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LETTER TO THE EDITOR

On the nature of large fluctuations in equilibrium systems: observation of an optimal force

D G Luchinsky†

School of Physics and Chemistry, Lancaster University, Lancaster, LA1 4YB, UK

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Abstract. An analogue electronic experiment is used to demonstrate that large fluctuations in a thermal equilibrium system exhibit time-reversal symmetry and, furthermore, that they arise through the action of an *optimal force* that can be predicted on the basis of Hamiltonian fluctuation theory.

Large fluctuations play a fundamental role in, for example, chemical reactions, nucleation at phase transitions, mutations in DNA sequences, stochastic resonance, protein transport in biological cells and failures of electronic devices. They also lie at the root of many discussions of the origin of macroscopic irreversibility [1–6] and of the properties of far from equilibrium systems [7–10]. The theory of large fluctuations, based on path integral [3, 11] or Hamiltonian [12, 13] formulations of the problem, has proved very successful in various applications to non-equilibrium systems (see, e.g., [9, 10, 14–19]).

In spite of the long-standing theoretical interest in the fundamental character of large fluctuations, there have been almost no relevant experiments. Indeed, the very possibility of such experiments has sometimes been doubted [4] on the grounds that large fluctuations are by definition very rare events, and therefore difficult to investigate. It has recently been shown, however, that optimal paths [10] (or instantons [9]), one of the central concepts of the theory of large fluctuations, are physical observables [20, 21], thus exposing to experimental scrutiny many fundamental assumptions and conclusions of the theory. One such assumption is the existence of an optimal force corresponding to the optimal path of a dynamical variable [11]. It is this assumption that makes possible the calculation of the optimal path itself [14, 17]; and for some applications a simultaneous knowledge of both optimal path and the optimal force is important [18]. However, the assumption has never been tested experimentally and its validity for large deviations of the system from the state of thermodynamic equilibrium is not immediately clear. It is particularly important to verify the statement that the optimal force 'dies' at the maximum of large fluctuations (see, e.g., [18]), and thus that the optimal force is *asymmetrical* in time, whereas the average growth and decay of large fluctuations in equilibrium systems are *symmetrical* [3, 7, 9, 10].

The Hamiltonian formulation is well understood to be a counterpart of the path integral (or Lagrangian) formulation of the theory, but the identification of the momentum of the auxiliary Hamiltonian system as a physical observable related to the optimal force has not

† Permanent address: Russian Research Institute for Metrological Service, Ozernaya 46, 119361 Moscow, Russia.

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been clearly established, even in the theoretical literature (see, e.g., [16, 19]). Thus it is especially important to seek further insight. In this letter, we report the preliminary results of a novel *experimental* approach to the problem, applied to the analysis of large fluctuations in an electronic analogue circuit model [22]. We demonstrate the predicted symmetry between the average growth and decay of fluctuations and the existence of the optimal force, and we provide experimental insight into the relationship between the optimal path of the random force and the momentum of the auxiliary Hamiltonian system.

Consider one-dimensional Brownian motion within a force field $K(x)$ subject to white Gaussian noise $\xi(t)$ in the limit of low noise intensity, $D \to 0$:

$$\dot{x} = K(x) + \xi(t)$$
$$\langle \xi(t) \rangle = 0 \qquad \langle \xi(t)\xi(0) \rangle = D\delta(t). \tag{1}$$

The variable x might represent, for example, the local energy density [2] or entropy [5] in a solid or gas, a current or voltage in an electrical circuit (see below), the phase of the order parameter in a superconducting quantum interference device (SQUID) [23], or the number density of a species in a chemical reaction [10], or the phase of a nonlinear optical interferometer [24]. A fluctuation occurs in two distinct sections, as it first grows towards some remote state x_f, and subsequently relaxes back towards x_s corresponding to the stable state S in the close vicinity of which the system spends most of its time. The latter section can easily be understood [3] as a relaxation of the macroscopic variable x towards its stable value along a deterministic trajectory corresponding to the phenomenological law (1) with $D = 0$. The initial growth process of the fluctuation is intuitively much less obvious, however, and has been the subject of continuing controversy (see, e.g., [2, 25]). The theory of large fluctuations suggests that, for systems in thermal equilibrium (Markovian processes obeying the property of detailed balance), not only the average growth and decay of fluctuations [3, 7, 9, 10], but also the entire evolution of the corresponding distributions should be symmetrical in time [6]. It also predicts [7–10, 15–21], however, that the optimal force should be asymmetrical in time, being non-zero during the growth, 'dying' at the maximum, and remaining zero during the decay of a large fluctuation.

To investigate experimentally the statistics of large fluctuations, and the relationship between their symmetry and the asymmetry of the optimal force, we have built an electronic model of (1) with $K(x) = x - x^3$ using standard techniques [22]. We drive it with zero-mean quasi-white Gaussian noise from a noise generator, digitize the response $x(t)$, and analyse it with a digital data processor. Such a system can be regarded as being in equilibrium at a characteristic temperature that is related to the noise intensity D. Because properties such as time symmetry and detailed balance (or the lack of them) are fundamental characteristics of the motion, the technique is equally applicable to the analogue electronic circuits studied in the present experiments, or to natural systems, or to technological ones: provided they are governed by the same equations, identical behaviour is to be anticipated. The value of $x(t)$ is monitored continuously until eventually, as shown in figure 1, a large fluctuation occurs bringing the system to the pre-selected remote state x_f. The interesting region of the path—including the fluctuational part f coming to x_f, as well as the relaxational part r leading back towards S—is then stored. An ensemble-average of such paths, built up over a period of time (typically weeks), creates the distribution $P_f(x, t)$, which provides very detailed information about the nature of the large rare fluctuations occurring in the system: $P_f(x, t)$ is shorthand for $P(x_i, t_i; x, t; x_f, t_f)$, the probability of the system being at x at time t if it started from x_i at time t_i and arrived at x_f at time t_f, setting $t_f = 0$ and $x_i = x_s$ at $t_i = -\infty$; unlike the prehistory distribution [20, 21],

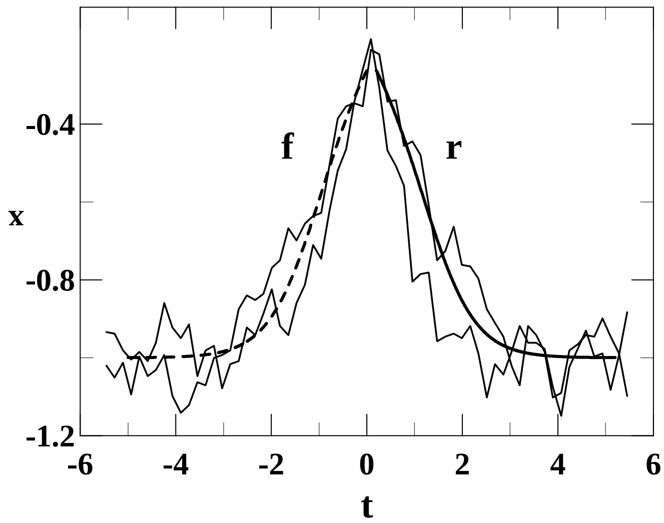

Figure 1. Fluctuational behaviour measured and calculated for a model equilibrium system: a double-well Duffing oscillator with $K(x) = x - x^3$, for $D = 0.014$. (a) Two typical fluctuations (jagged lines) from the stable state at $S = -1$ to the remote state $x_f = -0.1$, and back again, are compared with the deterministic (noise-free) relaxational path from x_f to S (full, smooth, curve) and its time-reversed ($t \to -t$) mirror image (broken curve). The fluctuational and relaxational parts of the trajectory are labelled f and r respectively.

$t > t_f$ is considered as well as $t < t_f$. In this sense, $P_f(x, t)$ is a complete-history probability density for the fluctuations coming to x_f, encompassing the whole duration of the system's excursion away from the stable state S. Figure 2 shows a distribution $P_f(x, t)$ built up through this procedure. The relaxational and fluctuational parts of the distribution are found to be symmetrical in time (a more detailed comparison including the higher moments will be given elsewhere). The top plane shows time-reversed curves (see below) drawn through data points that represent the first moment of the evolving distribution. In the macroscopic limit, where the width of the distribution would tend towards zero (because effectively $D \to 0$) we would therefore observe only the positions of the ridges (the first moments in the $D \to 0$ limit: see [7]), and the paths to/from x_f would themselves become reversible in time as was first proved theoretically by Onsager for a quadratic potential [3].

We note here that the experimental verification of the latter symmetry is important in itself, not only because it clarifies the physical interpretation of the concept of the optimal path [9, 10], but also because it is often discussed qualitatively in relation to physical interpretations of the Boltzmann principle [2] and of the second law of thermodynamics [5].

These results can be interpreted in terms of the Hamiltonian (or equivalent path-integral) theory of large fluctuations [7, 12, 13], whose conceptual basis we now summarize succinctly. To emphasize the generality of the approach, we consider a system with a multi-dimensional configuration space driven by the time dependent and in general non-gradient force field $\boldsymbol{K}(\boldsymbol{x}, t)$ (see, e.g., [8, 10, 16]). The corresponding Fokker–Planck equation for the probability density $P(\boldsymbol{x}, t)$ is

$$\frac{\partial P(\boldsymbol{x}, t)}{\partial t} = -\boldsymbol{\nabla} \cdot (\boldsymbol{K}(\boldsymbol{x}, t) P(\boldsymbol{x}, t)) + \frac{D}{2} \boldsymbol{\nabla}^2 P(\boldsymbol{x}, t). \tag{2}$$

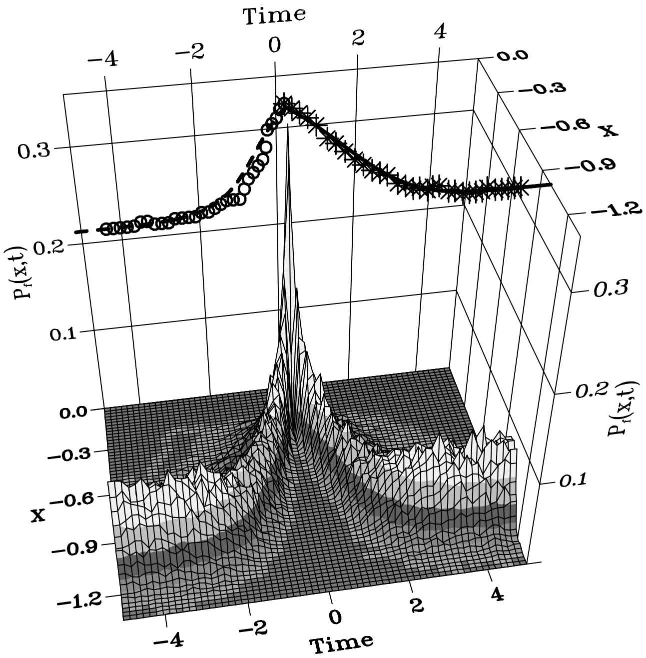

Figure 2. The probability distribution $P_f(x, t)$ built up by ensemble-averaging a sequence of trajectories like those in figure 1. The top-plane plots the positions of the ridges (first moments) of $P_f(x, t)$ for the fluctuational (open circles) and relaxational (asterisks) parts of the trajectory for comparison with theoretical predictions (curves) based on (4).

It can be solved in the limit of weak noise intensity by use of the WKB (eikonal) approximation

$$P(\boldsymbol{x}, t) = z(\boldsymbol{x}, t) \exp\left(-\frac{s(\boldsymbol{x}, t)}{D}\right). \tag{3}$$

Here $z(\boldsymbol{x}, t)$ is a prefactor, and $s(\boldsymbol{x}, t)$ is a classical action satisfying the Hamilton–Jacobi equation, which can be solved by integrating the Hamiltonian equations of motion

$$\begin{aligned} &\dot{\boldsymbol{x}} = \boldsymbol{p} + \boldsymbol{K} \qquad \dot{\boldsymbol{p}} = -\frac{\partial \boldsymbol{K}}{\partial \boldsymbol{x}}\boldsymbol{p} \\ &H(\boldsymbol{x}, \boldsymbol{p}, t) = \boldsymbol{p}\boldsymbol{K}(\boldsymbol{x}, t) + \frac{1}{2}\boldsymbol{p}^2 \qquad \boldsymbol{p} \equiv \nabla s \end{aligned} \tag{4}$$

with Hamiltonian $H(\boldsymbol{x}, \boldsymbol{p}, t)$ for appropriate boundary conditions [13, 16, 18]. Equations (4) have two different types of solution, depending on $\boldsymbol{p}$. For $\boldsymbol{p} = 0$, the set of all trajectories approaching the stable state S forms the stable invariant manifold of S. On this surface, the dynamics of (4) reduce to $\dot{\boldsymbol{x}} = \boldsymbol{K}$, which also describes relaxation of the system to S in the absence of noise. One may expect that the finite noise intensity in a real system will just give rise to a distribution about this deterministic path. The solutions of (4) with $\boldsymbol{p} \neq 0$, corresponding to the set of trajectories leaving S, form the unstable invariant manifold of S. These trajectories are interpreted as *optimal paths* along which the system will move with overwhelming probability during a fluctuation from S to a given remote state x_f. For a one-dimensional equilibrium system with a stationary force field without singularities, $K(x) = -U'(x)$ where $U(x)$ is a potential. Then the classical action is $2U(x)$ and the momentum is $p = 2U'(x)$. It can be seen from equations (4) [7] that in this case the two solutions for x (with $p = 0$ and $p \neq 0$) are mirror images of each other, as required by symmetry between past and future [3]. (Note that the same is *not* true of non-equilibrium systems for which the outward and returning paths are predicted to be [9, 10], and have very recently been shown to be [26], irreversible.) If we interpret the ($D \to 0$) theory as relating to the ridges (first moments) of the distribution, we can then compare the prediction with the data of figure 2. It is immediately evident that the ridges of the measured distribution are in excellent agreement with the symmetrical deterministic paths found from (4), plotted as the broken and full curves on the top-plane.

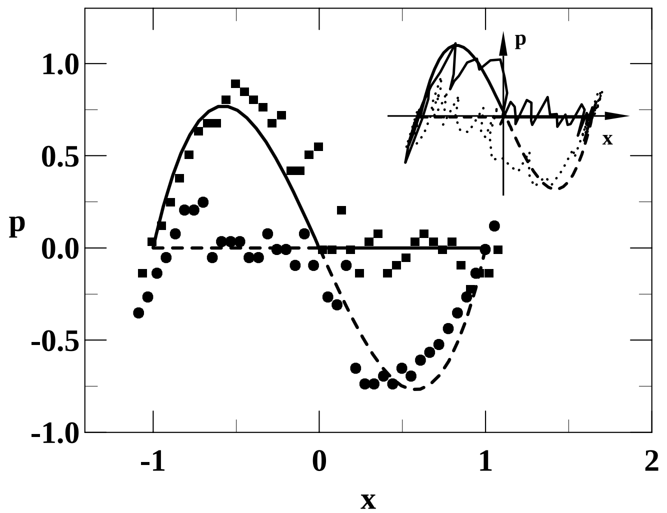

Figure 3. Demonstration of time-*irreversible* features of the fluctuations. The inset shows $p(x)$ measured for two typical transitional paths from $x = -1$ to $x = 1$ (full jagged line) and in the opposite direction (dotted jagged line). The main figure shows the paths traced out by the ridges (first moments) of the $P_f(p, x)$ distribution created from an ensemble average of such transitions. The transitional path from $x = -1$ to $x = 1$ is shown by squares, and the reverse transition by filled circles. The full and broken curves are the corresponding paths predicted from (4).

An immediate question arising from the Hamiltonian theory relates to the physical significance of the quantity p, which plays the role of a momentum in (4). Intuitively, one may infer that momenta appear in the theory because the coordinate corresponding to each degree of freedom of the original macroscopic system gets accelerated by interaction with the medium. This point is often glossed over in the theoretical literature, with some authors describing p as a mere 'theoretical abstraction'. In the particular case of our analogue experiment, however, where the noise is external, p can be identified [27] as the averaged value of the force driving the fluctuation—which is of course accessible to experimental measurement (as is also the case for the random force in Monte Carlo simulations of stochastic processes). Thus it becomes possible to perform direct tests of Feynman's proposition [11] of a one-to-one correspondence between the noise and the response of the system, and of the extension [14, 17, 18] of this idea to the prediction of an *optimal force* giving rise to any given optimal fluctuational path. We have therefore made simultaneous measurements of $x(t)$ and of the corresponding trajectories of the random force $\xi(t)$ in the analogue model of (1) during transitions between the potential wells, i.e. setting

$x_f = 0$ on the local potential maximum. Examples of actual trajectories during escapes from each of the potential wells are shown in the inset of figure 3, where they are compared to the theoretical escape paths obtained from equations (4) in the phase space (x, p) of the auxiliary Hamiltonian system. A distribution was built up by ensemble-averaging a few hundred such trajectories, and the positions of the maxima of this distribution are shown in figure 3 for comparison with the theoretical escape trajectories. We emphasize that, in the limit of weak noise, such escape events are extremely rare. Although the statistics of these events are consequently rather poor, the data clearly demonstrate: (i) that the averaged value of the force driving the fluctuation follows closely the deterministic trajectory corresponding to the *optimal force*; (ii) that p can be related to this *optimal force*; (iii) that, as anticipated, $p \neq 0$ during the fluctuational part of the path and $p = 0$ within experimental error during the relaxational part; and (iv) that the Hamiltonian theory (curves) describes very well both parts of the fluctuation.

It is also of interest to note that time reversal symmetry can be regarded as arising from a degeneracy between the projections of two different curves in an extended (by the p-dimension) phase space onto the space of the dynamical variables of an equilibrium system. Such an extension of the phase space may seem an unnecessary complication for a system in equilibrium, as in the present case, but it provides the key to understanding fluctuations in far-from-equilibrium systems, where the degeneracy is lifted by the presence of an external field [26].

The results have shown that large fluctuations in a thermal equilibrium system exhibit time-reversal symmetry and, furthermore, that they arise through the action of an *optimal force* that can be related to the momentum p introduced by Hamiltonian fluctuation theory (see e.g. [9, 10, 13–19]) which is asymmetrical in time. The same technique is being applied successfully to non-equilibrium systems [26]. It not only promises possible insights into long-standing questions [2, 5] about the role of fluctuations in irreversibility, but it is also quite generally applicable to a very wide range of ideas and problems in fluctuation theory that as yet remain untested by experiment.

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