ENTROPIC FLUCTUATIONS IN GAUSSIAN DYNAMICAL SYSTEMS

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We study nonequilibrium statistical mechanics of a Gaussian dynamical system and compute in closed form the large deviation functionals describing the fluctuations of the entropy production observable with respect to the reference state and the nonequilibrium steady state. The entropy production observable of this model is an unbounded function on the phase space, and its large deviation functionals have a surprisingly rich structure. We explore this structure in some detail.

Keywords: nonequilibrium statistical mechanics, entropy production, Gallavotti–Cohen symmetry, fluctuation relations, large deviations.

1. Introduction

In this paper, we prove and elaborate the results announced in Section 9 of [23]. We consider a dynamical system described by a real separable Hilbert space $\mathcal{K}$ and the equation of motion

$$\frac{d}{dt}x_t = \mathcal{L}x_t, \qquad x_0 \in \mathcal{K}, \tag{1}$$

where $\mathcal{L}$ is a bounded linear operator on $\mathcal{K}$. Let D be a strictly positive bounded symmetric operator on $\mathcal{K}$ and $(\mathfrak{X}, \omega_D)$ the Gaussian random field over $\mathcal{K}$ with zero mean value and covariance D. Eq. (1) induces a flow $\phi_{\mathcal{L}} = \{\phi_{\mathcal{L}}^t\}$ on $\mathfrak{X}$, and our starting point is the dynamical system $(\mathfrak{X}, \phi_{\mathcal{L}}, \omega_D)$ (its detailed construction is given in Section 2.1). We compute in closed form and under minimal regularity assumptions the nonequilibrium characteristics of this model by exploiting its Gaussian nature. In particular, we discuss the existence of a nonequilibrium steady state (NESS), compute the steady state entropy production, and study the large deviations of the entropy production observable w.r.t. both the reference state ω_D and the NESS. To emphasize the minimal mathematical structure behind the results, in the main body of the paper we have adopted an abstract axiomatic presentation. In Section 3, the results are illustrated on the example of the one-dimensional harmonic crystal. For additional information and a pedagogical introduction to the theory of entropic fluctuations in classical nonequilibrium statistical mechanics, we refer the reader to the reviews [23, 27].

There are very few models for which the large deviation functionals of the entropy production observable can be computed in a closed form, and we hope that our results may serve as a guide for future studies. In addition, an important characteristic of a Gaussian dynamical system is that its entropy production observable is an unbounded function on the phase space. This unboundedness has dramatic effects on the form and regularity properties of the large deviation functionals that require modifications of the celebrated fluctuation relations [12, 13, 15, 16]. Although this topic has received a considerable attention in the physics literature [1, 2, 6, 14, 19, 30–32], to the best of our knowledge, it has not been studied in the mathematically rigorous literature on the subject. Thus, another goal of this paper is to initiate a research program dealing with mathematical theory of extended fluctuation relations in nonequilibrium statistical mechanics, which emerge when some of the usual regularity assumptions (such as compactness of the phase space, boundedness of the entropy production observable, smoothness of the time reversal map) are not satisfied.

The paper is organized as follows. In Section 2.1 we introduce Gaussian dynamical systems. In Section 2.2 we define the entropy production observable and describe its basic properties. In Section 2.3 we introduce the NESS. Our main results are stated in Sections 2.4 and 2.5. The entropy production observable is defined as the phase space contraction rate of the reference measure ω_D under the flow $\phi_{\mathcal{L}}$, and in Section 2.6 we examine the effects of a perturbation of the reference measure on the large deviation theory. In Section 3 we illustrate our results on two classes of examples, toy models and harmonic chains. The proofs are given in Section 4.

The focus of this paper is the mathematics of the large deviation theory of the entropy production observable. The physical implications of our results will be discussed in the continuation of this paper [24].

2. The model and results

2.1. Gaussian dynamical systems

In order to setup our notation, we start with some basic facts about classical Gaussian dynamical systems. We refer the reader to [9] for a more detailed introduction to this subject.