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LETTER TO THE EDITOR

Variational and potential formulation for stochastic partial differential equations

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Online at stacks.iop.org/JPhysA/39/L93**Abstract**

Recently there has been interest in finding a potential formulation for stochastic partial differential equations (SPDEs). The rationale behind this idea lies in obtaining all the dynamical information of the system under study from one single expression. In this letter we formally provide a general Lagrangian formalism for SPDEs using the Hojman *et al* method. We show that it is possible to write the corresponding effective potential starting from an *s*-equivalent Lagrangian, and that this potential is able to reproduce all the dynamics of the system once a special differential operator has been applied. This procedure can be used to study the complete time evolution and spatial inhomogeneities of the system under consideration, and is also suitable for the statistical mechanics description of the problem.

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Structural development in cosmology and biology, pattern-formation, symmetry breaking, population dynamics, chemical chaos and turbulence [1–4], are just a few cases of a wide spectrum of phenomena for which self-regulation, oscillation, adaptiveness and multi-equilibrium behaviours can be adequately modelled by means of stochastic partial differential equations (SPDEs). Few general techniques are available for their study, but due to its importance and versatility, efforts have been made to find a formalism from which all the relevant physical information of the system can be obtained [5, 6, 10–13].

Thus, effective actions can be found, for example, by means of the Martin–Siggia–Rose formalism [5], a perturbative procedure that makes use of both physical and ‘conjugate’ (auxiliary) fields (for details concerning the difficulties of the method, see [6]). On the other hand, a variational formalism has been devised by Gambár and Márkus (see for example [7–9]) as groundwork for proposing a field theory for non-equilibrium thermodynamical systems, giving valuable information about the entropy in terms of current densities and thermodynamic

forces. Also, Hochberg *et al* have proposed in a series of papers [6, 10, 11] a ‘direct’ approach, finding effective actions and potentials for SPDEs using a functional integral formalism similar in structure to those of quantum field theory. But as reported [12], the associated effective potential does not provide information about the time evolution and spatial inhomogeneities of the system under consideration, and the effective action is very difficult to calculate exactly. More recently Ao [13] has reported a worth consulting novel approach for constructing potentials associated with SPDEs.

It is not surprising that variational formulations for SPDEs are not abundant in the literature. Indeed, it is widely accepted that a variational principle cannot be constructed for an arbitrary differential equation [14]. There is a strict mathematical theorem that shows its existence for a given situation, and whose application reduces the number of equations in physics that have a Lagrangian–Hamiltonian formulation [15, 16]. However, there are several methods in the literature devised to circumvent this condition and even some proposals for modified variational principles [14, 17–19].

Nonetheless, there is an interesting different approach, known as the inverse problem of the variational calculus (see, for example, [20]). It consists in studying the existence and uniqueness (or multiplicity) of Lagrangians for systems of differential equations, i.e. finding the Lagrangian, if it exists, from the equations of motion, instead of the traditional approach. This procedure has become quite useful and one important result is that of Hojman *et al* [21], who have proven that it is possible to construct the Lagrangian for any regular mechanical system as a linear combination of its own equations of motion. This particular construction, for example, is much wider than the traditional definition $L = T - V$, which is only true when the ‘forces’ involved are derivable from position-dependent potentials (or in some cases from velocity-dependent potentials); therefore it may be used for general non-conservative systems. Its application to the study of SPDEs may provide additional understanding of the internal structure of these phenomena and also enables the use of a well-known mathematical machinery to find conserved quantities, equilibria and stability cases, and other dynamical properties.

The aim of this letter is to establish a variational and effective potential formalism for the study of SPDEs with arbitrary additive noise function. This approach has the particular advantages that it provides Lagrange–Hamilton functionals in a very direct way starting from the equations of motion, and that the effective potential deduced is able to take account of the stability and equilibria conditions, temporal evolution, anisotropies and inhomogeneities of the system.

We will consider in this work SPDEs that can be written as

$$\delta\psi^i - \Phi^i(\psi^j) - \xi^i = 0 \quad (1)$$

for $i, j = 1, \dots, m$ where m is the number of degrees of freedom, $\psi^i \equiv \psi^i(q^j, t)$ denotes the components of a vector field whose arguments are, in the general case, spatial coordinates q^j and time t ; δ is an arbitrary linear space or time (or both) differential operator that does not depend on the field ψ^i ; $\Phi^i(\psi^j)$ is any, usually nonlinear, deterministic forcing term and $\xi^i \equiv \xi^i(q^j, t)$ is a random function of its arguments describing the stochastic force (noise) in the system. In table 1 some particular cases of δ operators and Φ^i functions are presented (a_p are the coefficients of the polynomial of order p while κ and ω are real scalars; for details see [6] and references therein). Hereafter, Einstein summation convention and Euclidian metric tensor are assumed. The (additive) noise functions to be considered here are completely arbitrary.

It is important to bear in mind that even when it is true that different sorts of noise and different behaviours of the underlying deterministic partial differential equations (hyperbolic,

Table 1. Some operators and dissipation functions.

Operator	δ	Function	$\Phi^i(\psi^j)$
D'Alembertian	$\partial_t^2 - \nabla^2$	Polynomial	$a_p[\psi^i]^p$
Diffusion	$\partial_t - \kappa \nabla^2$	Burgers (noisy)	$\frac{\omega}{2} (\nabla \psi^i)^2$
Temporal	∂_t	Purely dissipative	$-\frac{\delta H(\psi^j)}{\delta \psi^i}$

parabolic, linear or nonlinear) require different techniques to find the corresponding solutions, those may be unnecessary, as we will presently show, for obtaining a variational/effective potential formulation of the problem.

The equation of motion for a mechanical system arises from a set of m differential equations. For conceptual reasons, it is suitable to rewrite (1) as equations of motion in the variational sense

$$G^i \equiv \ddot{\psi}^i - F^i(\dot{\psi}^j, \partial_k \psi^j, \psi^j, t) = 0 \quad (2)$$

where F^i behaves as 'forces' (both deterministic and stochastic) divided by unitary mass and may include spatial derivatives of the field; the dot stands for total temporal derivative.

In the inverse problem of the variational calculus the Lagrangian $L(\dot{\psi}^j, \psi^j, t)$ is constructed such that relations (2) can be effectively deduced via Euler–Lagrange equations. The existence of such a Lagrangian is studied using the Helmholtz conditions [22]

$$\left. \begin{aligned} \frac{\partial G_i}{\partial \dot{\psi}^j} + \frac{\partial G_j}{\partial \dot{\psi}^i} &= \frac{d}{dt} \left(\frac{\partial G_i}{\partial \dot{\psi}^j} + \frac{\partial G_j}{\partial \dot{\psi}^i} \right) \\ \frac{\partial G_i}{\partial \dot{\psi}^j} - \frac{\partial G_j}{\partial \dot{\psi}^i} &= \frac{1}{2} \frac{d}{dt} \left(\frac{\partial G_i}{\partial \dot{\psi}^j} - \frac{\partial G_j}{\partial \dot{\psi}^i} \right) \end{aligned} \right\}. \quad (3)$$

Nevertheless, these conditions do not give any warranty about uniqueness. Two Lagrangians are said to be solution-equivalent (or s-equivalent) if they differ only by a global multiplicative constant, η , and a total time derivative of some gauge $\Lambda(\dot{\psi}^j, \psi^j, t)$:

$$\eta L = \tilde{L} - \frac{d\Lambda}{dt}. \quad (4)$$

The different systems of equations they provide, however, have exactly the same equations of motion.

The Hojman *et al* method enables us to write \tilde{L} as a linear combination of the known equations of motion; then for $i, j = 1, \dots, m$,

$$\tilde{L} = \mu_i [\ddot{\psi}^i - F^i] \quad (5)$$

where

$$\mu_i(\dot{\psi}^j, \psi^j, t) \equiv D_1 \frac{\partial D_2}{\partial \dot{\psi}^i} + \dots + D_{2m-1} \frac{\partial D_{2m}}{\partial \dot{\psi}^i} \quad (6)$$

$$= -\frac{\partial \Lambda}{\partial \dot{\psi}^i}. \quad (7)$$

In equation (6) the quantities under partial derivative (D_{2m}) are constants of motion of the system, while the corresponding coefficients (D_{2m-1}) are arbitrary functions whose arguments

are constants of motion. There are plenty of ways to write these D_{2m} functions. For instance, one possible form for the D_{2m-1} functions, given the D_{2m} conserved quantities, is presented in [20].

When the conserved quantities are unknown the problem is reduced to find μ_i such that the following system

$$\left. \begin{aligned} \frac{\partial \mu_i}{\partial \dot{\psi}^j} &= \frac{\partial \mu_j}{\partial \dot{\psi}^i} \\ \frac{\bar{d}}{dt} \left(\frac{\bar{d}}{dt} \mu_i + \mu_j \frac{\partial F^j}{\partial \dot{\psi}^i} \right) - \mu_j \frac{\partial F^j}{\partial \dot{\psi}^i} &= 0 \end{aligned} \right\} \quad (8)$$

is satisfied, and

$$\det \left[\frac{\partial}{\partial \dot{\psi}^j} \left(\frac{\bar{d}}{dt} \mu_i + \mu_k \frac{\partial F^k}{\partial \dot{\psi}^i} \right) + \frac{\partial \mu_j}{\partial \dot{\psi}^i} \right] \neq 0 \quad (9)$$

where the on-shell derivative $\frac{\bar{d}}{dt}$ is defined such that it behaves as a usual total time derivative taking into consideration that, on the shell, equation (2) is always true.

It is important to remark that this method is useful for both second-order and first-order differential equations [21]. For further details the reader is exhorted to review [20, 21] and the references therein.

By virtue of equation (5), the general Lagrangian for SPDEs of the form (1) can be written as

$$\tilde{L} = \mu_i (\delta \psi^i - \Phi^i - \xi^i), \quad (10)$$

where the μ_i parameters must be determined for each case in study.

It can be shown that the $2m$ constants of motion of equation (10) can be formally cast in

$$D^{(2i-1)} = \psi^i - \int \dot{\psi}^i dt \quad (11)$$

$$D^{(2i)} = \dot{\psi}^i - \int F^i dt. \quad (12)$$

It is clear that equations (11) and (12) must satisfy conditions (8) and (9) of the Hojman *et al* method.

Once the Lagrangian (10) is completely determined, the corresponding Hamiltonian can be found trivially by the usual Legendre transformation, and, as will be shown in the following lines, also the effective potential can be written straightforwardly.

Let us now define the following differential operator

$$\nabla_i^* \equiv \frac{1}{\dot{\psi}^j} \left(\frac{\bar{d}}{dt} \right)_i^j. \quad (13)$$

Then, let us require that the effective potential, V_{eff} , be such that

$$\nabla_i^* V_{\text{eff}} = -F_i. \quad (14)$$

Note that if $V_{\text{eff}} \equiv V_{\text{eff}}(\dot{\psi}^j, \psi^j, t)$, then

$$\left(\frac{\bar{d}}{dt} \right)_i^j \equiv \delta_i^j \frac{\partial}{\partial t} + \dot{\psi}^j \frac{\partial}{\partial \psi^i} + F^j \frac{\partial}{\partial \dot{\psi}^i} \quad (15)$$

and thus, in the conservative case, i.e. $V_{\text{eff}} \equiv V_{\text{eff}}(\psi) = V$, equation (14) provides (from now on the symbol \doteq indicates that the relation is valid only in special cases)

$$\overset{*}{\nabla}_i V_{\text{eff}} \doteq \frac{\partial V}{\partial \psi^i} = -F_i \quad (16)$$

which is equivalent to the standard relation $\nabla_i V = -F_i$ when the vector field ψ^i coincides with the spatial coordinate q^i .

Now, we are interested in finding a gauge $\Lambda = \lambda$ such that equations (10) and (5) provide an s-equivalent Lagrangian, L , that can be written as the difference between some function (kinetic energy) T_{eff} and the effective potential V_{eff} . In consequence (for the sake of simplicity, $\eta = 1$)

$$V_{\text{eff}} = T_{\text{eff}} - \mu_i(\delta\psi^i - \Phi^i - \xi^i) + \frac{d\lambda}{dt}. \quad (17)$$

For a general non-conservative system, T_{eff} can be written as [23]

$$T_{\text{eff}} \equiv \alpha A(\psi^i) + \beta B(\dot{\psi}^i, \psi^i) + \gamma G(\dot{\psi}^i \dot{\psi}_i, \psi^i), \quad (18)$$

and thus it is necessary to determine the scalars α, β, γ and the functions $A(\psi^i)$, $B(\dot{\psi}^i, \psi^i)$, $G(\dot{\psi}^i \dot{\psi}_i, \psi^i)$ to completely define V_{eff} .

It should be useful to write the kinetic energy of the system in the traditional quadratic form

$$T_{\text{eff}} \doteq \frac{1}{2} \dot{\psi}^i \dot{\psi}_i. \quad (19)$$

In order to do so, it is necessary to find the corresponding gauge first. Equation (14) provides the necessary constraint; thus, by taking the nabla-star derivative at both sides of equation (17) we obtain, for non-coupled equations,

$$\overset{*}{\nabla}_i \left[\frac{d\lambda}{dt} - \mu_j(\delta\psi^j - \Phi^j - \xi^j) \right] = -(F_i + \ddot{\psi}_i). \quad (20)$$

Solving this equation for the time derivative of the gauge λ , we have

$$\frac{d\lambda}{dt} = - \int \dot{\psi}^i (F_i + \ddot{\psi}_i) dt + \mu_i(\delta\psi^i - \Phi^i - \xi^i) + V_0 \quad (21)$$

where V_0 is an arbitrary constant of integration. Consequently, following equation (17)

$$V_{\text{eff}} \doteq V_0 + \frac{1}{2} \dot{\psi}^i \dot{\psi}_i - \int \dot{\psi}^i (F_i + \ddot{\psi}_i) dt \quad (22)$$

which is the general effective potential for equation (1) given the choice (19) for the kinetic energy.

In summary, we have presented in this letter a novel way to provide both variational and effective potential formulations for general SPDEs with additive noise function. There are several useful applications of this result. Once the Hamiltonian is obtained, for example, quantization of systems described by equation (1) follows straightforwardly. Also, the Hamilton–Jacobi approach may help to solve the equations of motion of a system via a convenient, if possible, variable separation.

The effective potential (17) is constructed such that it contains all the dynamical information of the system. In general, it may have explicit dependence on time, on the field itself and on the derivatives of the field; certainly, the nabla-star operator identifies the contribution of each functional dependence by means of specific terms, as can be seen in equation (15).

As reported [12, 13], in other approaches the effective potential is useful only for stationary or static regimes; the approach presented here can be used to study those cases, the complete

temporal evolution of (1) and also the equilibria and stability states. The present potential formulation is based on a classical mechanics approach; there is no need of auxiliary or ghost fields. Nor Fokker–Planck equations neither special assumptions about the additive noise function are invoked in the construction.

The important relation between the effective potential (17) and the statistical mechanics deserves a detailed discussion, and it will be treated elsewhere. However, it can be shown that this potential appears in the steady state solution of the corresponding Fokker–Planck equation (or even the Klein–Kramers equation) [2], a Boltzmann–Gibbs distribution

$$\rho_0(\psi^i) = \frac{1}{Z} \exp(-V_{\text{eff}}(\psi^i)) \quad (23)$$

with Z as the partition function.

A detailed application of this procedure to several particular cases of SPDEs, such as Langevin, inhomogeneous Klein–Gordon, and diffusion equations from a mechanical, statistical and quantum point of view is in course of preparation.

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