{18}$$

where

$$\Delta_{\mathbf{AB}}(t,t') := \frac{1}{2}\mathrm{Tr}\left[\left(\int_0^{t'} e^{-i(t-t')\mathcal{L}}[\mathbf{B},e^{-i(t'-s)\mathcal{L}}\mathcal{C}_s(\mathbf{H},\rho)]ds\right)\mathbf{A}\right], \tag{19}$$

and $\theta(t)$ is a Heaviside function defined by $\theta(t) = 1$ for $t \geqslant 0$ and $\theta(t) = 0$ for $t < 0$.

In a physical sense, the term $\mathrm{Tr}(\sigma'_\beta[\mathbf{A}(t),\mathbf{B}(t')])$ can be related to an antisymmetric correlation [4], where the correlation is usually defined as a two-epoch time correlation function between operators $\mathbf{A}$ and $\mathbf{B}$ in a given state. In this case,

$$C_{\mathbf{AB}}(t,t') := \langle \mathbf{A}(t)\mathbf{B}(t')\rangle_{\sigma'_\beta}. \tag{20}$$

One can then define symmetric and antisymmetric correlations, respectively, by

$$C^-_{\mathbf{AB}}(t,t') := \langle [\mathbf{A}(t),\mathbf{B}(t')]\rangle_{\sigma'_\beta}, \tag{21}$$

$$C^+_{\mathbf{AB}}(t,t') := \langle \{\mathbf{A}(t),\mathbf{B}(t')\}\rangle_{\sigma'_\beta}, \tag{22}$$

where $\{\mathbf{A},\mathbf{B}\} := \mathbf{AB} + \mathbf{BA}$. Thus, the modified form of the Kubo formula can be written as

$$\chi_{\mathbf{AB}}(t,t') = 2i\theta(t-t')[C^-_{\mathbf{AB}}(t,t') + \Delta_{\mathbf{AB}}(t,t')]. \tag{23}$$

We remark that, from a typical setup of a linear response, $h_{\mathbf{B}}(t)$ is set to be zero for $t < t'$ and then turned on at t' to preserve the causality of the measurement, i.e., the effect from the probe cannot influence the system before they are in contact at the time $t = t'$ [30,31]. In other words, from Eq. (19), it can be said that the system is in an adjusted equilibrium state at the initial time $t = 0$ and evolves until $t = t'$. Then, it makes weak contact with the bath, and they evolve together until the present time t. All relevant information on the evolution of the system and of the concerned operators is therefore contained in Eq. (23).

Now consider the conditions to obtain the standard FDR from Eq. (23). Using the shorthand notation $(t,t') \to (t)$ when $t' = 0$, so that $C_{\mathbf{AB}}(t,t') \to C_{\mathbf{AB}}(t)$, we obtain

$$C_{\mathbf{AB}}(t) = \mathrm{Tr}[\sigma'_\beta \mathbf{A}(t)\mathbf{B}] = \frac{\mathrm{Tr}[\mathbf{U}(t)\mathbf{B}\mathbf{U}^\dagger(i\beta)\mathbf{U}^\dagger(t)\mathbf{A}]}{\mathrm{Tr}[\mathbf{U}(i\beta)]}, \tag{24}$$

or equivalently,

$$C_{\mathbf{AB}}(t) = C_{\mathbf{BA}}(-t-i\beta). \tag{25}$$

One can see that the relation above is another version of the Kubo-Martin-Schwinger (KMS) condition, and the evolution along imaginary time arises here. It is important to note that, in Eq. (24), the operator $\mathbf{A}(t)$ can be written as a Heisenberg operator $\mathbf{U}^\dagger(t)\mathbf{A}\mathbf{U}(t)$, where $\mathbf{U}(t) = e^{-it\mathbf{H}}$ is a unitary evolution generated by the mean Hamiltonian $\mathbf{H}$, because the contribution from $\eta_{\sigma'_\beta}(t')$ vanishes at $t' = 0$. Furthermore, one can verify that $\Delta_{\mathbf{AB}}(t) = 0$ [32], and Eq. (23) becomes

$$\chi_{\mathbf{AB}}(t) = 2i\theta(t)C^-_{\mathbf{AB}}(t). \tag{26}$$

To see the modification of FDR, we consider the Fourier transform of Eq. (26). Toward that end, we define the Fourier transform of an integrable function $g(t)$ as

$$\hat{g}(\lambda) \equiv \mathcal{F}[g(t)] := \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{-it\lambda}g(t)\,dt,$$

where λ is a real number. It can be verified that the complex conjugate of $C^-_{\mathbf{AB}}(t)$ is equal to $C^-_{\mathbf{AB}}(-t)$. Consequently, the imaginary part of the linear-response function $\hat{\chi}_{\mathbf{AB}}(\lambda)$ in the frequency domain can be written as

$$\mathrm{Im}\hat{\chi}_{\mathbf{AB}}(\lambda) = \hat{C}^-_{\mathbf{AB}}(\lambda) \tag{27}$$

$$= (1-e^{-\beta\lambda})\hat{C}_{\mathbf{AB}}(\lambda) \tag{28}$$

as a direct consequence of Eq. (25). Similarly, one finds that

$$\hat{C}^+_{\mathbf{AB}}(\lambda) = (1+e^{-\beta\lambda})\hat{C}_{\mathbf{AB}}(\lambda). \tag{29}$$

Finally, we obtain

$$\mathrm{Im}\hat{\chi}_{\mathbf{AB}}(\lambda) = \tanh\left(\frac{\beta\lambda}{2}\right)\hat{C}^+_{\mathbf{AB}}(\lambda), \tag{30}$$

which corresponds to the power of energy dissipation as noted in Ref. [30]. The modified fluctuation-dissipation relation in Eq. (30) is structurally similar to the standard FDR given in Refs. [2,30] in the sense that it is extracted from a new Gibbs state, namely the adjusted equilibrium state σ'_β. However, we emphasize that only the average of the random potential affects the adjusted equilibrium state, resulting in the shifting of the measured energy. For the case $\mathbf{V} = \mathbf{0}$, despite having external random fluctuation, the adjusted equilibrium σ'_β coincides with σ_β, and Eq. (30) is exactly the standard FDR as expected.

IV. DISCUSSION

In this section, we will discuss our proposed model and its connection to the previous work in the literature. From our ideas of investigating a family of systems with random fluctuation, constructing an adjusted equilibrium state, and the mean dynamics, there are interesting results and tools to enable a better understanding of the dynamics out of equilibrium. The main topics for discussion are the consequences and interpretation of these ideas, especially the adjusted equilibrium, which is imperative in our derivations of the modified Kubo formula and the FDR. Also, a suggestion regarding an extension of this work from the viewpoint of stochastic path integrals and a brief discussion on the adiabaticity of the dynamics concerning the probability formulation are included at the end of this section.

A. Contribution from the random term

According to the derivation of the modified FDR in Sec. III B, it is advantageous to use the mean dynamics in Eq. (9), as this enables us to review a great deal of previous work regarding the modified FDR. For example, the correlation in the standard FDR is replaced by a composition of the former correlation, which involves the system's interaction with the bath, and another term that appears from the nonautonomous effects due to the random term. As is often suggested in the literature, the role of the latter term is to explain the behaviors of the considered system out of the equilibrium regime. One idea is that the extra contribution to the response function is due to the dynamical activity; the time-symmetric part of the action from the bath vanishes in equilibrium due to the causality argument (that is, the response must not occur before a measurement [33]). However, when the system is out of equilibrium or there are other parameters not considered, the dynamical activity seems to result in a certain amount of energy dissipation [23–25,34]. This has also been interpreted as the total entropy production from the dynamics, where the correlation term in the FDR is treated as the entropy production of the medium or the considered system analogous to S_0 [26,31].

In our case, the extra term arises from the presence of the nonhomogeneous term

$$\mathcal{C}_t(\mathbf{H},\rho) = \mathbb{E}_\omega([\delta \mathbf{H}_\omega(t),\rho_\omega(t)])$$

in the governing equation of the mean dynamics. One can see that it stores information on the external random potential at any time through which the system evolves. Recall Eq. (19),

$$\Delta_{\mathbf{AB}}(t,t') = \frac{1}{2}\mathrm{Tr}\left[\left(\int_0^{t'} e^{-i(t-t')\mathcal{L}}[\mathbf{B},e^{-i(t'-s)\mathcal{L}}\mathcal{C}_s(\mathbf{H},\rho)]ds\right)\mathbf{A}\right], \quad (31)$$

for the explicit form of the extra term in the Kubo formula. It can be seen that all actions along the dynamics are included in the expression at the time in which they act. There are two time evolutions therein. One evolves and accumulates the effects from the nonhomogeneous term $\mathcal{C}_s(\mathbf{H},\rho)$, interacting with a bath via the operator $\mathbf{B}$, from time s to the measurement time t'. The other evolution, i.e., $e^{-i(t-t')\mathcal{L}}$, causes the system and bath to evolve together until the final time t; see Fig. 1. Therefore, it reflects the memory effects of the whole evolution, equipped with the nonhomogeneous term from the random potential, resulting in the measured response function. In essence, the added random term disturbs the measured quantity, causing it to deviate from a modeled value in any experiment. Other than in the limit $t' \to 0$, taking the state to the adjusted equilibrium state at the measurement time, as shown in Eq. (26), the standard FDR in Eq. (30) is valid.

Furthermore, since the extra term $\Delta_{\mathbf{AB}}(t,t')$ appears in the Kubo formula as a deviation from an antisymmetric correlation that one can expect from the usual measurement process without a noisy environment, it can therefore quantify the degree of the deviation (violation) from the standard FDR.

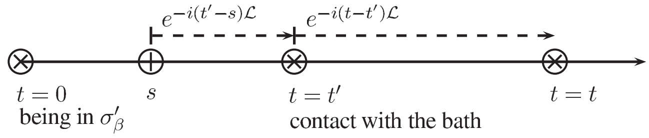

FIG. 1. Schematic illustration of the system's time evolution. The system is in the adjusted equilibrium σ'_β at time $t=0$, and it begins to contact with the bath at time $t=t'$. During time $0 \leqslant s \leqslant t'$, the system experiences random effects from the nonhomogeneous term that accumulate until time t'.

In this sense, the nonhomogeneous term $\mathcal{C}_t(\mathbf{H},\rho)$ plays an important role as it is the integrand for $\Delta_{\mathbf{AB}}(t,t')$. Simply speaking, the average deviation of random realizations affects the deviation of the modified FDR from the standard one.

B. Reference state

The crucial concern of this work, as already mentioned, is that the equilibrium state, which maximizes the von Neumann entropy, is not well-defined because of a lack of information over the entire time domain. Although the Gibbs state can be defined for the specific Hamiltonian at the specific time, the time dependence of the Hamiltonian results in ambiguity of the equilibrium state in the model since the Gibbs state defined here inherits the time dependence from the Hamiltonian. In other words, when the Hamiltonian changes, the preferred direction of the dynamics in the state space, which is expected to reach a state of maximum entropy, also changes. Thus, the equilibrium state in this sense depends on time and the dynamics as equilibration becomes questionable.

However, in the literature, this definition of the equilibrium state is still used for other proposes. For example, one can define an instantaneous equilibrium state, an accompanying state (in a closed system), or a poised state [35–38], each of which corresponds to the Hamiltonian at a specific time and for a specific configuration ω in our formulation, i.e., the Gibbs state of the form $\frac{e^{-\beta\mathbf{H}_\omega}}{\mathrm{Tr}(e^{-\beta\mathbf{H}_\omega})}$. From this point of view, the dynamics of the system can be viewed as a deviation of the trajectories of the states driven by the random and time-dependent dynamical equations from those of the accompanying state. Since the preferred direction of the dynamics changes with respect to the accompanying state, the deviation therefore involves the entropy production along the path dynamics [36]. In fact, the accompanying states do not constitute the reference states in the same manner as the attractors of the governing dynamics, but instead their trajectories can be viewed as attracting paths for the sake of maximizing entropy production.

Another advantage of using the accompanying state is well demonstrated in Ref. [38]. There is a formulation of the fluctuation relation of the nonautonomous Lindblad-like dynamics. In that work, the accompanying state, defined as an element in the kernel of the Lindblad-like generator, is proven to satisfy a modified dynamics given by another set of governing equations. After using perturbation, the fluctuation relation is derived in terms of the accompanying states and their time derivatives. Consequently, the standard FDR is recovered from the obtained fluctuation relation in the linear-response regime where the Lindblad-like generator is reduced to the time-independent Lindblad generator. [See Eqs. (21) and (39) and the subsequent discussion in Ref. [38].]

Unlike in Ref. [38], we consider the nonautonomous system governed by a family of Schrödinger-type or Liouville–von Neumann equations with random realizations of the potential. After determining the expectation over all the realizations to obtain the mean dynamics, the resulting equation is still nonautonomous, but the effects from the randomness are gathered in the nonhomogeneous term $\mathcal{C}_t(\mathbf{H},\rho)$. The ambiguity of the Gibbs state suggests that the definition of the external potential alone is inadequate to analyze the dynamics and the reference state. Therefore, we assume that the averaged energy taken over all realizations of the Hamiltonian is a constant of motion [39], so that we can construct a single adjusted equilibrium state, which is the Gibbs state of the mean Hamiltonian $\mathbf{H}$, as the reference state. It can be seen that the adjusted equilibrium state satisfies the definition of the accompanying state for the mean Hamiltonian. Ultimately, when the system is in weak contact with the bath, we obtain the modified Kubo formula in Eq. (23), which is reduced to the standard FDR in Eq. (30).

Indeed, it is shown that even when the time dependence is dropped for the mean Hamiltonian, making the homogeneous part time-independent, the violation of the standard FDR can be obtained from the random effects residing in the nonhomogeneous part of the mean dynamics. Moreover, the adjusted equilibrium state can well describe whether the violation of the standard FDR occurs and to what degree, as we already discussed following Eq. (23). This suggests that the adjusted equilibrium state is a good candidate for the reference state of the time-dependent dynamics with a time-independent energy.

C. Additional random potential as unobserved degrees of freedom

We revisit the model under consideration: $\mathbf{H}_\omega(t) = \mathbf{H}_0 + \mathbf{V}_\omega(t)$, where $\mathbf{H}_0$ is a constant (background) Hamiltonian and $\mathbf{V}_\omega(t)$ is a potential operator acting on a wave function φ by $\mathbf{V}_\omega(t)\varphi = v_\omega(t)\varphi$, where $v_\omega(t)$ is a random smooth function. The presence of the random external potential introduces unknown degrees of freedom. Unlike the bath or reservoir model, all dynamical properties of the external system S_ω, such as the relaxation time, the dimension, or the volume, are not specified in a way that enables the considered system S_0 to evolve to equilibrium. This idea is analogous to having unobserved degrees of freedom. A similar model was analyzed by Budini *et al.* in Ref. [40] to derive the non-Markovian master equation, which suggests that the presence of additional degrees of freedom, e.g., a random disturbance in the composite system, provides memory effects in the master equation [40].

In this work, we can see the inherited memory effects in Eq. (16) and its consequent Kubo formula in Eq. (23) when employing the time-dependent random potential instead of using the Hermitian operators to capture the unobserved degrees of freedom associated with the system with random coupling, as was done in Ref. [40]. Indeed, one can formulate a similar scheme by setting $\mathbf{V}_\omega(t) = \lambda_\omega \mathbf{Q}$, where $\mathbf{Q}$ is a Hermitian operator and λ_ω is a random real number representing the coupling constant, and by using the non-Markovian master equation instead of Eq. (9). In our case, it can be seen that the potential can be reduced to being time-independent, and the adjusted equilibrium state can be defined because the average over all the realizations of the Hamiltonian yields a constant of motion.

D. Nonhomogeneous part as a generator of random dynamics

Now we introduce a possible extension of our formulation. Since the commutator obeys the Lie structure, the term $\mathcal{C}_t(\mathbf{H},\cdot)$ can be analyzed as a Lie derivative. Then, the deviated Hamiltonian $\delta\mathbf{H}_\omega(t) := \mathbf{H}_\omega(t) - \mathbf{H}$ appearing in $\mathcal{C}_t(\mathbf{H},\cdot)$ will generate another dynamics, and its derivative represents changes of a physical quantity related to randomness. For example, for a particular realization ω, let us consider

$$[\delta\mathbf{H}_\omega(t),\cdot]$$

as an operator on Hilbert space. For definiteness, let $\mathcal{B}_0(\mathcal{H})$ denote an algebra of all bounded operators on $\mathcal{H}$ together with the Hilbert-Schmidt inner product $(\mathbf{A},\mathbf{B}) = \mathrm{Tr}[\mathbf{A}^\dagger\mathbf{B}]$. In this sense, the set of trace class operators $\mathcal{B}_1(\mathcal{H}) := \{\mathbf{A} \in \mathcal{B}(\mathcal{H}) : \mathrm{Tr}(\mathbf{A}) < \infty\}$ forms a separable Hilbert space $\breve{\mathcal{H}}$ ([41], p. 33), and any density operator ρ can be viewed as a vector in $\breve{\mathcal{H}}$. Then $[\delta\mathbf{H}_\omega(t),\cdot]$ defines an action on $\breve{\mathcal{H}}$ denoted by $\mathcal{R}_\omega(\cdot) := i[\delta\mathbf{H}_\omega(t),\cdot]$, so that

$$(\rho,\mathcal{R}_\omega(\rho)) = i\,\mathrm{Tr}(\rho[\delta\mathbf{H}_\omega(t),\rho]) = 0$$

following the cyclic invariance of the trace function. By the Lumer-Phillips theorem, the operator $\mathcal{R}_\omega(\cdot)$ is dissipative and can be a generator of a contraction semigroup on $\breve{\mathcal{H}}$ (Theorem 2.5 in [42]). However, the semigroup given here is determined up to a configuration ω, as is a dynamical parameter (denoted by τ_ω) of the evolution. Therefore,

$$\frac{\partial\rho}{\partial\tau_\omega} = \mathcal{R}_\omega(\rho), \tag{32}$$

yielding another governing equation for the density operator ρ. In the case of a countable number of configurations, Eqs. (8) and (9) become a multidimensional problem in parameters. When the number of configurations is uncountable, the description of the problem in this direction can be considered as a version of the path integral or stochastic dynamics, whose derivations can potentially be used to investigate the dynamics of dissipative systems.

E. Adiabaticity of dynamics

There remain interesting topics concerning the adiabatic property of the dynamics which can simply be quantified by the entropy function $S(\rho) := -\mathrm{Tr}(\rho\ln\rho)$. First of all, let us consider the case $\mathcal{C}_t(\mathbf{H},\rho) = 0$, which occurs, for instance, when the random fluctuation is absent. Thus, only the effect from the bath contributes to the entropy production. With perturbation from the bath, the entropy production can be expressed as [43]

$$Ent_{\mathbf{B}}(t) := -i\beta h_{\mathbf{B}}(t)\mathrm{Tr}\{\rho(t)[\mathbf{H},\mathbf{B}]\}, \tag{33}$$

where the reference state is chosen to be the adjusted equilibrium state σ'_β. Because the entropy production above is of linear order of $h_{\mathbf{B}}$, the evolution is still close to the adiabatic regime where the entropy production is identically zero. On the contrary, for the case $\mathcal{C}_t(\mathbf{H},\rho) \neq 0$, the evolution map corresponding to Eq. (9) may not admit group or even semi-group properties in general. The definition of entropy production in Eq. (33) is therefore not well-defined for this case, and one can expect nonadiabatic effects in some situations.

Although the exact form of the entropy production becomes more complicated for the mean dynamics due to the fact that it is out of equilibrium, we can show that the entropy production in our case is increasing with time. To demonstrate this point, consider again Eq. (7). Because the entropy function is concave and invariant under a unitary transformation [28], it follows that

$$S[\rho(t)] = S\{\mathbb{E}_\omega[\rho_\omega(t)]\} \geqslant \mathbb{E}_\omega\{S[\rho_\omega(t)]\}$$
$$= \mathbb{E}_\omega\{S[\rho(0)]\} = S[\rho(0)].$$

Hence, the difference of the entropy $S[\rho(t)] - S[\rho(0)]$, treated as the overall entropy production along the dynamics up to time t, is non-negative. In particular, the equality holds for the δ distribution (a single path with probability 1) or when the entropy function is linear. Since the entropy function is nonlinear and usually the distribution over the configuration space is non-δ, the overall entropy production is strictly positive, yielding that the mean dynamics is strictly nonadiabatic.

Apart from the mean dynamics, the evolution of the system is unitary for a specific realization ω, and the entropy is unchanged. However, when one cannot know exactly in which state the system lies, i.e., when one cannot know exactly the equation of the dynamics by which the system is governed, the unknown random potential will affect the dynamics, and the mean dynamics is preferred. For example, an experimenter can do a number of measurements in which each one is significantly different from the rest since they are governed by different Hamiltonians resulting from random effects. One can say that the average of the measurements will reflect the information on the mean Hamiltonian, and the random contribution will appear in the modified Kubo formula.

V. CONCLUSION

In conclusion, we consider a family of Liouville–von Neumann equations indexed by configurations in a probability space to represent a system inheriting random fluctuation. By taking the average over all random realizations, the mean dynamics is obtained as another Liouville–von Neumann equation but with a nonhomogeneous term. The homogeneous term is consistent with the mean behavior of all realizations, while the nonhomogeneous one corresponds to the effects of the noisy environment. Under the condition that the average of the Hamiltonians over all realizations, called the mean Hamiltonian, is constant in time, we can construct a suitable reference state, called the adjusted equilibrium state, which is simply the Gibbs state for the mean Hamiltonian. After the system is in contact with a bath and a perturbation is taken in a linear order, we obtain a linear-response function, and consequently the modified Kubo formula and the FDR, with two contributions from different causes. One is an antisymmetric cross correlation between two observables expected from the contact with the bath, while the other arises from the existence of randomness. The latter can be expressed as an accumulation of the nonhomogeneous term in the governing equation of the mean dynamics, signaling the propagation of a noisy environment and interacting with the cross correlation at later times. Furthermore, we find that the modified Kubo formula yields the modified FDR in the case in which the probe contacts the system when the latter has not yet reached an equilibrium state, but instead is in an adjusted equilibrium state. When random fluctuation is absent, the standard FDR and Kubo formula are recovered as expected.

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