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Complementary relations in non-equilibrium stochastic processes

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ABSTRACT

We present novel complementary relations in non-equilibrium stochastic processes. Specifically, by utilising path integral formulation, we derive statistical measures (entropy, information, and work) and investigate their dependence on variables (x, v), reference frames, and time. In particular, we show that the equilibrium state maximises the simultaneous information quantified by the product of the Fisher information based on x and v while minimising the simultaneous disorder/uncertainty quantified by the sum of the entropy based on x and v as well as by the product of the variances of the PDFs of x and v. We also elucidate the difference between Eulerian and Lagrangian entropy. Our theory naturally leads to Hamilton–Jacobi relation for forced-dissipative systems.

1. Introduction

Information theory provides one of the most useful frameworks in statistical modelling with broad application [1–4]. One of popular measures of information is entropy, which quantifies the uncertainty in a random variable X, and thus the degree of disorder in a system described by the variable X. In sharp contrast, Fisher information [1] measures the amount of information an observable random variable X carries about an unknown parameter θ upon which the probability of X depends. As the inverse of the Fisher information is a lower bound on the variance of any unbiased estimator of θ through Cramer–Rao inequality [1], Fisher information increases as the variance decreases. Alternatively, the Fisher information increases with the gradient of the probability density function (PDF) in parameter space – the narrower the PDF, the higher Fisher information. Thus, Fisher information quantifies the degree of order (certainty) or self-organisation in a system.

A great effort has been made on the generalisation of information theory from equilibrium to non-equilibrium systems (e.g. see [6,7]). Noteworthy controversial issues include the proper definition of entropy and Fisher information in strongly non-equilibrium (nonlinear) systems and the existence of universal principle such as maximum/minimum entropy (or entropy production) (e.g. see [8] and the references therein) that governs the time evolution of such systems. The main aim of this Letter is to focus on some of the issues which could be important in settling these controversies but yet have received less attention in non-equilibrium stochastic processes.

Specifically, first, we report on how these concepts could depend on dynamic variables of PDFs. To this end, it is worth noting that the entropy computed from the PDF of a continuous variable – the so-called differential or continuous entropy – has the property different from discrete entropy for a discrete variable. For instance, the value of differential entropy can be negative and depends on the resolution [9]. This is basically because PDF itself is not the physical probability and it needs to be multiplied by a support to become the probability. Furthermore, differential entropy is not invariant under the change of variables such as Fourier transform from the position x to the momentum p space, with different values of entropy in position and momentum representations. In fact, this is closely related to Heisenberg's uncertainty principle. In quantum mechanics where the PDF is determined by the square of the magnitude of wave function, Heisenberg's uncertainty principle makes position x and momentum p stochastic variables, leading to the opposite behaviour of the (Shannon) Boltzmann entropy projected to x ($S_B(x)$) and p ($S_B(p)$), respectively. However, the sum of $S_B(x)$ and $S_B(p)$ was shown to satisfy the following interesting Hirschman's inequality [1,5]

$$S_B(x) + S_B(p) \geq \ln[\pi e\hbar/2]\,, \tag{1}$$

where e and $\hbar$ are Naperian base and Planck constant divided by 2π, respectively.

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In this Letter, by considering a classical stochastic process far from equilibrium, we compare entropy obtained from the PDF of the position and the velocity, show how they evolve in time, and establish complementary relation between them through inequality similar to Eq. (1). Similar complementary relation is also illustrated through Fisher information. Second, we show that entropy-related concepts including entropy production and flux depend on reference frames by using PDFs given by Eulerian vs Lagrangian variables. Mathematically, we utilise path integral formulation for the PDFs in order to compute statistical quantity computed along particle trajectory. Note that technical difficulty in computation of path-dependent measures might have been responsible for the lack of attention to this problem in the past. The remainder of this Letter is organised as follows: Section 2 presents the formulation of the problem, summarising key results on PDFs. Section 3 provides complementary relations in information through entropy and Fisher information. Eulerian vs Lagrangian entropy and work and related concepts are discussed in Section 4 where an error in a recent publication [10] is identified. Our conclusions and discussion are found in Section 5. Appendices A–E contain mathematical details including the derivation of Hamilton–Jacobi relation.

2. Formulation of the problems

We consider a strongly out-of-equilibrium initial state where particles are localised in space at $x = x_0$ at time $t = 0$ and investigate how they relax towards equilibrium under the potential $V(x)$ and stochastic noise f, governed by,

$$\frac{dx}{dt} = -\frac{dV}{dx} + f. \tag{2}$$

For simplicity, f is assumed to have a short memory time as $\langle f(t)f(t')\rangle = D\delta(t-t')$ and zero mean value $\langle f\rangle = 0$. Here, angular brackets $\langle\rangle$ denote average over f. D represents the mean square amplitude of f [11]. For our purpose of presenting complementary relations, it turns out to be sufficient to take the simplest case of $V(x) = \mu x^2/2$ (μ is constant). While finding PDFs of position is rather trivial (e.g. [12]) in this case, the computation of path-dependent statistical measures and velocity PDFs necessitates a more complicated analysis such as path integral formulation, which is summarised in Appendix A.

2.1. Saddle-point solutions

Following path integral formulation (e.g. [13–18]), the transition probability $p(x_f, t_f; x_0, 0)$ between initial position x_0 at $t = 0$ and final positions x_f at final time $t = t_f$ is formally expressed as the integral over all paths whose contribution decreases exponentially e^{-S} as the value of action S increases [see Eq. (A.1)]. A particular path that minimises S in Eq. (A.1) thus contributes most to the path integral – this so-called saddle-point solution is found by solving Eq. (A.2) with the boundary conditions that $x = x_0$ at $t = 0$ and $x = x_f$ at $t = t_f$ as:

$$x(t) = e^{-\mu t}x_0 + \frac{e^{\mu t} - e^{-\mu t}}{e^{\mu t_f} - e^{-\mu t_f}}[x_f - x_0 e^{-\mu t_f}]. \tag{3}$$

For our initial condition where $x = x_0$ at $t = 0$, x_0 is fixed while x_f is a random variable due to the stochastic forcing f. Eq. (3) enables us to find velocity along particle trajectory as

$$\frac{dx}{dt} = v(t) = -\mu e^{-\mu t}x_0 + \mu\frac{(e^{\mu t} + e^{-\mu t})}{(e^{\mu t_f} - e^{-\mu t_f})}[x_f - x_0 e^{-\mu t_f}]. \tag{4}$$

By replacing t by 0 and t_f in Eq. (4), we obtain the initial velocity v_0 and final velocity v_f at $t = 0$ and t_f, respectively, as

$$v_0 = \frac{\mu}{1 - e^{-2\mu t_f}}\left[-(1 + e^{-2\mu t_f})x_0 + 2x_f e^{-\mu t_f}\right], \tag{5}$$

$$v_f = \frac{\mu}{1 - e^{-2\mu t_f}}\left[(1 + e^{-2\mu t_f})x_f - 2x_0 e^{-\mu t_f}\right]. \tag{6}$$

Eqs. (5)–(6) reveal that for a fixed x_0, v_0 is totally uncertain and non-local, depending on random variable x_f at later time $t = t_f$. Likewise, v_f is also random and non-local, depending on random variable x_f and the earlier position x_0. This is because the saddle-point solution is obtained for the boundary conditions $x = x_0$ at $t = 0$ and $x = x_f$ at $t = t_f$ where x_0 is fixed in our problem while x_f is random due to the action of stochastic forcing f. That is, for the fixed x_0, v_0, v_f and x_f are all stochastic.

2.2. PDFs of position x and velocity v

Our initial condition $x = x_0$ at $t = 0$ gives a highly localised initial PDF given by a delta-function $p(x = x_0, 0) = \delta(x - x_0)$. PDFs of x_f and v_f follow from Eqs. (A.3) and (6) and $p(v_f, t_f) = p(x_f, t_f)\frac{dx_f}{dv_f}$ as

$$p(x_f, t_f) = \sqrt{\beta_x}\exp[-\beta_x(x_f - x_0 e^{-\mu t_f})^2], \tag{7}$$

$$p(v_f, t_f) = \sqrt{\frac{\beta_v}{\mu^2}}\exp[-\beta_v(\frac{v_f}{\mu} + x_0 e^{-\mu t_f})^2]. \tag{8}$$

Here, $\beta_x = \frac{\mu}{D(1-e^{-2\mu t_f})}$ and $\beta_v = \frac{\mu}{D}\frac{(1-e^{-2\mu t_f})}{(1+e^{-2\mu t_f})^2}$ are inverse temperature associated with x_f and v_f, respectively, which depend on time t_f. Note that $\beta_x \to \infty$ and $\beta_v \to 0$ as $t \to 0$ while $\beta_x \sim \beta_v \to \mu/D$ as $t \to \infty$, meaning that PDF of x (v) becomes broader (narrower) towards equilibrium. Eqs. (7)–(8) give us the following useful mean values as:

$$\langle x_f\rangle = x_0 e^{-\mu t_f}, \langle(\delta x_f)^2\rangle = \frac{1}{2\beta_x}, \tag{9}$$

$$\langle v_f\rangle = -\mu x_0 e^{-\mu t_f}, \langle(\delta v_f)^2\rangle = \mu^2\frac{1}{2\beta_v}, \tag{10}$$

where $\delta x_f = x_f - \langle x_f\rangle$ and $\delta v_f = v_f - \langle v_f\rangle$. In Eq. (9), $\langle x_f\rangle = x_0 e^{-\mu t}$ illustrates the exponential relaxation of $\langle x_f\rangle$ from x_0 while $\langle(\delta x_f)^2\rangle$ represents the mean square fluctuation of x_f which increases in time as $p(x, t)$ becomes broader. In Eq. (10), $\langle v_f\rangle = -\mu x_0 e^{-\mu t} = -\mu\langle x_f\rangle$ represents the relaxation of the mean velocity associated with $\langle x_f\rangle$ while $\langle(\delta v_f)^2\rangle$ decreases in time as $p(v, t)$ becomes narrower. Specifically, Eq. (10) gives $\langle(\delta v_f)^2\rangle \to \infty$ as $t \to 0$ in sharp contrast to the behaviour of $\langle(\delta x_f)^2\rangle \to 0$ as $t \to 0$; $\langle(\delta v_f)^2/\mu^2\rangle \to D/2\mu$ and $\langle(\delta x_f)^2\rangle \to D/2\mu$ as $t \to \infty$. While each mean square fluctuation varies considerably in time, the product of the two exhibits much less variation as:

$$\langle(\delta v_f)^2\rangle\langle(\delta x_f)^2\rangle = \frac{\mu^2}{4\beta_x\beta_v} = \frac{D^2(1 + e^{-2\mu t_f})^2}{4} \geq \left[\frac{D}{2}\right]^2. \tag{11}$$

The last inequality in Eq. (11) establishes an interesting complementary relation, which is equivalent to the uncertainty relation between x and p in quantum mechanics. The lower bound in Eq. (11) is set by the strength D of the forcing f and corresponds to $\hbar$ in quantum mechanics. Alternatively, D sets the accuracy in simultaneous determination of x and v (see also [1]). Our result thus explicitly shows that the uncertainty in the simultaneous measurement of x and v decreases in time towards its minimum equilibrium value.

As β_x and β_v are related to statistical measures such as entropy S_B, free energy F (see Appendix A), etc., their disparate values result in the difference in statistical measures depending on x and v descriptions, as discussed in Section 3.