frontiers in Physics

ORIGINAL RESEARCH
published: 15 October 2020
doi: 10.3389/fphy.2020.567523

Generalized Fluctuation-Dissipation Theorem for Non-equilibrium Spatially Extended Systems

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The fluctuation-dissipation theorem (FDT) connecting the response of the system to external perturbations with the fluctuations at thermodynamic equilibrium is a central result in statistical physics. There has been effort devoted to extending the FDT in several different directions since its original formulation. In this work we establish a generalized form of the FDT for spatially extended non-equilibrium stochastic systems described by continuous fields. The generalized FDT is formulated with the aid of the non-equilibrium force decomposition in the potential landscape and flux field theoretical framework. The general results are substantiated in the setting of the Ornstein-Uhlenbeck (OU) process and further illustrated by a more specific example worked out in detail. The key feature of this generalized FDT for non-equilibrium spatially extended systems is that it represents a ternary relation rather than a binary relation as the FDT for equilibrium systems does. In addition to the response function and the time derivative of the field-field correlation function that are present in the equilibrium FDT, the field-flux correlation function also enters the generalized FDT. This additional contribution originates from detailed balance breaking that signifies the non-equilibrium irreversible nature of the steady state. In the special case when the steady state is an equilibrium state obeying detailed balance, the field-flux correlation function vanishes and the ternary relation in the generalized FDT reduces to the binary relation in the equilibrium FDT.

Keywords: fluctuation-dissipation theorem, spatially extended system, stochastic field equation, non-equilibrium steady state, non-equilibrium force decomposition

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Specialty section:
This article was submitted to Interdisciplinary Physics, a section of the journal Frontiers in Physics

Received: *29 May 2020*
Accepted: *26 August 2020*
Published: *15 October 2020*

Citation:
Wu W and Wang J (2020) Generalized Fluctuation-Dissipation Theorem for Non-equilibrium Spatially Extended Systems. Front. Phys. 8:567523. doi: 10.3389/fphy.2020.567523

1. INTRODUCTION

The fluctuation-dissipation theorem (FDT) is a cornerstone in equilibrium statistical physics, which establishes a connection between the response of the system to external perturbations and the correlation of fluctuations at thermodynamic equilibrium [1]. Thus it is a very useful tool for investigating the properties of the system at thermodynamic equilibrium. Since its first derivation from fundamental postulates [2], important progress has been made in testing the boundary of its range of applications [3–5] and finding possible directions of extension [6–16]. Much effort has been devoted to the study of the violation of the FDT in systems out of equilibrium, for instance, in glassy systems [3], granular matter [4] and colloidal suspensions [5]. There has been growing interest in recent years to construct modified forms of the FDT beyond its original range of applications [6–16]. Deviations of the form of the FDT in out-of-equilibrium systems from the equilibrium FDT have been investigated [6–9]. Effort has also been directed to modifying the forms of the FDT around non-equilibrium steady states [10–15]. Restoring equilibrium forms of the FDT in non-equilibrium regimes has also attracted much attention [10, 12]. Study also been carried out to generalize the FDT to non-stationary states and other directions [16]. The logic behind the equilibrium FDT based on a stochastic approach and the reason for its violation due to detailed balance breaking in non-equilibrium systems will be clarified in section 2.3.

In this work we study the FDT for non-equilibrium spatially extended systems governed by stochastic field equations. Spatially extended systems are systems with a large number of degrees of freedom distributed across space, so that spatial extension (spatial distribution or spatial inhomogeneity) plays an important role in the behavior, function and dynamics of the system. Spatially extended systems are ubiquitous in the natural and the human world. Many physical, chemical and biological systems are spatially distributed and spatial inhomogeneity is an important factor in the system dynamics. Examples of spatially extended systems with the spatial-temporal dynamics of self-organization and pattern formation include the growing interface described by the Kardar-Parisi-Zhang (KPZ) equation [17], the Turing pattern in chemical morphogenesis [18], the Rayleigh-Bénard convection in fluids [19], Drosophila embryo differentiation in developmental biology [20], and plant distribution dynamics in ecological systems [21]. At the macroscopic scale, the spatially extended system can usually be characterized by continuous fields, with the granularity of its components ignored. The deterministic dynamics of a large class of spatially extended systems with local interactions can be studied in terms of partial differential equations (PDEs). Non-local interactions are also possible in the non-relativistic physics of spatially extended systems, which are typically described by integro-differential equations. Peridynamics as a non-local theory of continuum mechanics is an example of this type of dynamics that has become popular in recent years [22]. In a noisy world, stochastic fluctuations with internal or external origins are unavoidable. There are many situations in which the roles of noise on the dynamics of spatially extended systems cannot be ignored, necessitating a stochastic description of the system dynamics [23–27]. Stochastic partial-differential equations (SPDEs) are a common tool for studying the stochastic dynamics of spatially extended system with local interactions [24, 25]. More generally, spatially extended systems with local or non-local interactions under the influence of stochastic fluctuations can be described by stochastic field equations in the form of stochastic differential equations in infinite-dimensional spaces [23, 27], with SPDEs included as an important special class. Alternatively, master equations have also been employed to investigate the stochastic dynamics of spatially extended systems [25, 26]. Furthermore, open systems (including open spatially extended systems) that constantly exchange matter, energy or information with the environments can sustain non-equilibrium steady states that break detailed balance and time reversal symmetry [25, 28–30]. Systems with non-equilibrium steady states have been an active research area in recent years [31–36]. Much effort has been devoted to the development of non-equilibrium thermodynamics based on Markovian stochastic dynamics described by Langevin equations, Fokker-Planck equations and master equations [29–36]. Spatially extended systems capable of sustaining non-equilibrium steady states typically exhibit spatial-temporal dynamics of pattern formation and self-organization [17–21]. Field-theoretic techniques [37] and approaches based on the non-equilibrium potential landscape [26, 27, 38, 39], among others, have been utilized to study the non-equilibrium dynamics of spatially extended systems.

The formulation of the FDT for spatially extended stochastic systems with non-equilibrium steady states are complicated by several factors. Spatially extended systems have many degrees of freedom and much more complicated spatial-temporal dynamics compared to spatially homogeneous systems. Study of these types of systems typically requires field-theoretic descriptions. The stochastic nature of the system dynamics arising from intrinsic or external fluctuations also adds to the difficulty in the description and investigation of the property and dynamics of the system. Furthermore, spatially extended systems sustaining non-equilibrium steady states have an intrinsic non-equilibrium nature signified by the violation of detailed balance and time reversal symmetry, which makes them even more difficult to handle than equilibrium systems obeying detailed balance and time reversal symmetry. Therefore, it is a challenging task to develop a reasonably general formulation of the FDT for spatially extended systems with an intrinsic non-equilibrium nature governed by stochastic field dynamics.

The objective of the present work is to establish such a reasonably general formulation of the FDT for spatially extended non-equilibrium stochastic systems in such a way that, on the one hand, the formulated FDT highlights its qualitative distinction from the equilibrium FDT due to the non-equilibrium nature of the steady state, and on the other hand, its connection to the equilibrium FDT is as transparent as possible. This objective is achieved with the help of the non-equilibrium force decomposition in the potential landscape and flux field theoretical framework [26, 27, 33, 36, 40]. The non-equilibrium force decomposition relates the driving force of the system to the defining characteristics of non-equilibrium steady states [33], which plays an important role in the study of the global dynamics and non-equilibrium thermodynamics of spatially extended stochastic systems in the context of this theoretical framework [27, 36]. Its extension into the concept of non-equilibrium trinity offered some fresh insights into the turbulence dynamics [40]. In this work it also facilitates the formulation of the generalized FDT. We first formulate the generalized FDT in the general setting of spatially extended systems governed by stochastic field equations. Then we substantiate the general formulation in the more special setting of the Ornstein-Uhlenbeck (OU) process for spatially extended systems, and further study in detail a more specific example based on a modified version of the stochastic cable equation (SCE) [41] to illustrate the general results.

The form of the generalized FDT obtained in this work has a structure that is qualitatively different from the FDT for equilibrium spatially extended systems. Yet its connection to the equilibrium FDT is also transparent. In addition to the response function and the time derivative of the field-field correlation function, which are exactly the two quantities related by the FDT for equilibrium spatially extended systems, there is an additional quantity, the field-flux correlation function, which enters the generalized FDT and transforms it into a ternary relation. The additional contribution of the field-flux correlation function arises from detailed balance breaking that characterizes the non-equilibrium nature of the steady state without time reversal symmetry. For equilibrium systems obeying detailed balance this additional contribution vanishes and the generalized FDT reduces to the usual equilibrium FDT.

The rest of this article is organized as follows. In section 2, we develop the generalized FDT for spatially extended systems in a general setting within the context of the potential landscape and flux field theoretical framework. Then we demonstrate and verify the generalized FDT for a class of spatially extended systems described by the OU Process in section 3. A more specific spatially extended system governed by a modified version of the SCE is studied in detail in section 4 to further illustrate the generalized FDT. Finally, the conclusion is given in section 5.

2. GENERAL FORMULATION OF THE GENERALIZED FDT

In this section, we formulate the generalized FDT for stochastic spatially extended systems in a general setting. We first set up the background by introducing the field dynamical equation and the functional Fokker-Planck equation (FFPE). Then we briefly present the potential landscape and flux field framework, with an emphasis on the non-equilibrium force decomposition that will be used to formulate the generalized FDT. After that the generalized FDT is established step by step by putting together the various ingredients needed for the formulation, namely the time-dependent perturbation, the linear response function, and the correlation function. We end this section with discussions on the physical meaning and the implications of the generalized FDT.

2.1. Field Dynamical Equation

Consider a general spatially extended system, with its state at time t described by the continuous vector field $\boldsymbol{\phi}(\mathbf{x},t) = (\phi_1(\mathbf{x},t),\cdots,\phi_i(\mathbf{x},t),\cdots,\phi_n(\mathbf{x},t))$. If there is only one component, then the vector field reduces to a scalar field. We focus on fields that are even variables (i.e., do not change sign) under time reversal. Examples of such even-variable fields include the height field of the growing interface in the KPZ equation [17], the concentration field of a chemical substance in the Turing pattern [18], the population density field of a biological species [21], and the electric potential field on a neuron fiber [41]. The velocity field as in the Rayleigh-Bénard convection [19] is an example of an odd-variable field that changes sign under time reversal. The state space (or phase space) of the spatially extended system is an infinite-dimensional function space, consisting of the field configurations that may be subject to certain boundary conditions or other technical requirements [23]. Each field configuration (the field $\boldsymbol{\phi}(\mathbf{x})$ in this entirety) represents a "point" in this infinite-dimensional state space.

From the dynamical system perspective, the autonomous deterministic dynamics of the spatially extended system takes place in the infinite-dimensional state space, which, in general, can be described by the deterministic field dynamical equation

$$\partial_t \boldsymbol{\phi}(\mathbf{x},t) = \mathbf{F}(\mathbf{x})[\boldsymbol{\phi}], \tag{1}$$

where $\mathbf{F}(\mathbf{x})[\boldsymbol{\phi}]$, short for $\mathbf{F}(\mathbf{x})[\boldsymbol{\phi}(\mathbf{y},t)]$, is the deterministic driving force governing the deterministic dynamics of the spatially extended system. The notation $[\boldsymbol{\phi}]$ represents functional dependence (i.e., dependence on the field configuration as a whole) and $(\mathbf{x})$ denotes spatial dependence. Mathematically, $\mathbf{F}(\mathbf{x})[\boldsymbol{\phi}(\mathbf{y},t)]$ is a vector-field-valued functional, which takes in the state of the system at time t described by the vector field $\boldsymbol{\phi}(\mathbf{y},t)$ as a whole, and spits out another vector field $\mathbf{F}(\mathbf{x})$ that determines the time rate of change of the state of the system at time t, i.e., $\partial_t\boldsymbol{\phi}(\mathbf{x},t)$. Equation (1) is an extension of the deterministic dynamics of dynamical systems with a finite-dimensional state space, and it represents a very general formulation of the deterministic dynamics of spatially extended systems with an infinite-dimensional state space. (In accord with $\boldsymbol{\phi}(\mathbf{x})$, we assume $\mathbf{F}(\mathbf{x})$ to be even variables under time reversal, though.) PDEs modeling the deterministic dynamics of spatially extended systems with local interactions are an important class of the dynamics in Equation (1). In this case, the vector field $\mathbf{F}(\mathbf{x})$ is determined by the vector field $\boldsymbol{\phi}(\mathbf{y},t)$ with $\mathbf{y}$ limited to the vicinity of $\mathbf{x}$, so that $\mathbf{F}(\mathbf{x})[\boldsymbol{\phi}(\mathbf{y},t)] = \mathbf{F}(\boldsymbol{\phi}(\mathbf{x},t),\nabla\boldsymbol{\phi}(\mathbf{x},t),\nabla\nabla\boldsymbol{\phi}(\mathbf{x},t),\cdots,\nabla^k\boldsymbol{\phi}(\mathbf{x},t))$, where k indicates the highest order of the differential operator. For instance, in the case of the diffusion equation $\partial_t\boldsymbol{\phi}(\mathbf{x},t) = D\nabla^2\boldsymbol{\phi}(\mathbf{x},t)$, $\mathbf{F}(\mathbf{x})[\boldsymbol{\phi}] = D\nabla^2\boldsymbol{\phi}(\mathbf{x},t)$ has the form of a differential operator (of second order) acting on the field. More generally, Equation (1) can also model the deterministic dynamics of spatially extended systems with non-local interactions by using a non-local functional $\mathbf{F}(\mathbf{x})[\boldsymbol{\phi}(\mathbf{y},t)]$, where the value of $\mathbf{F}(\mathbf{x})$ at $\mathbf{x}$ is not necessarily determined by $\boldsymbol{\phi}(\mathbf{y},t)$ at $\mathbf{y}$ near $\mathbf{x}$, but may depend on $\mathbf{y}$ that is far away from $\mathbf{x}$. A simple example of the non-local dynamics is of the form $\partial_t\boldsymbol{\phi}(\mathbf{x},t) = -\int \boldsymbol{\gamma}(\mathbf{x},\mathbf{y})\cdot\boldsymbol{\phi}(\mathbf{y},t)d\mathbf{y}$. In this case, $\mathbf{F}(\mathbf{x})[\boldsymbol{\phi}(\mathbf{y},t)] = -\int \boldsymbol{\gamma}(\mathbf{x},\mathbf{y})\cdot\boldsymbol{\phi}(\mathbf{y},t)d\mathbf{y}$ has the form of an integral operator acting on the field. This dynamics in general represents non-local interactions as the field at location $\mathbf{x}$ is instantaneously influenced by the field at another location $\mathbf{y}$ that may be far away from $\mathbf{x}$. The two examples given above are both linear dynamics. In general, the dynamics can also be non-linear in the field.

When stochastic fluctuations are important to the system dynamics, a stochastic description is required. We consider the stochastic dynamics of spatially extended systems that can be described by the following form of stochastic field equations [23, 25, 27, 36, 40]

$$\partial_t \boldsymbol{\phi}(\mathbf{x},t) = \mathbf{F}(\mathbf{x})[\boldsymbol{\phi}] + \boldsymbol{\zeta}(\mathbf{x},t), \tag{2}$$

where the stochastic driving force $\boldsymbol{\zeta}(\mathbf{x},t)$ is the space-dependent additive Gaussian white noise in time with zero mean,

$\langle \boldsymbol{\zeta}(\mathbf{x}, t) \rangle = \mathbf{0}$, and has the correlation

$$\langle \boldsymbol{\zeta}(\mathbf{x}, t)\boldsymbol{\zeta}(\mathbf{x}', t') \rangle = 2\mathbf{D}(\mathbf{x}, \mathbf{x}')\delta(t - t'). \tag{3}$$

In the above we used the dyadic notation in which the dyadic product $\mathbf{ab}$ of two vectors $\mathbf{a}$ and $\mathbf{b}$ returns a matrix with elements $[\mathbf{ab}]_{ij} = a_i b_j$. The spatial correlator $\mathbf{D}(\mathbf{x}, \mathbf{x}')$ characterizes the spatial correlation of the stochastic driving force $\boldsymbol{\zeta}(\mathbf{x}, t)$, which is assumed to be independent of the field $\boldsymbol{\phi}(\mathbf{x})$ (thus additive noise). By allowing $\mathbf{D}(\mathbf{x}, \mathbf{x}')$ to be generalized functions that include Dirac delta functions and its derivatives of various orders, the space-time Gaussian white noise, e.g., $\langle \boldsymbol{\zeta}(\mathbf{x}, t)\boldsymbol{\zeta}(\mathbf{x}', t') \rangle = 2\mathbf{D}(\mathbf{x})\delta(\mathbf{x} - \mathbf{x}')\delta(t - t')$, is contained in Equation (3) as an important class of stochastic driving forces with local correlations in space. In general, the form of Equation (3) allows the stochastic driving force to have non-local correlations in space. The KPZ equation, which is a non-linear SPDE [17], is a special example of the above stochastic field equation.

2.2. Functional Fokker-Planck Equation

The stochastic field equation in Equation (2) is a Langevin equation in the infinite-dimensional state space (the field configuration space). Its solution traces a stochastic trajectory in the state space. The evolution of the corresponding probability distribution in the state space is governed by the FFPE [24, 25, 27, 36, 40]

$$\begin{aligned} \partial_t P_t[\boldsymbol{\phi}] = &- \int d\mathbf{x}\, \delta_{\boldsymbol{\phi}(\mathbf{x})} \cdot \big(\mathbf{F}(\mathbf{x})[\boldsymbol{\phi}] P_t[\boldsymbol{\phi}]\big) \\ &+ \iint d\mathbf{x} d\mathbf{x}' \delta_{\boldsymbol{\phi}(\mathbf{x})} \cdot \mathbf{D}(\mathbf{x}, \mathbf{x}') \cdot \delta_{\boldsymbol{\phi}(\mathbf{x}')} P_t[\boldsymbol{\phi}], \end{aligned} \tag{4}$$

where $P_t[\boldsymbol{\phi}] \equiv P[\boldsymbol{\phi}, t]$ is the (transient) probability distribution functional and $\delta_{\boldsymbol{\phi}(\mathbf{x})} \equiv \delta/\delta\boldsymbol{\phi}(\mathbf{x})$ is the short notation for the vector-valued functional derivative. The FFPE is an extension of the Fokker-Planck equation (FPE) for systems with a finite-dimensional state space to spatially extended systems with an infinite-dimensional state space. The two terms on the right-hand side (RHS) of the FFPE represent the drift and the diffusion, respectively, in the state space. The drift vector is given by the deterministic driving force $\mathbf{F}(\mathbf{x})[\boldsymbol{\phi}]$ in the stochastic field equation, and the diffusion matrix $\mathbf{D}(\mathbf{x}, \mathbf{x}')$ is determined by the spatial correlator of the stochastic driving force.

The FFPE has the symbolic form

$$\partial_t P_t = L P_t, \tag{5}$$

where L is the generator of the probability evolution dynamics. It is an operator in the state space with the form

$$\begin{aligned} L = &- \int d\mathbf{x}\, \delta_{\boldsymbol{\phi}(\mathbf{x})} \cdot \mathbf{F}(\mathbf{x})[\boldsymbol{\phi}] \\ &+ \iint d\mathbf{x} d\mathbf{x}' \delta_{\boldsymbol{\phi}(\mathbf{x})} \cdot \mathbf{D}(\mathbf{x}, \mathbf{x}') \cdot \delta_{\boldsymbol{\phi}(\mathbf{x}')}. \end{aligned} \tag{6}$$

The operator L acts on functionals of the field in a way similar to that on the RHS of Equation (4). Its adjoint in the state space is given by

$$\begin{aligned} L^\dagger = &\int d\mathbf{x}\, \mathbf{F}(\mathbf{x})[\boldsymbol{\phi}] \cdot \delta_{\boldsymbol{\phi}(\mathbf{x})} \\ &+ \iint d\mathbf{x} d\mathbf{x}' \delta_{\boldsymbol{\phi}(\mathbf{x})} \cdot \mathbf{D}(\mathbf{x}, \mathbf{x}') \cdot \delta_{\boldsymbol{\phi}(\mathbf{x}')}. \end{aligned} \tag{7}$$

The FFPE can also be reformulated into a continuity equation in the state space

$$\partial_t P_t[\boldsymbol{\phi}] = - \int d\mathbf{x}\, \delta_{\boldsymbol{\phi}(\mathbf{x})} \cdot \mathbf{J}_t(\mathbf{x})[\boldsymbol{\phi}], \tag{8}$$

where $\mathbf{J}_t(\mathbf{x})[\boldsymbol{\phi}]$ is the probability flux field with the expression

$$\mathbf{J}_t(\mathbf{x})[\boldsymbol{\phi}] = \mathbf{F}(\mathbf{x})[\boldsymbol{\phi}] P_t[\boldsymbol{\phi}] - \int d\mathbf{x}'\, \mathbf{D}(\mathbf{x}, \mathbf{x}') \cdot \delta_{\boldsymbol{\phi}(\mathbf{x}')} P_t[\boldsymbol{\phi}]. \tag{9}$$

It is instructive to observe the time reversal property of the FFPE in the form of Equation (8). The left-hand side (LHS) of the equation changes sign when time is reversed since ∂_t changes sign while the probability density P_t does not. In contrast, the RHS of the equation does not change sign for even-variable systems considered in this work. Therefore, the time reversal symmetry of the FFPE is broken, except for the special case of a vanishing probability flux field.

2.3. Potential Landscape and Flux Field

Steady states that do not vary with time are of interest. Equilibrium steady states obey the detailed balance condition which characterizes the time reversal symmetry of the underlying dynamics. Open systems constantly exchanging matter, energy or information with the environments can sustain non-equilibrium steady states that break detailed balance and time reversal symmetry [31]. The presence of matter, energy or information flow is a distinguishing feature of non-equilibrium steady states, which is reflected on the dynamical level by the irreversible steady-state probability flux that signifies detailed balance breaking and time irreversibility in non-equilibrium steady states.

When the drift vector (the deterministic driving force) and the diffusion matrix (the correlator of the stochastic driving force) satisfy certain conditions, the FPE has a unique steady-state probability distribution completely determined by the drift vector and the diffusion matrix, which every initial probability distribution converges to in the long time limit [28]. (The conditions for the existence of such a steady-state probability distribution, however, is likely to be violated by glassy systems.) For the FFPE described by Equation (4), we assume that the conditions for the existence and uniqueness of the steady state are fulfilled. We denote the steady-state probability distribution functional as $P_s[\boldsymbol{\phi}]$.

Accordingly, the steady-state probability flux field reads

$$\mathbf{J}_s(\mathbf{x})[\boldsymbol{\phi}] = \mathbf{F}(\mathbf{x})[\boldsymbol{\phi}] P_s[\boldsymbol{\phi}] - \int d\mathbf{x}'\, \mathbf{D}(\mathbf{x}, \mathbf{x}') \cdot \delta_{\boldsymbol{\phi}(\mathbf{x}')} P_s[\boldsymbol{\phi}]. \tag{10}$$

As a result of the steady-state condition, $\partial_t P_s[\boldsymbol{\phi}] = 0$, the steady-state probability flux field satisfies the 'divergence-free' condition in the state space:

$$\int d\mathbf{x}\, \delta_{\boldsymbol{\phi}(\mathbf{x})} \cdot \mathbf{J}_s(\mathbf{x})[\boldsymbol{\phi}] = 0, \tag{11}$$

which means it is a solenoidal vector field in the state space. Non-vanishing $\mathbf{J}_s$ breaks the time reversal symmetry of the FFPE and is a signature of non-equilibrium steady states with time irreversibility.

For systems sustaining non-equilibrium steady states, according to Equation (10), the driving force has the following potential-flux decomposed form, referred to as the *non-equilibrium force decomposition* [27, 33, 36, 40]:

$$\mathbf{F}(\mathbf{x})[\boldsymbol{\phi}] = -\int d\mathbf{x}'\, \mathbf{D}(\mathbf{x}, \mathbf{x}') \cdot \delta_{\boldsymbol{\phi}(\mathbf{x}')} U[\boldsymbol{\phi}] + \mathbf{V}_s(\mathbf{x})[\boldsymbol{\phi}], \tag{12}$$

where $U[\boldsymbol{\phi}] = -\ln P_s[\boldsymbol{\phi}]$ is the potential landscape associated with the steady-state probability distribution functional, and $\mathbf{V}_s(\mathbf{x})[\boldsymbol{\phi}] = \mathbf{J}_s(\mathbf{x})[\boldsymbol{\phi}]/P_s[\boldsymbol{\phi}]$ is the steady-state probability flux velocity. Non-vanishing $\mathbf{V}_s(\mathbf{x})[\boldsymbol{\phi}]$ is also a signature of detailed balance breaking and time irreversibility in non-equilibrium steady states as $\mathbf{J}_s(\mathbf{x})[\boldsymbol{\phi}]$ is. For the special case of equilibrium systems with detailed balance, $\mathbf{V}_s(\mathbf{x})[\boldsymbol{\phi}]$ vanishes and, as a result, the driving force $\mathbf{F}(\mathbf{x})[\boldsymbol{\phi}]$ has the form, $\mathbf{F}(\mathbf{x})[\boldsymbol{\phi}] = -\int d\mathbf{x}'\, \mathbf{D}(\mathbf{x}, \mathbf{x}') \cdot \delta_{\boldsymbol{\phi}(\mathbf{x}')} U[\boldsymbol{\phi}]$, which is a generalized functional gradient of the potential landscape in the state space. This form that relates the potential landscape $U[\boldsymbol{\phi}]$ (the steady-state probability distribution $P_s[\boldsymbol{\phi}]$), the stochastic fluctuation characterized by the diffusion matrix $\mathbf{D}(\mathbf{x}, \mathbf{x}')$, and the irreversible dissipative driving force $\mathbf{F}(\mathbf{x})[\boldsymbol{\phi}]$ is the ultimate origin of the equilibrium FDT. However, this structure of the driving force is qualitatively changed by the presence of non-vanishing $\mathbf{V}_s(\mathbf{x})[\boldsymbol{\phi}]$ for systems sustaining non-equilibrium steady states that violate detailed balance and time reversal symmetry. As a consequence, the generalized FDT for non-equilibrium systems with detailed balance breaking also has a qualitatively different structure compared to the equilibrium FDT.

The structure of the driving force in relation to the characteristics of non-equilibrium steady states, namely the non-equilibrium force decomposition in Equation (12), is critical for the understanding of the effects of detailed balance breaking on the global dynamics and the non-equilibrium thermodynamics of stochastic spatially extended systems in the framework of the potential landscape and flux field theory [27, 36]. Its extension into the concept of non-equilibrium trinity and the implications thereof for turbulence dynamics can be found in [40]. In this work the non-equilibrium force decomposition also plays a key role in the formulation of the generalized FDT, where the effect of detailed balance breaking on the qualitative structural change of the FDT is highlighted. In the following we proceed to formulate this generalized FDT step by step.

2.4. Time-Dependent Perturbation

Suppose that we perturb the system in such a way that the stochastic field equation becomes

$$\partial_t \boldsymbol{\phi}(\mathbf{x}, t) = \mathbf{F}(\mathbf{x})[\boldsymbol{\phi}] + h(t)\mathbf{e}_j \delta(\mathbf{x} - \mathbf{x}') + \boldsymbol{\zeta}(\mathbf{x}, t), \tag{13}$$

where $\mathbf{e}_j = (0, \cdots, 1, \cdots, 0)$ is the standard base vector with the element 1 at the j-th component and 0 otherwise. The form of the perturbation in Equation (13) means the perturbative force is applied locally at the position $\mathbf{x}'$ on the j-th component of the field, with a magnitude $h(t)$ that may vary with time but is independent of the system state (the field $\boldsymbol{\phi}$).

The FFPE for the perturbed system then becomes

$$\partial_t P = L(t)P = [L + L_{\text{ext}}(t)]P, \tag{14}$$

where $L_{\text{ext}}(t)$ is the perturbation operator with the expression

$$L_{\text{ext}}(t) = -h(t)\delta_{\phi_j(\mathbf{x}')} \tag{15}$$

according to Equation (6) and the form of the perturbative force.

The formal solution of the perturbed FFPE is given by

$$P(t) = \hat{T} e^{\int_{t_0}^{t} (L + L_{\text{ext}}(t'))dt'} P(t_0), \tag{16}$$

where $\hat{T}$ is the time-ordering operator. When $L_{\text{ext}}(t)$ is small, the perturbation expansion yields [28]

$$P(t) = e^{L(t-t_0)} P(t_0) + \int_{t_0}^{t} dt' e^{L(t-t')} L_{\text{ext}}(t') e^{L(t'-t_0)} P(t_0). \tag{17}$$

For systems initially in the steady state (i.e., $P(t_0) = P_s$) as considered in this article, this reduces to

$$P(t) = P_s + \int_{t_0}^{t} dt' e^{L(t-t')} L_{\text{ext}}(t') P_s, \tag{18}$$

where we have used the steady-state FFPE for the unperturbed system, $LP_s = 0$. Written more specifically, the perturbative solution reads

$$P_t[\boldsymbol{\phi}] = P_s[\boldsymbol{\phi}] + \int_{t_0}^{t} dt' h(t') e^{L(t-t')} \left(-\delta_{\phi_j(\mathbf{x}')}\right) P_s[\boldsymbol{\phi}]. \tag{19}$$

2.5. Linear Response Function

As the system is perturbed, it responds to the perturbation by changing the time evolution of its states and thus also the observables depending on the states. The response of the system can be studied by investigating how the observables of the system vary before and after the perturbation. We choose the basic observable of the field $\phi_i(\mathbf{x})$, namely the i-th component of the field at the location $\mathbf{x}$, and investigate how its average changes in response to the perturbative force applied at the j-th component of the field at the location $\mathbf{x}'$. The change of the average of this observable in response to the perturbation is given by

$$\begin{aligned}&\delta\langle\phi_i(\mathbf{x})\rangle(t)\\=&\langle\phi_i(\mathbf{x})\rangle_{\text{pert}}-\langle\phi_i(\mathbf{x})\rangle_s\\=&\int\phi_i(\mathbf{x})(P_t[\boldsymbol{\phi}]-P_s[\boldsymbol{\phi}])\mathcal{D}\boldsymbol{\phi}\\=&\int\phi_i(\mathbf{x})\left[\int_{t_0}^{t}dt'h(t')e^{L(t-t')}\left(-\delta_{\phi_j(\mathbf{x}')}\right)P_s[\boldsymbol{\phi}]\right]\mathcal{D}\boldsymbol{\phi}\\=&\int_{t_0}^{t}dt'h(t')R_{ij}(\mathbf{x},\mathbf{x}',t-t'),\end{aligned}\tag{20}$$

where $\langle\phi_i(\mathbf{x})\rangle_{\text{pert}}$ is the average of the observable at the perturbed state, $\langle\phi_i(\mathbf{x})\rangle_s$ is that at the unperturbed steady state, and $\int\mathcal{D}\boldsymbol{\phi}$ represents functional integration in the state space. In the above we have used the perturbative solution in Equation (19). Thus the linear response function can be identified as

$$R_{ij}(\mathbf{x},\mathbf{x}',t)=\theta(t)\int\phi_i(\mathbf{x})e^{Lt}\left(-\delta_{\phi_j(\mathbf{x}')}\right)P_s[\boldsymbol{\phi}]\mathcal{D}\boldsymbol{\phi},\tag{21}$$

where $\theta(t)$ is the step function taking the value 1 for $t\geq 0$ and 0 otherwise. $R_{ij}(\mathbf{x},\mathbf{x}',t)$ characterizes how the i-th component of the field at the location $\mathbf{x}$ responds, after the lapse of time t, to a perturbative impulse force applied on the j-th component of the field at the location $\mathbf{x}'$, when the system is initially prepared at the steady state. The linear response function can also be rewritten in the matrix form

$$\mathbf{R}(\mathbf{x},\mathbf{x}',t)=\theta(t)\int\boldsymbol{\phi}(\mathbf{x})e^{Lt}\left(-\delta_{\boldsymbol{\phi}(\mathbf{x}')}\right)P_s[\boldsymbol{\phi}]\mathcal{D}\boldsymbol{\phi}.\tag{22}$$

2.6. Correlation Functions

For spatially extended systems, observables in general are functionals of the field $\boldsymbol{\phi}(\mathbf{x})$. The correlation function of two general observables $A[\boldsymbol{\phi}]$ at time t and $B[\boldsymbol{\phi}]$ at time t' in the steady state is denoted by $\langle A(t)B(t')\rangle_s$. Since the steady state has time translation invariance, the correlation function only depends on the time difference $t-t'$. Without loss of generality, we only need to consider $\langle A(t)B(0)\rangle_s$.

Following the derivation for systems without spatial extension [28], the expression of the correlation function for spatially extended systems can be found as follows (for $t\geq 0$):

$$\begin{aligned}&\langle A(t)B(0)\rangle_s\\=&\iint A[\boldsymbol{\phi}]W[\boldsymbol{\phi},t;\boldsymbol{\phi}',0]B[\boldsymbol{\phi}']\mathcal{D}\boldsymbol{\phi}\mathcal{D}\boldsymbol{\phi}'\\=&\iint A[\boldsymbol{\phi}]P[\boldsymbol{\phi},t|\boldsymbol{\phi}',0]B[\boldsymbol{\phi}']P_s[\boldsymbol{\phi}']\mathcal{D}\boldsymbol{\phi}\mathcal{D}\boldsymbol{\phi}'\\=&\iint A[\boldsymbol{\phi}]\left(e^{Lt}\delta[\boldsymbol{\phi}-\boldsymbol{\phi}']\right)B[\boldsymbol{\phi}']P_s[\boldsymbol{\phi}']\mathcal{D}\boldsymbol{\phi}\mathcal{D}\boldsymbol{\phi}'\\=&\int A[\boldsymbol{\phi}]e^{Lt}\left(B[\boldsymbol{\phi}]P_s[\boldsymbol{\phi}]\right)\mathcal{D}\boldsymbol{\phi},\end{aligned}\tag{23}$$

where $W[\boldsymbol{\phi},t;\boldsymbol{\phi}',0]$ and $P[\boldsymbol{\phi},t|\boldsymbol{\phi}',0]$ are the joint probability distribution and the transition probability distribution in the state space, respectively, and $\delta[\boldsymbol{\phi}-\boldsymbol{\phi}']$ is the Dirac delta function in the state space. For readers concerned with the use of such highly singular function(al)s as $\delta[\boldsymbol{\phi}-\boldsymbol{\phi}']$, a family of Gaussian distributions on the (infinite-dimensional) state space [23] can be used to approximate the delta function.

The correlation function has the equivalent expression

$$\langle A(t)B(0)\rangle_s=\int\left(e^{L^\dagger t}A[\boldsymbol{\phi}]\right)B[\boldsymbol{\phi}]P_s[\boldsymbol{\phi}]\mathcal{D}\boldsymbol{\phi},\tag{24}$$

where we have performed integration by parts in the state space. One may define the time-dependent observable $A[\boldsymbol{\phi},t]=e^{L^\dagger t}A[\boldsymbol{\phi}]$ with its time evolution generated by the operator $L^\dagger$. Note that the time evolution of the probability distribution is generated by the operator L. The situation here resembles the relation between the Heisenberg picture and the Schrödinger picture in quantum mechanics.

The correlation function of the field is of particular importance, which has the following expressions (for $t\geq 0$):

$$\begin{aligned}\langle\boldsymbol{\phi}(\mathbf{x},t)\boldsymbol{\phi}(\mathbf{x}',0)\rangle_s&=\int\left(e^{L^\dagger t}\boldsymbol{\phi}(\mathbf{x})\right)\boldsymbol{\phi}(\mathbf{x}')P_s[\boldsymbol{\phi}]\mathcal{D}\boldsymbol{\phi}\\&=\int\boldsymbol{\phi}(\mathbf{x})e^{Lt}\left(\boldsymbol{\phi}(\mathbf{x}')P_s[\boldsymbol{\phi}]\right)\mathcal{D}\boldsymbol{\phi}.\end{aligned}\tag{25}$$

We will also need the time derivative of the field correlation function to formulate the generalized FDT. Direct calculation yields

$$\begin{aligned}&\frac{\partial}{\partial t}\langle\boldsymbol{\phi}(\mathbf{x},t)\boldsymbol{\phi}(\mathbf{x}',0)\rangle_s\\=&\int\boldsymbol{\phi}(\mathbf{x})Le^{Lt}\left(\boldsymbol{\phi}(\mathbf{x}')P_s[\boldsymbol{\phi}]\right)\mathcal{D}\boldsymbol{\phi}\\=&\int\left(L^\dagger\boldsymbol{\phi}(\mathbf{x})\right)e^{Lt}\left(\boldsymbol{\phi}(\mathbf{x}')P_s[\boldsymbol{\phi}]\right)\mathcal{D}\boldsymbol{\phi}\\=&\int\mathbf{F}(\mathbf{x})[\boldsymbol{\phi}]e^{Lt}\left(\boldsymbol{\phi}(\mathbf{x}')P_s[\boldsymbol{\phi}]\right)\mathcal{D}\boldsymbol{\phi}\\=&\langle\mathbf{F}(\mathbf{x},t)\boldsymbol{\phi}(\mathbf{x}',0)\rangle_s,\end{aligned}\tag{26}$$

where we have used $L^\dagger\boldsymbol{\phi}(\mathbf{x})=\mathbf{F}(\mathbf{x})[\boldsymbol{\phi}]$. This can be shown using the expression of $L^\dagger$ in Equation (7).

However, the simple relation in Equation (26) is not sufficient for the purpose of formulating the generalized FDT. We need to relate the time derivative of the field correlation function to $\langle\boldsymbol{\phi}(\mathbf{x},t)\mathbf{F}(\mathbf{x}',0)\rangle_s$ instead of $\langle\mathbf{F}(\mathbf{x},t)\boldsymbol{\phi}(\mathbf{x}',0)\rangle_s$ for reasons that will become clear later. For equilibrium steady states with detailed balance and time reversal symmetry, these two correlation functions $\langle\boldsymbol{\phi}(\mathbf{x},t)\mathbf{F}(\mathbf{x}',0)\rangle_s$ and $\langle\mathbf{F}(\mathbf{x},t)\boldsymbol{\phi}(\mathbf{x}',0)\rangle_s$ are equal to each other as will be shown later. For non-equilibrium steady states violating detailed balance, $\langle\boldsymbol{\phi}(\mathbf{x},t)\mathbf{F}(\mathbf{x}',0)\rangle_s$ and $\langle\mathbf{F}(\mathbf{x},t)\boldsymbol{\phi}(\mathbf{x}',0)\rangle_s$ differ from each other, which is a manifestation of time irreversibility in non-equilibrium steady states.

Given the above considerations, we calculate the time derivative of the field correlation function in an alternative way as follows:

$$
\begin{aligned}
&\frac{\partial}{\partial t}\langle \boldsymbol{\phi}(\mathbf{x},t)\boldsymbol{\phi}(\mathbf{x}',0)\rangle_s \\
&=\int \boldsymbol{\phi}(\mathbf{x})e^{Lt}L\left(\boldsymbol{\phi}(\mathbf{x}')P_s\right)\mathcal{D}\boldsymbol{\phi} \\
&=\int \left(e^{L^\dagger t}\boldsymbol{\phi}(\mathbf{x})\right)P_s^{-1}L\left(P_s\boldsymbol{\phi}(\mathbf{x}')\right)P_s\mathcal{D}\boldsymbol{\phi} \\
&=\int \left(e^{L^\dagger t}\boldsymbol{\phi}(\mathbf{x})\right)\left[\left(P_s^{-1}LP_s\right)\boldsymbol{\phi}(\mathbf{x}')\right]P_s\mathcal{D}\boldsymbol{\phi} \\
&=\int \left(e^{L^\dagger t}\boldsymbol{\phi}(\mathbf{x})\right)\left(\widetilde{L}\boldsymbol{\phi}(\mathbf{x}')\right)P_s\mathcal{D}\boldsymbol{\phi},
\end{aligned}
\tag{27}
$$

where

$$
\widetilde{L}=P_s^{-1}LP_s=L^\dagger-2\int d\mathbf{x}\mathbf{V}_s(\mathbf{x})[\boldsymbol{\phi}]\cdot\delta_{\boldsymbol{\phi}(\mathbf{x})}. \tag{28}
$$

The last expression of the operator $\widetilde{L}$ is proven in the **Appendix**, with the help of the non-equilibrium force decomposition in Equation (12). Given this expression of $\widetilde{L}$, we further derive

$$
\begin{aligned}
\widetilde{L}\boldsymbol{\phi}(\mathbf{x}')&=L^\dagger\boldsymbol{\phi}(\mathbf{x}')-2\mathbf{V}_s(\mathbf{x}')[\boldsymbol{\phi}] \\
&=\mathbf{F}(\mathbf{x}')[\boldsymbol{\phi}]-2\mathbf{V}_s(\mathbf{x}')[\boldsymbol{\phi}].
\end{aligned}
\tag{29}
$$

Therefore, we obtain the alternative expression of the time derivative of the field correlation function:

$$
\begin{aligned}
\frac{\partial}{\partial t}\langle \boldsymbol{\phi}(\mathbf{x},t)\boldsymbol{\phi}(\mathbf{x}',0)\rangle_s =&\langle \boldsymbol{\phi}(\mathbf{x},t)\mathbf{F}(\mathbf{x}',0)\rangle_s \\
&-2\langle \boldsymbol{\phi}(\mathbf{x},t)\mathbf{V}_s(\mathbf{x}',0)\rangle_s.
\end{aligned}
\tag{30}
$$

This is the relation needed in the formulation of the generalized FDT.

We remark that the two expressions of $\partial_t\langle \boldsymbol{\phi}(\mathbf{x},t)\boldsymbol{\phi}(\mathbf{x}',0)\rangle$ in Equations (26) and (30) imply the following interesting result in the form of asymmetry of the correlation function:

$$
\begin{aligned}
&\langle \boldsymbol{\phi}(\mathbf{x},t)\mathbf{F}(\mathbf{x}',0)\rangle_s-\langle \mathbf{F}(\mathbf{x},t)\boldsymbol{\phi}(\mathbf{x}',0)\rangle_s \\
=&2\langle \boldsymbol{\phi}(\mathbf{x},t)\mathbf{V}_s(\mathbf{x}',0)\rangle_s.
\end{aligned}
\tag{31}
$$

For equilibrium steady states, $\mathbf{V}_s$ vanishes and $\langle \boldsymbol{\phi}(\mathbf{x},t)\mathbf{F}(\mathbf{x}',0)\rangle_s=\langle \mathbf{F}(\mathbf{x},t)\boldsymbol{\phi}(\mathbf{x}',0)\rangle_s$. This symmetry of the correlation function is a reflection of time reversal symmetry in equilibrium states, which is broken for non-equilibrium steady states with non-vanishing $\mathbf{V}_s$. It may be possible to test this relation in experiments, at least the qualitative character of the asymmetry of the correlation functions.

2.7. Generalized FDT

Now we are in a position to formulate the generalized FDT for stochastic spatially extended systems sustaining non-equilibrium steady states. First notice that the linear response function in Equation (22) can be rewritten in the following form:

$$
\begin{aligned}
\mathbf{R}(\mathbf{x},\mathbf{x}',t)&=\theta(t)\int \boldsymbol{\phi}(\mathbf{x})e^{Lt}\left(-\delta_{\boldsymbol{\phi}(\mathbf{x}')}\right)P_s[\boldsymbol{\phi}]\mathcal{D}\boldsymbol{\phi} \\
&=\theta(t)\int \boldsymbol{\phi}(\mathbf{x})e^{Lt}\left(\delta_{\boldsymbol{\phi}(\mathbf{x}')}U[\boldsymbol{\phi}]\right)P_s[\boldsymbol{\phi}]\mathcal{D}\boldsymbol{\phi},
\end{aligned}
\tag{32}
$$

where $U[\boldsymbol{\phi}]=-\ln P_s[\boldsymbol{\phi}]$ is the potential landscape. The RHS of this equation also has the form of a correlation function, namely $\theta(t)\langle \boldsymbol{\phi}(\mathbf{x},t)\delta_{\boldsymbol{\phi}(\mathbf{x}',0)}U\rangle_s$. Hence, this relation may be considered as a FDT as it relates the response function to the correlation function. However, this form of FDT does not provide insight into some important questions, such as how the non-equilibrium nature of the system affects the FDT. Neither does it relate the response function to (the time derivative of) the field-field correlation function as the equilibrium FDT for spatially extended systems does.

To gain insight into how the FDT is affected by detailed balance breaking that characterizes the non-equilibrium nature of the steady states, we invoke the non-equilibrium force decomposition in Equation (12). Inverting the diffusion matrix in the state space, it can be reformulated as

$$
\begin{aligned}
\delta_{\boldsymbol{\phi}(\mathbf{x}')}U[\boldsymbol{\phi}]=-&\int d\mathbf{x}''\mathbf{D}^{-1}(\mathbf{x}',\mathbf{x}'') \\
&\cdot\left(\mathbf{F}(\mathbf{x}'')[\boldsymbol{\phi}]-\mathbf{V}_s(\mathbf{x}'')[\boldsymbol{\phi}]\right),
\end{aligned}
\tag{33}
$$

where $\mathbf{D}^{-1}(\mathbf{x}',\mathbf{x}'')$ is the state-space matrix inversion of $\mathbf{D}(\mathbf{x}',\mathbf{x}'')$ defined by

$$
\int \mathbf{D}^{-1}(\mathbf{x},\mathbf{x}')\mathbf{D}(\mathbf{x}',\mathbf{x}'')d\mathbf{x}'=\mathbf{I}\delta(\mathbf{x}-\mathbf{x}''). \tag{34}
$$

Here $\mathbf{I}$ is the $n\times n$ identity matrix. With the help of the above form of the non-equilibrium force decomposition, Equation (32) is brought into the form

$$
\begin{aligned}
\mathbf{R}(\mathbf{x},\mathbf{x}',t)=-\theta(t)\int &\left[\langle \boldsymbol{\phi}(\mathbf{x},t)\mathbf{F}(\mathbf{x}'',0)[\boldsymbol{\phi}]\rangle_s\right. \\
&\left.-\langle \boldsymbol{\phi}(\mathbf{x},t)\mathbf{V}_s(\mathbf{x}'',0)\rangle_s\right]\mathbf{D}^{-1}(\mathbf{x}'',\mathbf{x}')d\mathbf{x}''.
\end{aligned}
\tag{35}
$$

To further bring it closer to the form of the equilibrium FDT, in which the time derivative of the field-field correlation function appears, we use the alternative expression of the time derivative of the field-field correlation function in Equation (30) (its derivation also used the non-equilibrium force decomposition) to obtain

$$
\begin{aligned}
\mathbf{R}(\mathbf{x},\mathbf{x}',t)\;=\;&-\theta(t)\int\left[\frac{\partial}{\partial t}\langle \boldsymbol{\phi}(\mathbf{x},t)\boldsymbol{\phi}(\mathbf{x}'',0)\rangle_s+2\langle \boldsymbol{\phi}(\mathbf{x},t)\mathbf{V}_s(\mathbf{x}'',0)\rangle_s\right. \\
&\left.-\langle \boldsymbol{\phi}(\mathbf{x},t)\mathbf{V}_s(\mathbf{x}'',0)\rangle_s\right]\mathbf{D}^{-1}(\mathbf{x}'',\mathbf{x}')d\mathbf{x}'' \\
=&-\theta(t)\int\left[\frac{\partial}{\partial t}\langle \boldsymbol{\phi}(\mathbf{x},t)\boldsymbol{\phi}(\mathbf{x}'',0)\rangle_s\right. \\
&\left.+\langle \boldsymbol{\phi}(\mathbf{x},t)\mathbf{V}_s(\mathbf{x}'',0)\rangle_s\right]\mathbf{D}^{-1}(\mathbf{x}'',\mathbf{x}')d\mathbf{x}''.
\end{aligned}
\tag{36}
$$

We have thus finally formulated the *generalized FDT* for stochastic spatially extended systems sustaining non-equilibrium steady states:

$$
\begin{aligned}
\mathbf{R}(\mathbf{x},\mathbf{x}',t)=-\theta(t)\int&\left[\frac{\partial}{\partial t}\langle \boldsymbol{\phi}(\mathbf{x},t)\boldsymbol{\phi}(\mathbf{x}'',0)\rangle_s\right. \\
&\left.+\langle \boldsymbol{\phi}(\mathbf{x},t)\mathbf{V}_s(\mathbf{x}'',0)\rangle_s\right]\mathbf{D}^{-1}(\mathbf{x}'',\mathbf{x}')d\mathbf{x}''.
\end{aligned}
\tag{37}
$$

2.8. Discussion

We first consider some special forms of the generalized FDT. For diffusion matrices (spatial correlators of the stochastic force) of the particular form $\mathbf{D}(\mathbf{x}, \mathbf{x}') = D\mathbf{I}\delta(\mathbf{x} - \mathbf{x}')$, the generalized FDT reads

$$\mathbf{R}(\mathbf{x}, \mathbf{x}', t) = -\frac{\theta(t)}{D}\left[\frac{\partial}{\partial t}\langle\boldsymbol{\phi}(\mathbf{x}, t)\boldsymbol{\phi}(\mathbf{x}', 0)\rangle_s + \langle\boldsymbol{\phi}(\mathbf{x}, t)\mathbf{V}_s(\mathbf{x}', 0)\rangle_s\right]. \tag{38}$$

For equilibrium states with detailed balance indicated by $\mathbf{V}_s = 0$, the generalized FDT further reduces to the more familiar form of the equilibrium FDT:

$$\mathbf{R}(\mathbf{x}, \mathbf{x}', t) = -\frac{\theta(t)}{D}\frac{\partial}{\partial t}\langle\boldsymbol{\phi}(\mathbf{x}, t)\boldsymbol{\phi}(\mathbf{x}', 0)\rangle_{eq}, \tag{39}$$

which relates the response function to the time derivative of the field-field correlation function.

If the system under consideration is not spatially extended, but one that can be described by a finite-dimensional state vector $\mathbf{X}$, then the generalized FDT in Equation (37) reduces to the following form:

$$\mathbf{R}(t) = -\theta(t)\left[\frac{d}{dt}\langle\mathbf{X}(t)\mathbf{X}(0)\rangle_s + \langle\mathbf{X}(t)\mathbf{V}_s(0)\rangle_s\right]\mathbf{D}^{-1}. \tag{40}$$

Some modified forms of the FDT in the literature have a close connection to the above form but may differ in certain aspects [11, 13, 15].

Now we discuss the implications of the generalized FDT. Compared to the FDT for equilibrium spatially extended systems preserving detailed balance and time reversal symmetry, the generalized FDT for non-equilibrium spatially extended systems in Equation (37) has a qualitatively different structure. It is no longer a binary relation that connects the response function to the field-field correlation function (field correlation for short). Instead, the generalized FDT is a *ternary relation* that connects three objects together, namely the response function, the field correlation, and the additional flux correlation (or field-flux correlation function). The flux correlation originates from detailed balance breaking and time irreversibility in non-equilibrium steady states. It vanishes for systems obeying detailed balance with equilibrium steady states, which reduces the ternary relation of the generalized FDT to the binary relation of the equilibrium FDT. We note that the feature of the generalized FDT for non-equilibrium steady states as a ternary relation instead of a binary relation also carries over to systems that are not spatially extended, as is evident from Equation (40).

One way to understand the physical meaning of the generalized FDT is to interpret the flux correlation as a form of dissipative response associated with detailed balance breaking in non-equilibrium steady states, which contributes to how the system responds to perturbations in totality. In other words, the total response of the system to perturbations described by the response function consists of a part that is related to the fluctuations at the steady state characterized by the field correlation and another part that is associated with the non-equilibrium nature of the steady state quantified by the flux correlation. For systems with a stable steady state, it is typical that the system responds to perturbations that kick the system out of the steady state by going through a transient relaxation process that brings the system back to the steady state. This dissipative relaxation process the system goes through in response to perturbations can be characterized by the response function. The steady state is the reference state on which this relaxation process is targeted. When the steady state of the system is a non-equilibrium state violating detailed balance, the target state which the system relaxes back to in general has changed compared to that of the equilibrium steady state obeying detailed balance. In addition, the conditions for sustaining non-equilibrium steady states may also affect the dynamical process of the transient relaxation (e.g., how fast the system relaxes back to the steady state). Therefore, it is not surprising that the non-equilibrium nature of the steady state reflected by the flux correlation affects how the system responds to perturbations. This is the rationale behind the interpretation of the flux correlation as part of the response function associated with the non-equilibrium nature of the steady state signified by detailed balance breaking.

To further appreciate the physical meaning of the generalized FDT from a different perspective, we reformulate it into the following form

$$\begin{aligned}-\theta(t)\frac{\partial}{\partial t}\langle\boldsymbol{\phi}(\mathbf{x}, t)\boldsymbol{\phi}(\mathbf{x}', 0)\rangle_s = \int \mathbf{R}(\mathbf{x}, \mathbf{x}'', t)\mathbf{D}(\mathbf{x}'', \mathbf{x}')d\mathbf{x}'' \\ + \theta(t)\langle\boldsymbol{\phi}(\mathbf{x}, t)\mathbf{V}_s(\mathbf{x}', 0)\rangle_s.\end{aligned} \tag{41}$$

We simply inverted back the diffusion matrix and grouped the response function and the flux correlation together. The logic here is to interpret the response function and the flux correlation as two ‘sources’ of fluctuations characterized by the field correlation. This logic is based on the distinction of two basic types of non-equilibrium processes, namely the transient and the steady-state non-equilibrium processes. When a system is in a state different from the steady state (e.g., kicked out of the steady state by an external perturbation), it goes through the transient process of relaxing back to the steady state, which is an irreversible dissipative non-equilibrium process. However, for systems capable of sustaining non-equilibrium steady states, the steady state itself also has an intrinsic non-equilibrium nature with an arrow of time indicated by the irreversible probability flux. Even if the system remains in the steady state without going through the transient relaxation process, it is still going through the non-equilibrium steady-state process with time irreversibility. These two basic types of non-equilibrium processes both have associated fluctuations. The transient relaxation of the system back to the steady state upon perturbation characterized by the response function is associated with the fluctuations *around* the steady state. The flux correlation originating from detailed balance breaking in non-equilibrium steady states is associated with the fluctuations inherent *within* non-equilibrium steady-state processes.

With these two connections established, we can now interpret the generalized FDT in the form of Equation (41) as follows. The field correlation (also its time derivative) is a characterization of the non-equilibrium fluctuations of the stochastic spatially extended system, which come from two different sources corresponding to two basic types of non-equilibrium processes. One part of the non-equilibrium fluctuations originates from the process of transient relaxation back to the steady state characterized by the response function. The other part of the non-equilibrium fluctuations captured by the flux correlation arises from the inherent fluctuations within the steady-state non-equilibrium processes with detailed balance breaking. The latter part exists only for systems sustaining non-equilibrium steady states with an intrinsic arrow of time.

For inherently equilibrium systems that obey detailed balance, the steady state is an equilibrium state. The fluctuations around the equilibrium state characterized by the field correlation is directly linked to the transient process of relaxing back to equilibrium upon perturbation captured by the response function. However, for intrinsically non-equilibrium systems violating detailed balance, the steady state itself form a stationary non-equilibrium background embedded with intrinsic non-equilibrium fluctuations, upon which transient relaxation of returning to the steady state takes place. As a result, the field correlation characterizing non-equilibrium fluctuations around the non-equilibrium steady state can no longer be directly connected to the response function, as it only captures the part of fluctuations associated with relaxing back to the background upon perturbation. The flux correlation describing the intrinsic non-equilibrium fluctuations within the stationary background itself also has to be taken into account.

In general, the non-equilibrium nature of the steady state (reflected by the flux correlation) affects both the response of the system to perturbations (e.g., by changing the target the system relaxes back to) and fluctuations of the system at the steady state (e.g., due to the presence of fluctuations associated with non-equilibrium steady-state processes). The particular example in section 4 also demonstrates this point. Thus it is a matter of perspective whether to interpret the flux correlation as part of the response function or part of the field correlation. After all, it is the ternary relation quantified by the generalized FDT that has the final word on how the response function and the field correlation should be related to each other by the additional flux correlation when the steady state of the system is non-equilibrium in nature.

The qualitative structural change of the FDT from a binary relation to a ternary relation and its physical significance discussed above also have experimental implications. For equilibrium systems obeying detailed balance, once we experimentally measure the response of the system to designed disturbances that kick the system out of equilibrium, we also have information on the fluctuations of the system around equilibrium, vice versa, as implied by the binary relation of the equilibrium FDT. In contrast, for systems with non-equilibrium steady states, experimentally obtaining information on the response of the system relaxing back to the steady state after being perturbed is not sufficient to derive information on the field correlation that characterizes fluctuations of the system at the steady state, as dictated by the ternary relation of the generalized FDT. Two elements are needed to derive information on the third in the ternary relation. Experimentally, the field correlation and the response function are relatively easier to access. The difference between the two, according to the generalized FDT, can be used to infer the flux correlation that contains quantitative information on the non-equilibrium nature of the steady state with detailed balance breaking. In addition, the asymmetry of correlation functions in the form of Equation (31) is also useful for obtaining such information in experiments.

3. ORNSTEIN-UHLENBECK PROCESS OF SPATIALLY EXTENDED SYSTEMS

We study the general OU process for stochastic spatially extended systems to demonstrate the generalized FDT developed in the previous section. Due to some special features in the OU process, the steady state of the FFPE can be solved in principle and thus we can verify the generalized FDT for this type of process.

3.1. Stochastic Field Dynamics

The essential feature of the OU process is that the deterministic force is linear in the state variables and the stochastic force is independent of the state variables [28]. For stochastic spatially extended systems with the field $\boldsymbol{\phi}(\mathbf{x})$ as the state variables, the OU process is governed by the following form of stochastic field equation [23, 36]:

$$\partial_t \boldsymbol{\phi}(\mathbf{x}, t) = -\int \boldsymbol{\gamma}(\mathbf{x}, \mathbf{x}') \cdot \boldsymbol{\phi}(\mathbf{x}', t) d\mathbf{x}' + \boldsymbol{\zeta}(\mathbf{x}, t), \tag{42}$$

where $\boldsymbol{\zeta}(\mathbf{x}, t)$ is Gaussian white noise in time with zero mean and has the correlation

$$\langle \boldsymbol{\zeta}(\mathbf{x}, t) \boldsymbol{\zeta}(\mathbf{x}', t') \rangle = 2\mathbf{D}(\mathbf{x}, \mathbf{x}') \delta(t - t'). \tag{43}$$

In the most general form $\boldsymbol{\gamma}(\mathbf{x}, \mathbf{x}')$ and $\mathbf{D}(\mathbf{x}, \mathbf{x}')$ may also be time-dependent, which is not considered here.

The deterministic driving force in Equation (42) has the form of an integral operator acting on the field. This form is actually general for linear forces, if the integral kernel $\boldsymbol{\gamma}(\mathbf{x}, \mathbf{x}')$ is allowed to be generalized functions involving the Dirac delta function and its derivatives of various orders. For instance, for the diffusion equation $\partial_t \boldsymbol{\phi}(\mathbf{x}, t) = D\nabla^2 \boldsymbol{\phi}(\mathbf{x}, t)$, its driving force has the form $-\hat{\gamma}\boldsymbol{\phi}$ where $\hat{\gamma} = -D\nabla^2$ is a differential operator. But $\hat{\gamma}$ can be equivalently interpreted as an integral operator with the integral kernel $\gamma(\mathbf{x}, \mathbf{x}') = -D\nabla^2 \delta(\mathbf{x} - \mathbf{x}')$. We shall interpret the integral kernel $\boldsymbol{\gamma}(\mathbf{x}, \mathbf{x}')$ in Equation (42) and in the rest of the paper in this general sense. We also use the notation $\hat{\boldsymbol{\gamma}}$ to represent the corresponding integral operator so that the deterministic driving force can also be written as $-\hat{\boldsymbol{\gamma}}\boldsymbol{\phi}$. By interpreting $\mathbf{D}(\mathbf{x}, \mathbf{x}')$ as an integral kernel (allowed to be generalized functions), we can also associate with it an operator $\hat{\mathbf{D}}$.

3.2. Functional Fokker-Planck Equation

The FFPE associated with the stochastic field dynamics in Equation (42) has the form

$$\begin{aligned} \partial_t P_t[\boldsymbol{\phi}] = &\iint d\mathbf{x} d\mathbf{x}' \delta_{\boldsymbol{\phi}(\mathbf{x})} \cdot \left(\boldsymbol{\gamma}(\mathbf{x}, \mathbf{x}') \cdot \boldsymbol{\phi}(\mathbf{x}') P_t[\boldsymbol{\phi}] \right) \\ &+ \iint d\mathbf{x} d\mathbf{x}' \delta_{\boldsymbol{\phi}(\mathbf{x})} \cdot \mathbf{D}(\mathbf{x}, \mathbf{x}') \cdot \delta_{\boldsymbol{\phi}(\mathbf{x}')} P_t[\boldsymbol{\phi}]. \end{aligned} \tag{44}$$

In the symbolic form of the FFPE $\partial_t P = LP$, the operator L has the expression

$$L = \iint d\mathbf{x}d\mathbf{x}'\, \delta_{\boldsymbol{\phi}(\mathbf{x})} \cdot \boldsymbol{\gamma}(\mathbf{x},\mathbf{x}') \cdot \boldsymbol{\phi}(\mathbf{x}') + \iint d\mathbf{x}d\mathbf{x}'\, \delta_{\boldsymbol{\phi}(\mathbf{x})} \cdot \mathbf{D}(\mathbf{x},\mathbf{x}') \cdot \delta_{\boldsymbol{\phi}(\mathbf{x}')}. \tag{45}$$

Its adjoint reads

$$L^\dagger = -\iint d\mathbf{x}d\mathbf{x}'\, \boldsymbol{\phi}(\mathbf{x}') \cdot \boldsymbol{\gamma}^T(\mathbf{x},\mathbf{x}') \cdot \delta_{\boldsymbol{\phi}(\mathbf{x})} + \iint d\mathbf{x}d\mathbf{x}'\, \delta_{\boldsymbol{\phi}(\mathbf{x})} \cdot \mathbf{D}(\mathbf{x},\mathbf{x}') \cdot \delta_{\boldsymbol{\phi}(\mathbf{x}')}, \tag{46}$$

where $\boldsymbol{\gamma}^T$ represents the transpose of the matrix $\boldsymbol{\gamma}$. The operators L and $L^\dagger$ are very different from the operators $\hat{\boldsymbol{\gamma}}$ and $\hat{\mathbf{D}}$ as these two types of operators are defined on different spaces. $\hat{\boldsymbol{\gamma}}$ and $\hat{\mathbf{D}}$ act on fields $\boldsymbol{\phi}(\mathbf{x})$, while L and $L^\dagger$ act on functionals of the field $A[\boldsymbol{\phi}]$.

Due to the particular features of the OU process, it allows for Gaussian solutions [28]. We are particularly interested in the steady state. When $\hat{\boldsymbol{\gamma}}$ and $\hat{\mathbf{D}}$ satisfy certain conditions [23], the steady-state solution exists and is unique. The steady-state probability distribution is a Gaussian distribution of the form

$$P_s[\boldsymbol{\phi}] = \mathcal{N} \exp\left\{-\frac{1}{2}\iint \boldsymbol{\phi}(\mathbf{x}) \cdot \boldsymbol{\Sigma}_s^{-1}(\mathbf{x},\mathbf{x}') \cdot \boldsymbol{\phi}(\mathbf{x}')d\mathbf{x}d\mathbf{x}'\right\}, \tag{47}$$

where $\mathcal{N}$ is the normalization constant and $\boldsymbol{\Sigma}_s(\mathbf{x},\mathbf{x}')$ is the covariance matrix in the state space. $\boldsymbol{\Sigma}_s^{-1}(\mathbf{x},\mathbf{x}')$ is the state-space matrix inverse of $\boldsymbol{\Sigma}_s(\mathbf{x},\mathbf{x}')$ defined similarly as $\mathbf{D}^{-1}(\mathbf{x},\mathbf{x}')$ in Equation (34).

The covariance matrix $\boldsymbol{\Sigma}_s(\mathbf{x},\mathbf{x}')$ is determined by the functional equation [28, 36]

$$\int \boldsymbol{\gamma}(\mathbf{x},\mathbf{x}'')\boldsymbol{\Sigma}_s(\mathbf{x}'',\mathbf{x}')d\mathbf{x}'' + \int \boldsymbol{\Sigma}_s(\mathbf{x},\mathbf{x}'')\boldsymbol{\gamma}^T(\mathbf{x}',\mathbf{x}'')d\mathbf{x}'' = 2\mathbf{D}(\mathbf{x},\mathbf{x}'), \tag{48}$$

which can be reformulated as the operator equation

$$\hat{\boldsymbol{\gamma}}\hat{\Sigma}_s + \hat{\Sigma}_s\hat{\boldsymbol{\gamma}}^\dagger = 2\hat{\mathbf{D}}. \tag{49}$$

Here $\hat{\Sigma}_s$ is the operator associated with $\boldsymbol{\Sigma}_s(\mathbf{x},\mathbf{x}')$ (interpreted as an integral kernel) and $\hat{\boldsymbol{\gamma}}^\dagger$ is the adjoint of $\hat{\boldsymbol{\gamma}}$. Equation (49) is an algebraic Lyapunov equation for operators, which has the solution

$$\hat{\Sigma}_s = 2\int_0^\infty e^{-\hat{\boldsymbol{\gamma}}\tau}\hat{\mathbf{D}}e^{-\hat{\boldsymbol{\gamma}}^\dagger\tau}d\tau, \tag{50}$$

if the integral converges. A sufficient condition is that the operator $\hat{\boldsymbol{\gamma}}$ has a complete biorthogonal set of eigenfunctions [28] and that its eigenvalues all have positive real parts.

3.3. Potential Landscape and Flux Field

With the steady-state probability distribution given in Equation (47), the potential landscape has the quadratic form

$$U[\boldsymbol{\phi}] = -\ln P_s[\boldsymbol{\phi}] = \frac{1}{2}\iint \boldsymbol{\phi}(\mathbf{x}) \cdot \boldsymbol{\Sigma}_s^{-1}(\mathbf{x},\mathbf{x}') \cdot \boldsymbol{\phi}(\mathbf{x}')d\mathbf{x}d\mathbf{x}', \tag{51}$$

up to an additive constant. Then the probability flux velocity field at the steady state can be obtained using the non-equilibrium force decomposition in Equation (12), which yields

$$\begin{aligned}\mathbf{V}_s(\mathbf{x})[\boldsymbol{\phi}] &= \mathbf{F}(\mathbf{x})[\boldsymbol{\phi}] + \int \mathbf{D}(\mathbf{x},\mathbf{x}') \cdot \delta_{\boldsymbol{\phi}(\mathbf{x}')}U[\boldsymbol{\phi}]d\mathbf{x}' \\ &= -\int \boldsymbol{\gamma}(\mathbf{x},\mathbf{x}') \cdot \boldsymbol{\phi}(\mathbf{x}')d\mathbf{x}' \\ &\quad + \int \left[\int \mathbf{D}(\mathbf{x},\mathbf{x}'')\boldsymbol{\Sigma}_s^{-1}(\mathbf{x}'',\mathbf{x}')d\mathbf{x}''\right] \cdot \boldsymbol{\phi}(\mathbf{x}')d\mathbf{x}'\end{aligned} \tag{52}$$

In operator notations, this reads $\mathbf{V}_s = -(\hat{\boldsymbol{\gamma}} - \hat{\mathbf{D}}\hat{\Sigma}_s^{-1})\boldsymbol{\phi}$.

Novanishing $\mathbf{V}_s$ is an indicator that the steady state is a non-equilibrium state with time irreversibility. The steady state is an equilibrium state if $\mathbf{V}_s$ vanishes. According to the expression of $\mathbf{V}_s$, this requires $\hat{\boldsymbol{\gamma}} = \hat{\mathbf{D}}\hat{\Sigma}_s^{-1}$. Combined with Equation (49) and eliminating $\hat{\Sigma}_s$ (assuming the relevant operators are invertible), we obtain

$$\hat{\boldsymbol{\gamma}}\hat{\mathbf{D}} = \hat{\mathbf{D}}\hat{\boldsymbol{\gamma}}^\dagger, \tag{53}$$

or, more explicitly,

$$\int \boldsymbol{\gamma}(\mathbf{x},\mathbf{x}'')\mathbf{D}(\mathbf{x}'',\mathbf{x}')d\mathbf{x}'' = \int \mathbf{D}(\mathbf{x},\mathbf{x}'')\boldsymbol{\gamma}^T(\mathbf{x}',\mathbf{x}'')d\mathbf{x}''. \tag{54}$$

This is the detailed balance condition for spatially extended OU processes (assuming even state variables). For the system to sustain non-equilibrium steady states, this detailed balance condition must be violated.

3.4. Response Function

The response function has the general expression in Equation (22), which is reproduced below for the reader's convenience

$$\mathbf{R}(\mathbf{x},\mathbf{x}',t) = \theta(t)\int \boldsymbol{\phi}(\mathbf{x})e^{Lt}\left(-\delta_{\boldsymbol{\phi}(\mathbf{x}')}\right)P_s[\boldsymbol{\phi}]\mathcal{D}\boldsymbol{\phi}. \tag{55}$$

We obtain the response function for the OU process in the following way. For $t \geq 0$, we have

$$\begin{aligned}\partial_t\mathbf{R}(\mathbf{x},\mathbf{x}',t) &= \int \boldsymbol{\phi}(\mathbf{x})Le^{Lt}\left(-\delta_{\boldsymbol{\phi}(\mathbf{x}')}\right)P_s[\boldsymbol{\phi}]\mathcal{D}\boldsymbol{\phi} \\ &= \int \left(L^\dagger\boldsymbol{\phi}(\mathbf{x})\right)e^{Lt}\left(-\delta_{\boldsymbol{\phi}(\mathbf{x}')}\right)P_s[\boldsymbol{\phi}]\mathcal{D}\boldsymbol{\phi} \\ &= -\int d\mathbf{x}''\,\boldsymbol{\gamma}(\mathbf{x},\mathbf{x}'')\mathbf{R}(\mathbf{x}'',\mathbf{x}',t),\end{aligned} \tag{56}$$

where we have used

$$L^\dagger\boldsymbol{\phi}(\mathbf{x}) = -\int d\mathbf{x}''\,\boldsymbol{\gamma}(\mathbf{x},\mathbf{x}'') \cdot \boldsymbol{\phi}(\mathbf{x}'') \tag{57}$$

for the OU process, according to the expression of $L^\dagger$ in Equation (46). Equation (56) needs to be supplemented with an initial condition. Setting $t = 0$ in Equation (55) and performing integration by parts in the state space, we find

$$\begin{aligned}\mathbf{R}(\mathbf{x},\mathbf{x}',0) &= \int \boldsymbol{\phi}(\mathbf{x})\left(-\delta_{\boldsymbol{\phi}(\mathbf{x}')}\right) P_s[\boldsymbol{\phi}]\mathcal{D}\boldsymbol{\phi} \\ &= \int \left(\delta_{\boldsymbol{\phi}(\mathbf{x}')}\boldsymbol{\phi}(\mathbf{x})\right) P_s[\boldsymbol{\phi}]\mathcal{D}\boldsymbol{\phi} \\ &= \mathbf{I}\delta(\mathbf{x}-\mathbf{x}'). \end{aligned} \tag{58}$$

The response function can be obtained by solving Equation (56) under the initial condition in Equation (58). In operator notations, the response function has the formal solution ($t \geq 0$)

$$\mathbf{R}(\mathbf{x},\mathbf{x}',t) = e^{-\hat{\boldsymbol{\gamma}}t}\mathbf{I}\delta(\mathbf{x}-\mathbf{x}'). \tag{59}$$

This is actually the Green's function of the deterministic dynamics of the OU process.

In fact, we can obtain the above result in a more direct way. Noticing that Equation (57) means $L^\dagger\boldsymbol{\phi}(\mathbf{x}) = -\hat{\boldsymbol{\gamma}}\boldsymbol{\phi}(\mathbf{x})$, we have

$$\begin{aligned}\mathbf{R}(\mathbf{x},\mathbf{x}',t) &= \theta(t)\int \left(e^{L^\dagger t}\boldsymbol{\phi}(\mathbf{x})\right)\left(-\delta_{\boldsymbol{\phi}(\mathbf{x}')}\right) P_s[\boldsymbol{\phi}]\mathcal{D}\boldsymbol{\phi} \\ &= \theta(t)\int \left(e^{-\hat{\boldsymbol{\gamma}}t}\boldsymbol{\phi}(\mathbf{x})\right)\left(-\delta_{\boldsymbol{\phi}(\mathbf{x}')}\right) P_s[\boldsymbol{\phi}]\mathcal{D}\boldsymbol{\phi} \\ &= \theta(t)e^{-\hat{\boldsymbol{\gamma}}t}\mathbf{I}\delta(\mathbf{x}-\mathbf{x}'). \end{aligned} \tag{60}$$

3.5. Field-Field Correlation Function

The field-field correlation function, with its general expression in Equation (25), can be calculated for the OU process as follows:

$$\begin{aligned}\langle\boldsymbol{\phi}(\mathbf{x},t)\boldsymbol{\phi}(\mathbf{x}',0)\rangle_s &= \int \left(e^{L^\dagger t}\boldsymbol{\phi}(\mathbf{x})\right)\boldsymbol{\phi}(\mathbf{x}')P_s[\boldsymbol{\phi}]\mathcal{D}\boldsymbol{\phi} \\ &= e^{-\hat{\boldsymbol{\gamma}}t}\int \boldsymbol{\phi}(\mathbf{x})\boldsymbol{\phi}(\mathbf{x}')P_s[\boldsymbol{\phi}]\mathcal{D}\boldsymbol{\phi} \\ &= e^{-\hat{\boldsymbol{\gamma}}t}\langle\boldsymbol{\phi}(\mathbf{x})\boldsymbol{\phi}(\mathbf{x}')\rangle_s \\ &= e^{-\hat{\boldsymbol{\gamma}}t}\boldsymbol{\Sigma}_s(\mathbf{x},\mathbf{x}'), \end{aligned} \tag{61}$$

where we have used the fact that the steady-state probability distribution of the OU process, given in Equation (47), is a Gaussian distribution with zero mean and has the covariance matrix $\langle\boldsymbol{\phi}(\mathbf{x})\boldsymbol{\phi}(\mathbf{x}')\rangle_s = \boldsymbol{\Sigma}_s(\mathbf{x},\mathbf{x}')$.

The time derivative of the field-field correlation function is then found to be

$$\begin{aligned}\frac{\partial}{\partial t}\langle\boldsymbol{\phi}(\mathbf{x},t)\boldsymbol{\phi}(\mathbf{x}',0)\rangle_s &= -e^{-\hat{\boldsymbol{\gamma}}t}\hat{\boldsymbol{\gamma}}\boldsymbol{\Sigma}_s(\mathbf{x},\mathbf{x}') \\ &= -e^{-\hat{\boldsymbol{\gamma}}t}\int d\mathbf{x}''\boldsymbol{\gamma}(\mathbf{x},\mathbf{x}'')\boldsymbol{\Sigma}_s(\mathbf{x}'',\mathbf{x}'), \end{aligned} \tag{62}$$

where we have spelled out the action of $\hat{\boldsymbol{\gamma}}$ on $\boldsymbol{\Sigma}_s(\mathbf{x},\mathbf{x}')$.

3.6. Field-Flux Correlation Function

With the expression of $\mathbf{V}_s(\mathbf{x})[\boldsymbol{\phi}]$ in Equation (52), the field-flux correlation function is calculated as follows:

$$\begin{aligned}&\langle\boldsymbol{\phi}(\mathbf{x},t)\mathbf{V}_s(\mathbf{x}',0)\rangle_s = \int \left(e^{L^\dagger t}\boldsymbol{\phi}(\mathbf{x})\right)\mathbf{V}_s(\mathbf{x}')[\boldsymbol{\phi}]P_s[\boldsymbol{\phi}]\mathcal{D}\boldsymbol{\phi} \\ &= e^{-\hat{\boldsymbol{\gamma}}t}\langle\boldsymbol{\phi}(\mathbf{x})\mathbf{V}_s(\mathbf{x}')\rangle_s \\ &= e^{-\hat{\boldsymbol{\gamma}}t}\int d\mathbf{x}''\langle\boldsymbol{\phi}(\mathbf{x})\boldsymbol{\phi}(\mathbf{x}'')\rangle_s\big[-\boldsymbol{\gamma}^T(\mathbf{x}',\mathbf{x}'') \\ &+ \int d\mathbf{x}'''\boldsymbol{\Sigma}_s^{-1}(\mathbf{x}'',\mathbf{x}''')\mathbf{D}(\mathbf{x}''',\mathbf{x}')\big] \\ &= e^{-\hat{\boldsymbol{\gamma}}t}\int d\mathbf{x}''\boldsymbol{\Sigma}_s(\mathbf{x},\mathbf{x}'')\big[-\boldsymbol{\gamma}^T(\mathbf{x}',\mathbf{x}'') \\ &+ \int d\mathbf{x}'''\boldsymbol{\Sigma}_s^{-1}(\mathbf{x}'',\mathbf{x}''')\mathbf{D}(\mathbf{x}''',\mathbf{x}')\big] \\ &= e^{-\hat{\boldsymbol{\gamma}}t}\big[-\int d\mathbf{x}''\boldsymbol{\Sigma}_s(\mathbf{x},\mathbf{x}'')\boldsymbol{\gamma}^T(\mathbf{x}',\mathbf{x}'') + \mathbf{D}(\mathbf{x},\mathbf{x}')\big]. \end{aligned} \tag{63}$$

3.7. Generalized FDT

Recall that the generalized FDT in Equation (37) has the form

$$\begin{aligned}\mathbf{R}(\mathbf{x},\mathbf{x}'',t) = -\theta(t)\int \bigg[&\frac{\partial}{\partial t}\langle\boldsymbol{\phi}(\mathbf{x},t)\boldsymbol{\phi}(\mathbf{x}',0)\rangle_s \\ &+\langle\boldsymbol{\phi}(\mathbf{x},t)\mathbf{V}_s(\mathbf{x}',0)\rangle_s\bigg]\mathbf{D}^{-1}(\mathbf{x}',\mathbf{x}'')d\mathbf{x}', \end{aligned} \tag{64}$$

where we have switched the symbols $\mathbf{x}'$ and $\mathbf{x}''$ for convenience. We verify this relation for the OU process.

The quantities in the square brackets read

$$\begin{aligned}&\frac{\partial}{\partial t}\langle\boldsymbol{\phi}(\mathbf{x},t)\boldsymbol{\phi}(\mathbf{x}',0)\rangle_s + \langle\boldsymbol{\phi}(\mathbf{x},t)\mathbf{V}_s(\mathbf{x}',0)\rangle_s \\ =&e^{-\hat{\boldsymbol{\gamma}}t}\bigg[-\int d\mathbf{x}''\boldsymbol{\gamma}(\mathbf{x},\mathbf{x}'')\boldsymbol{\Sigma}_s(\mathbf{x}'',\mathbf{x}') \\ &-\int d\mathbf{x}''\boldsymbol{\Sigma}_s(\mathbf{x},\mathbf{x}'')\boldsymbol{\gamma}^T(\mathbf{x}',\mathbf{x}'') + \mathbf{D}(\mathbf{x},\mathbf{x}')\bigg] \\ =&e^{-\hat{\boldsymbol{\gamma}}t}\left[-2\mathbf{D}(\mathbf{x},\mathbf{x}') + \mathbf{D}(\mathbf{x},\mathbf{x}')\right] \\ =&-e^{-\hat{\boldsymbol{\gamma}}t}\mathbf{D}(\mathbf{x},\mathbf{x}'), \end{aligned} \tag{65}$$

where we have used the expressions in Equations (62) and (63) as well as Equation (48) that determines $\boldsymbol{\Sigma}_s(\mathbf{x}-\mathbf{x}')$. Therefore, the RHS of the generalized FDT for the OU process has the expression

$$\begin{aligned}\text{RHS} &= \theta(t)e^{-\hat{\boldsymbol{\gamma}}t}\int \mathbf{D}(\mathbf{x},\mathbf{x}')\mathbf{D}^{-1}(\mathbf{x}',\mathbf{x}'')d\mathbf{x}' \\ &= \theta(t)e^{-\hat{\boldsymbol{\gamma}}t}\mathbf{I}\delta(\mathbf{x}-\mathbf{x}'') \\ &= \mathbf{R}(\mathbf{x},\mathbf{x}'',t) \\ &= \text{LHS}, \end{aligned} \tag{66}$$

where we have used the expression of the response function for the OU process in Equation (60). We have thus demonstrated that the generalized FDT holds true for a general OU process.

4. A PARTICULAR EXAMPLE: THE MODIFIED STOCHASTIC CABLE EQUATION

We further study a particular example of the OU process with explicitly solvable non-equilibrium steady states to demonstrate the generalized FDT. In this example we use a modified version of the SCE. The SCE is a stochastic differential equation that has been extensively used in theoretical neurobiology [23, 41]. It describes the evolution of the membrane potential of a spatially extended neuron under the influence of stochastic inputs. We studied this model in a previous work in the context of non-equilibrium thermodynamics, but the steady state of the system was found to be an equilibrium state with detailed balance and time reversal symmetry [36]. Thus the original form of this model is not suitable for illustrating the generalized FDT. However, we discovered in this work that with some modifications the SCE can also sustain non-equilibrium steady states. It is this modified stochastic cable equation (MSCE) that will be studied in this section.

4.1. Stochastic Field Dynamics

In its typical form, the original SCE is considered on a one-dimensional interval modeling the spatial extension of the neuron and has the form

$$\partial_t \phi(x,t) = \partial_x^2 \phi(x,t) - \phi(x,t) + \zeta(x,t), \tag{67}$$

where $\zeta(x,t)$ is space-time Gaussian white noise with zero mean and has the correlation

$$\langle \zeta(x,t)\zeta(x',t')\rangle = \delta(x-x')\delta(t-t'). \tag{68}$$

We modify the above equation and consider the following MSCE defined on the interval $[0,\pi]$:

$$\partial_t \phi(x,t) = \partial_x^2 \phi(x,t) - \phi(x,t) - 2\mu\partial_x\phi(x,t) + \zeta(x,t), \tag{69}$$

where the Gaussian white noise $\zeta(x,t)$ has the correlation

$$\langle \zeta(x,t)\zeta(x',t')\rangle = 2(1-\partial_x^2)\delta(x-x')\delta(t-t'). \tag{70}$$

The equation is supplemented with the Dirichlet boundary condition

$$\phi(0,t) = \phi(\pi,t) = 0. \tag{71}$$

There are two major differences between the MSCE and the SCE. One difference is the presence of an additional term, $-2\mu\partial_x\phi(x,t)$, in the deterministic dynamics. The other is the form of the correlation of the stochastic force. These differences allow the MSCE to sustain non-equilibrium steady states with detailed balance breaking and time irreversibility, in contrast with the original SCE that has equilibrium steady states preserving detailed balance. This crucial distinction will be demonstrated and discussed later.

4.2. Operator Analysis

The MSCE can be rewritten in the form

$$\partial_t \phi(x,t) = -\hat{\gamma}\phi(x,t) + \zeta(x,t) \tag{72}$$

with $\langle \zeta(x,t)\zeta(x',t')\rangle = 2D(x,x')\delta(t-t')$. In this form $\hat{\gamma}$ is an operator with the expression

$$\hat{\gamma} = 1 - \partial_x^2 + 2\mu\partial_x. \tag{73}$$

Note that $\hat{\gamma}$ is not a Hermitian operator, since its adjoint is given by

$$\hat{\gamma}^\dagger = 1 - \partial_x^2 - 2\mu\partial_x. \tag{74}$$

Thus $\hat{\gamma}$ can be decomposed into a Hermitian part

$$\hat{\gamma}_h = 1 - \partial_x^2 \tag{75}$$

and an anti-Hermitian part[1]

$$\hat{\gamma}_a = 2\mu\partial_x. \tag{76}$$

These two parts commute with each other, namely

$$[\hat{\gamma}_h, \hat{\gamma}_a] = 0, \tag{77}$$

as can be verified. We shall show later that the anti-Hermitian operator $\hat{\gamma}_a$ is directly related to the irreversible probability flux that signifies detailed balance breaking and time irreversibility in the steady state. For the special case $\mu = 0$, the anti-Hermitian part $\hat{\gamma}_a$ vanishes and $\hat{\gamma}$ reduces to the Hermitian operator in the SCE that has equilibrium steady states. The magnitude of the parameter μ can be interpreted as a measure of the distance from equilibrium or the degree of detailed balance breaking.

The non-Hermitian operator $\hat{\gamma}$ in general does not have a set of orthonormal eigenfunctions. However, a complete biorthogonal set of eigenfunctions can be found for this operator. This amounts to finding the eigenfunctions of both $\hat{\gamma}$ and $\hat{\gamma}^\dagger$. By solving the eigen-equation $\hat{\gamma}\varphi_n(x) = \lambda_n\varphi_n(x)$ under the specified boundary condition, we obtain the eigenvalues of $\hat{\gamma}$

$$\lambda_n = n^2 + \mu^2 + 1 \quad (n \geq 1), \tag{78}$$

and the corresponding eigenfunctions

$$\varphi_n(x) = \sqrt{\frac{2}{\pi}}\, e^{\mu x} \sin nx \quad (n \geq 1). \tag{79}$$

Notice that $\hat{\gamma}^\dagger$ can be obtained from $\hat{\gamma}$ simply by replacing μ with $-\mu$. Therefore, the eigen-equation $\hat{\gamma}^\dagger\psi_n(x) = \lambda_n\psi_n(x)$ can be solved with the same set of eigenvalues in Equation (78), and the corresponding eigenfunctions are given by

$$\psi_n(x) = \sqrt{\frac{2}{\pi}}\, e^{-\mu x} \sin nx \quad (n \geq 1). \tag{80}$$

These two sets of eigenfunctions are orthonormal with respect to each other in the sense that

$$\int_0^\pi \varphi_n(x)\psi_m(x)dx = \delta_{nm}. \tag{81}$$

[1]The definition of an operator and whether it is Hermitian or anti-Hermitian depend on the boundary condition. The operator ∂_x is anti-Hermitian under the Dirichlet boundary condition in Equation (71), but it is not anti-Hermitian under the Neumann boundary condition due to the presence of non-vanishing boundary terms when performing integration by parts.

They are also complete in the sense that

$$\sum_{n=1}^{\infty} \varphi_n(x)\psi_n(x') = \delta(x - x'). \tag{82}$$

This completeness relation (or resolution of the identity) can be derived from the completeness of the set of orthonormal functions $\{e_n(x) = \sqrt{2/\pi}\sin nx\}$ by a similarity transformation. By considering the Fourier analysis of the function $e^{-\mu x}f(x)$ in terms of $\{e_n(x)\}$, where $f(x)$ satisfies the given boundary condition, one can show the completeness relation in Equation (82) for the function $f(x)$.

The differential operator $\hat{\gamma}$ can also be represented as an integral operator, with the integral kernel

$$\gamma(x, x') = \hat{\gamma}\delta(x - x') = (1 - \partial_x^2 + 2\mu\partial_x)\delta(x - x'). \tag{83}$$

Using the completeness relation in Equation (82) and the fact that φ_n is the eigenfunction of $\hat{\gamma}$, it is easy to see that

$$\gamma(x, x') = \sum_{n=1}^{\infty} \lambda_n \varphi_n(x)\psi_n(x'). \tag{84}$$

The form of correlation of the stochastic force in Equation (70) means the diffusion matrix in the FFPE has the form

$$D(x, x') = (1 - \partial_x^2)\delta(x - x') = \hat{\gamma}_h\delta(x - x'), \tag{85}$$

where $\hat{\gamma}_h$ is the Hermitian part of $\hat{\gamma}$. By interpreting $D(x, x')$ as an integral kernel, we see that the associated operator $\hat{D}$ has the form

$$\hat{D} = \hat{\gamma}_h = 1 - \partial_x^2. \tag{86}$$

This particular choice of $D(x, x')$ or $\hat{D}$ allows the steady state of the system to be explicitly solved without interfering with its non-equilibrium nature as we shall see later.

4.3. Functional Fokker-Planck Equation

The FFPE in this case reduces to the following form

$$\begin{aligned} \partial_t P_t[\phi] = &\int dx\, \delta_{\phi(x)} \left(\hat{\gamma}\phi(x)P_t[\phi]\right) \\ &+ \int dx\, \delta_{\phi(x)}\hat{D}\delta_{\phi(x)}P_t[\phi], \end{aligned} \tag{87}$$

where $\hat{\gamma}$ and $\hat{D}$ are given by Equations (73) and (86), respectively.

The steady-state probability distribution functional $P_s[\phi]$ is a Gaussian distribution functional

$$P_s[\phi] = \mathcal{N}\exp\left\{-\frac{1}{2}\iint \phi(x)\Sigma_s^{-1}(x, x')\phi(x')dxdx'\right\}, \tag{88}$$

where the covariance matrix $\Sigma_s(x, x')$ with the associated operator $\hat{\Sigma}_s$ is determined by the equation (see Equation 49)

$$\hat{\gamma}\hat{\Sigma}_s + \hat{\Sigma}_s\hat{\gamma}^\dagger = 2\hat{D}. \tag{89}$$

As a result of the particular choice $\hat{D} = \hat{\gamma}_h = (\hat{\gamma} + \hat{\gamma}^\dagger)/2$, it is easy to see that the solution is given by

$$\hat{\Sigma}_s = \hat{I}, \tag{90}$$

namely the identity operator, which corresponds to $\Sigma_s(x, x') = \delta(x - x')$. (This result can also be obtained using the solution formula for $\hat{\Sigma}_s$ in Equation (50) and the biorthogonal expansion of $\hat{\gamma}$.) Therefore, the steady-state distribution is explicitly solved as

$$P_s[\phi] = \mathcal{N}\exp\left\{-\frac{1}{2}\int \phi^2(x)dx\right\}. \tag{91}$$

4.4. Potential Landscape and Flux Field

The potential landscape is given by

$$U[\phi] = -\ln P_s[\phi] = \frac{1}{2}\int \phi^2(x)dx, \tag{92}$$

up to an additive constant. The steady-state probability flux velocity field indicating detailed balance breaking can be calculated with the help of the non-equilibrium force decomposition:

$$\begin{aligned} V_s(x)[\phi] &= F(x)[\phi] + \hat{D}\delta_{\phi(x)}U[\phi] \\ &= -\hat{\gamma}\phi(x) + \hat{D}\phi(x) \\ &= -\hat{\gamma}_a\phi(x) = -2\mu\partial_x\phi(x), \end{aligned} \tag{93}$$

where we have used $\hat{D} = \hat{\gamma}_h$ and $\hat{\gamma} = \hat{\gamma}_h + \hat{\gamma}_a$.

In this particular case the steady-state probability flux that signifies detailed balance breaking and time irreversibility in the non-equilibrium steady state is directly determined by the anti-Hermitian part of the operator $\hat{\gamma}$ in the deterministic force. Notice that V_s is proportional to the parameter μ. The steady state of the system is a non-equilibrium state as long as $\mu \neq 0$, and the special case $\mu = 0$ reduces to the equilibrium case of the SCE. Hence, the magnitude of the parameter μ may be considered as a measure of the degree of detailed balance breaking or the distance from equilibrium.

4.5. Response Function

Specializing the response function for general OU process in Equation (60) to this one-dimensional example, we see that $R(x, x', t) = e^{-\hat{\gamma}t}\delta(x - x')$. The response function in this case can be calculated more explicitly using the completeness relation in Equation (82) as follows:

$$\begin{aligned} R(x, x', t) = e^{-\hat{\gamma}t}\delta(x - x') &= \sum_{n=1}^{\infty} e^{-\hat{\gamma}t}\varphi_n(x)\psi_n(x') \\ &= \sum_{n=1}^{\infty} e^{-\lambda_n t}\varphi_n(x)\psi_n(x') \\ &= \frac{2}{\pi}\sum_{n=1}^{\infty} e^{-(n^2+\mu^2+1)t+\mu(x-x')}\sin nx \sin nx' \\ &= B(x - x', t|\mu)R_0(x, x', t), \end{aligned} \tag{94}$$

where

$$B(x-x',t|\mu)=e^{-\mu^2t+\mu(x-x')} \tag{95}$$

and

$$R_0(x,x',t)=\frac{1}{\pi}\sum_{n=1}^{\infty}e^{-(n^2+1)t}\left[\cos n(x-x')-\cos n(x+x')\right]. \tag{96}$$

In the above we have written the response function in the product form

$$R(x,x',t)=B(x-x',t|\mu)R_0(x,x',t). \tag{97}$$

The function $R_0(x,x',t)$ is the equilibrium response function. This can be seen by setting $\mu=0$ (the equilibrium case) and noticing that $B(x-x',t|0)=1$. However, it does not seem to have a closed expression. For fixed x and x', the response generally decays with time. This can be seen from the expression in Equation (96) or the physical intuition that the deterministic dynamics is a damping dynamics that relaxes to equilibrium (the eigenvalues of $\hat{\gamma}$ are all positive). For fixed t and x', numerical investigation suggests that the response as a function of x is typically unimodal and vanishes at the boundary (the latter due to the Dirichlet boundary condition).

On the other hand, the function $B(x-x',t|\mu)$ fully captures the effect of detailed balance breaking on the response function. In the spatial dimension, this function has the exponential form $e^{\mu(x-x')}$, which increases or decreases the response exponentially, depending on the relative position between the response point x and the stimulus point x' and the sign of the parameter μ. On the other hand, in the temporal dimension the function has the form $e^{-\mu^2t}$, which shows that the response decays faster due to the presence of detailed balance breaking.

4.6. Field-Field Correlation Function

The field-field correlation function can be obtained as follows (Equation 61):

$$\begin{aligned}\langle\phi(x,t)\phi(x',0)\rangle_s&=\langle e^{L^\dagger t}\phi(x)\phi(x')\rangle_s\\&=e^{-\hat{\gamma}t}\langle\phi(x)\phi(x')\rangle_s\\&=e^{-\hat{\gamma}t}\Sigma_s(x-x').\end{aligned} \tag{98}$$

For this particular example we actually have, more specifically, $\Sigma_s(x-x')=\delta(x-x')$. Therefore,

$$\langle\phi(x,t)\phi(x',0)\rangle_s=e^{-\hat{\gamma}t}\delta(x-x')=R(x,x',t). \tag{99}$$

That is, the correlation function is equal to the response function in this special example. The effect of detailed balance breaking on the correlation function is thus the same as that analyzed for the response function.

Notice that this special scenario that the correlation function coincides with the response function does not mean the field-flux correlation in the generalized FDT vanishes, because what appears in the generalized FDT is not the field-field correlation function itself, but its time derivative. The time derivative of the field-field correlation function is given by

$$\frac{\partial}{\partial t}\langle\phi(x,t)\phi(x',0)\rangle_s=-\hat{\gamma}e^{-\hat{\gamma}t}\delta(x-x')=-\hat{\gamma}R(x,x',t), \tag{100}$$

which has the more specific expression

$$\frac{\partial}{\partial t}\langle\phi(x,t)\phi(x',0)\rangle_s=-\sum_{n=1}^{\infty}\lambda_ne^{-\lambda_nt}\varphi_n(x)\psi_n(x'). \tag{101}$$

4.7. Field-Flux Correlation Function

The field-flux correlation function associated with detailed balance breaking is obtained as follows:

$$\begin{aligned}&\langle\phi(x,t)V_s(x',0)\rangle_s\\=&e^{-\hat{\gamma}t}\langle\phi(x)V_s(x')\rangle_s=e^{-\hat{\gamma}t}\langle\phi(x)(-\hat{\gamma}_a')\phi(x')\rangle_s\\=&-e^{-\hat{\gamma}t}\hat{\gamma}_a'\Sigma_s(x-x')=-e^{-\hat{\gamma}t}\hat{\gamma}_a'\delta(x-x')\\=&e^{-\hat{\gamma}t}\hat{\gamma}_a\delta(x-x')=\hat{\gamma}_ae^{-\hat{\gamma}t}\delta(x-x')\\=&\hat{\gamma}_aR(x,x',t),\end{aligned} \tag{102}$$

where $\hat{\gamma}_a'=2\mu\partial_{x'}$. In the above we have used $V_s=-\hat{\gamma}_a\phi$, $\partial_{x'}\delta(x-x')=-\partial_x\delta(x-x')$, and $[\hat{\gamma}_a,\hat{\gamma}]=0$ implied by $[\hat{\gamma}_h,\hat{\gamma}_a]=0$ and $\hat{\gamma}=\hat{\gamma}_h+\hat{\gamma}_a$.

The field-flux correlation function has the following more specific expression

$$\begin{aligned}&\langle\phi(x,t)V_s(x',0)\rangle_s\\=&2\mu\partial_xR(x,x',t)\\=&2\mu\partial_x[B(x-x',t|\mu)R_0(x,x',t)]\\=&2\mu B(x-x',t|\mu)(\mu+\partial_x)R_0(x,x',t)\\=&2\mu e^{-\mu^2t+\mu(x-x')}(\mu+\partial_x)R_0(x,x',t).\end{aligned} \tag{103}$$

It vanishes in the special equilibrium case $\mu=0$.

4.8. Generalized FDT

The generalized FDT for this particular system has the form

$$R(x,x',t)=-\theta(t)\hat{D}^{-1}\left[\frac{\partial}{\partial t}\langle\phi(x,t)\phi(x',0)\rangle_s+\langle\phi(x,t)V_s(x',0)\rangle_s\right], \tag{104}$$

which is shown as follows. For $t\geq 0$, the RHS of the equation has the expression

$$\begin{aligned}\text{RHS}&=-\hat{D}^{-1}\left[\frac{\partial}{\partial t}\langle\phi(x,t)\phi(x',0)\rangle_s+\langle\phi(x,t)V_s(x',0)\rangle_s\right]\\&=-\hat{D}^{-1}\left[-\hat{\gamma}R(x,x',t)+\hat{\gamma}_aR(x,x',t)\right]\\&=\hat{D}^{-1}(\hat{\gamma}-\hat{\gamma}_a)R(x,x',t)=\hat{D}^{-1}\hat{\gamma}_hR(x,x',t)\\&=\hat{D}^{-1}\hat{D}R(x,x',t)=R(x,x',t),\end{aligned} \tag{105}$$

which is equal to the LHS of Equation (104). In the above we have used the expression of the time derivative of the correlation function in Equation (100), the expression of the field-flux correlation function in Equation (102), and the fact that $\hat{D} = \hat{\gamma}_h$ by construction.

We have thus demonstrated that the MSCE model satisfies the generalized FDT in the form of Equation (104). It is worthwhile noting that this particular form of the generalized FDT, with an operator $\hat{D}^{-1}$ acting on functions of x on the right, is specific to this example due to some special features in the model. Although in this special example it is also equivalent to the general form of the FDT given in Equation (37), this is not generally true when a different system is considered. In a more general setting the form of the generalized FDT in Equation (37) or its alternative form in Equation (41) still applies. In addition, we have also shown in this particular example that detailed balance breaking indicated by the parameter μ, which characterizes the non-equilibrium nature of the steady state, affects both the response function and the field correlation as they are both dependent on μ. It is the ternary relation quantified by the generalized FDT that determines how the response function and field correlation are related to each other by the flux correlation in non-equilibrium steady states.

In addition, we note that in this particular example of the MSCE, the deterministic dynamics, $\partial_t \phi = -\hat{\gamma}\phi$, is a purely damping dynamics, since the eigenvalues of $\hat{\gamma}$ are all positive. As a result, the steady state of the deterministic system (the fixed "point" in the state space) is the zero field configuration, $\phi(x) = 0$. Therefore, there is no pattern formation in this system, which also has to do with the linear nature of the system. In this respect, nonlinear spatially extended systems with the spatial-temporal dynamics of pattern formation and self-organization represent more interesting systems [17–21]. However, these systems are also more difficult to handle. In the context of the potential landscape and flux field theory, the non-equilibrium force decomposition, $\mathbf{F}(\mathbf{x})[\boldsymbol{\phi}] = -\int d\mathbf{x}'\mathbf{D}(\mathbf{x},\mathbf{x}')\cdot \delta_{\boldsymbol{\phi}(\mathbf{x}')}U[\boldsymbol{\phi}] + \mathbf{V}_s(\mathbf{x})[\boldsymbol{\phi}]$, plays a central role in the study of the global dynamics of spatially extended systems in the state space [27]. In particular, the flux $\mathbf{V}_s(\mathbf{x})[\boldsymbol{\phi}]$ that signifies detailed balance breaking is the part of the driving force that is essential for the non-equilibrium dynamics of the system, which is closely related to the manifestation of pattern formation and self-organization in nonlinear spatially extended systems. In this work, we have also demonstrated how the flux $\mathbf{V}_s(\mathbf{x})[\boldsymbol{\phi}]$ is manifested in the generalized FDT for non-equilibrium spatially extended systems, altering the structure of equilibrium FDT and transforming it into a ternary relation. Therefore, the flux $\mathbf{V}_s(\mathbf{x})[\boldsymbol{\phi}]$ can serve as a bridge that connects the spatial-temporal dynamics of pattern formation and self-organization to the generalized FDT of non-equilibrium spatially extended systems. This line of research will be pursued in the future.

5. CONCLUSION

In this work, we have established a generalized form of the FDT for spatially extended non-equilibrium stochastic systems. In formulating the generalized FDT, we invoked a key element in the potential landscape and flux field framework, namely the non-equilibrium force decomposition, which played an essential role in reaching the final form of the generalized FDT. We have also demonstrated the generalized FDT with spatially extended systems described by general OU processes and further studied in detail a particular example based on a modified version of the SCE to illustrate the general results. These more concrete studies have substantiated the validity of the generalized FDT.

The distinguishing feature of the generalized FDT formulated in this work is that it represents a ternary relation instead of a binary relation as in the equilibrium FDT. In addition to (the time derivative of) the field correlation and the response function, which also exist in the equilibrium FDT, there is an additional term, namely the flux correlation, which enters the generalized FDT and qualitatively alters the structure of the FDT by transforming it into a ternary relation. This additional contribution of the flux correlation originates from detailed balance breaking and inherent time irreversibility in non-equilibrium steady states, which is signified by the presence of steady-state irreversible probability flux that reflects the constant flows of matter, energy or information in and out of the system. The non-equilibrium nature of the steady state alters how the system responds to perturbations, for instance, by changing the target state that the system relaxes back to. It also affects the fluctuations of the system at the steady state due to the presence of fluctuations associated with non-equilibrium steady-state processes. Depending on the perspective taken, the flux correlation associated with the non-equilibrium nature of the steady state may either be interpreted as part of the system response to perturbations or part of the fluctuations at the non-equilibrium steady state. In the end, it is the ternary relation quantified by the generalized FDT that determines how the response function and the field correlation should be related to each other by the flux correlation when the steady state of the system has a non-equilibrium nature. In the special case when the steady state of the system is an equilibrium state with detailed balance, the contribution of flux correlation vanishes and the ternary relation in the generalized FDT reduces to the binary relation in the equilibrium FDT.

We have also discussed experimental implications of the generalized FDT in this work. For equilibrium spatially extended systems with detailed balance, information obtained from experiments on either the response function or the field correlation implies the other due to the binary relation of the equilibrium FDT. For spatially extended systems sustaining non-equilibrium steady states, however, the response function and the field correlation are no longer tightly connected to each other due to the ternary relation of the generalized FDT. Since they are relatively easier to access experimentally than the flux correlation, experimental information acquired on the response function and the field correlation can be used to infer the flux correlation that contains quantitative information on the non-equilibrium nature of the steady state of the system. The same type of information may be inferred from experimental data using the asymmetry relation of the correlation function derived in Equation (31) in this work.

Considering the generality of the setting in which the generalized FDT is derived, results obtained in the general setting in this work have a much wider range of applications beyond the more restricted setting of the OU process and the particular example used to substantiate the general results. A variety of physical, chemical and biological spatially extended systems capable of sustaining non-equilibrium steady states may be amenable to the generalized FDT derived in this work. When some of the restrictions in the general setting are further lifted, an even wider range of applications including more general types of systems may become accessible, which will be pursued in future work. Furthermore, we will also explore in the future the connection of the spatial-temporal dynamics of pattern formation and self-organization to the generalized FDT via the bridge established by the irreversible probability flux that signifies detailed balance breaking and time irreversibility in non-equilibrium spatially extended systems. The stochastic trajectory perspective of the FDT near equilibrium steady states and its extension to non-equilibrium steady states far from thermodynamic equilibrium will also be investigated.

DATA AVAILABILITY STATEMENT

All datasets presented in this study are included in the article/supplementary material.

AUTHOR CONTRIBUTIONS

WW and JW conceived the idea and wrote the paper. WW performed the formal analysis. JW surpervised the work. Both authors contributed to the article and approved the submitted version.

FUNDING

WW was supported by the National Natural Science Foundation of China (Grant No. 11905222) and the Scientific Instrument Developing Project of the Chinese Academy of Sciences (Grant No. YJKYYQ20180038).

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Conflict of Interest: The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

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APPENDIX

A. EXPRESSION OF THE OPERATOR $\widetilde{L}$

We introduced the operator $\widetilde{L} = P_s^{-1}LP_s$ in the main text. Here we prove the following result used in the main text:

$$\widetilde{L} = L^\dagger - 2\int d\mathbf{x}\mathbf{V}_s(\mathbf{x})[\boldsymbol{\phi}] \cdot \delta_{\boldsymbol{\phi}(\mathbf{x})}, \tag{A1}$$

where the expressions of L and $L^\dagger$ were given in Equations (6) and (7), respectively.

Consider an arbitrary functional $Q[\boldsymbol{\phi}]$ in the state space. We first calculate $L(P_sQ)$. Given the expression of L in Equation (6), direct calculation yields

$$\begin{aligned} &L(P_sQ)\\ &= - P_s[\boldsymbol{\phi}]\int d\mathbf{x}\,\mathbf{F}(\mathbf{x})[\boldsymbol{\phi}] \cdot \delta_{\boldsymbol{\phi}(\mathbf{x})}Q[\boldsymbol{\phi}]\\ &\quad + 2\iint d\mathbf{x}d\mathbf{x}'\left(\delta_{\boldsymbol{\phi}(\mathbf{x})}P_s[\boldsymbol{\phi}]\right) \cdot \mathbf{D}(\mathbf{x},\mathbf{x}') \cdot \left(\delta_{\boldsymbol{\phi}(\mathbf{x}')}Q[\boldsymbol{\phi}]\right)\\ &\quad + P_s[\boldsymbol{\phi}]\iint d\mathbf{x}d\mathbf{x}'\delta_{\boldsymbol{\phi}(\mathbf{x})} \cdot \mathbf{D}(\mathbf{x},\mathbf{x}') \cdot \delta_{\boldsymbol{\phi}(\mathbf{x}')}Q[\boldsymbol{\phi}]. \end{aligned} \tag{A2}$$

In obtaining the above result we have used the steady-state FFPE: $LP_s = 0$. Multiplying both sides of the above equation with P_s^{-1} and taking into account the definition $\widetilde{L} = P_s^{-1}LP_s$, we obtain

$$\begin{aligned} \widetilde{L}Q = &- \int d\mathbf{x}\,\mathbf{F}(\mathbf{x})[\boldsymbol{\phi}] \cdot \delta_{\boldsymbol{\phi}(\mathbf{x})}Q[\boldsymbol{\phi}]\\ &- 2\iint d\mathbf{x}d\mathbf{x}'\left(\delta_{\boldsymbol{\phi}(\mathbf{x})}U[\boldsymbol{\phi}]\right) \cdot \mathbf{D}(\mathbf{x},\mathbf{x}') \cdot \left(\delta_{\boldsymbol{\phi}(\mathbf{x}')}Q[\boldsymbol{\phi}]\right)\\ &+ \iint d\mathbf{x}d\mathbf{x}'\delta_{\boldsymbol{\phi}(\mathbf{x})} \cdot \mathbf{D}(\mathbf{x},\mathbf{x}') \cdot \delta_{\boldsymbol{\phi}(\mathbf{x}')}Q[\boldsymbol{\phi}], \end{aligned} \tag{A3}$$

where $U[\boldsymbol{\phi}] = -\ln P_s[\boldsymbol{\phi}]$ is the potential landscape introduced in the main text.

Given the expression of $L^\dagger$ in Equation (7) and comparing $\widetilde{L}Q$ with $L^\dagger Q$, it is readily seen that

$$\begin{aligned} &\widetilde{L}Q - L^\dagger Q\\ &= - 2\int d\mathbf{x}\,\mathbf{F}(\mathbf{x})[\boldsymbol{\phi}] \cdot \delta_{\boldsymbol{\phi}(\mathbf{x})}Q[\boldsymbol{\phi}]\\ &\quad - 2\iint d\mathbf{x}d\mathbf{x}'\left(\delta_{\boldsymbol{\phi}(\mathbf{x})}U[\boldsymbol{\phi}]\right) \cdot \mathbf{D}(\mathbf{x},\mathbf{x}') \cdot \left(\delta_{\boldsymbol{\phi}(\mathbf{x}')}Q[\boldsymbol{\phi}]\right) \end{aligned} \tag{A4}$$

Then we invoke the non-equilibrium force decomposition in Equation (12), which relates the driving force $\mathbf{F}(\mathbf{x})$ to the potential landscape $U[\boldsymbol{\phi}]$ and the probability flux velocity $\mathbf{V}_s(\mathbf{x})$. We thus obtain

$$\widetilde{L}Q - L^\dagger Q = -2\int d\mathbf{x}\,\mathbf{V}_s(\mathbf{x})[\boldsymbol{\phi}] \cdot \delta_{\boldsymbol{\phi}(\mathbf{x})}Q[\boldsymbol{\phi}], \tag{A5}$$

which is essentially the desired result in Equation (A1) since $Q[\boldsymbol{\phi}]$ is an arbitrary functional in the state space.