Brownian dynamics simulation of the prehistory problem

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The prehistory problem for the description of large fluctuations in a stochastic system with Gaussian white noise is studied by means of a numerical solution of the Langevin equation. Comparison of the results with analytical treatments provides an adequate test of the ideas underlying the concept of the optimal path. [S1063-651X(97)15002-4]

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The description of small-amplitude equilibrium fluctuations in stochastic systems is rather well established. On the other hand, the statistical description of rare events, like large-amplitude fluctuations, remains largely unexplored. These improbable events are thought to be important in the analysis of the dynamics of physical systems with multiple stable points, as, for instance, in optically bistable systems or in Josephson juctions. In recent years, the method of the optimal path has proven to be very useful for the investigation of large-amplitude fluctuations in noisy systems [1–3]. In particular, the stationary distribution, the activation energy, and the mean first passage time have been discussed for both white and colored noise, in the limit of very small noise strength. The expressions obtained are based on the idea of the existence of a most probable fluctuational path driving the system away from one of its steady points and closer to the boundaries of its region of attraction. The predictions of the theory have been tested repeatedly by comparison with numerical simulations [4].

A quantity appropriate for the investigation of the rare large excursions away from a stable point, the *prehistory probability density*, has been proposed by Dykman and coworkers [5–7]. It can be briefly presented as follows. Let us consider a system at equilibrium so that its one time probability density $P_1(x)$ does not change with time. Suppose that, as a consequence of a large fluctuation, the stochastic variable is observed to reach, for the first time at time t_f, the value x_f away from its steady stable value x_{st}. Then we seek for the probability density $p_h(x,t;x_f t_f)$ that the system has passed through a point x, intermediate between x_{st} and x_f, at an earlier time $t<t_f$. We will always consider that both x and x_f lie to the right or to the left of x_{st}, that is, we assume that either $x_{\mathrm{st}}<x<x_f$ or $x_{\mathrm{st}}>x>x_f$. Furthermore, in situations where several stationary stable points exist, one is interested in time ranges much smaller than the typical transition times between stable points, so that the final point x_f always lies within the same region of attraction as x and x_{st}.

The prehistory distribution can be formally expressed in terms of a path integral representation, whose explicit evaluation requires, in general, some type of approximation. Dykman and co-workers [5,7] expressed the prehistory distribution as the solution of a pertinent variational problem. In the limit of small noise intensities, it is found to be a Gaussian whose maximum moves in time along the optimal path, $x_{\mathrm{opt}}(t;x_f)$. That is, the pre-history probability density is given by

$$p_h(x,t;x_f,0)=[2\pi D\sigma(t;x_f)]^{-1/2}e^{-[x-x_{\mathrm{opt}}(t;x_f)]^2/2D\sigma(t;x_f)}. \tag{1}$$

The width of the Gaussian has been expressed as $D\sigma(t;x_f)$ so that the dispersion parameter $\sigma(t;x_f)$ is independent of the noise strength. The calculations of the two parameters characterizing the prehistory distribution, the optimal path, and the dispersion can be carried out explicitly in some cases. In particular, for a system whose dynamics is governed by the Langevin equation, in dimensionless form,

$$\dot{x}(t)=-U'(x)+\xi(t), \tag{2}$$

where $\xi(t)$ is a Gaussian white noise with

$$\langle\xi(t)\rangle=0, \quad \langle\xi(t)\xi(s)\rangle=D\delta(t-s), \tag{3}$$

and the optimal path is given by the solution of

$$\dot{x}_{\mathrm{opt}}=U'(x_{\mathrm{opt}}). \tag{4}$$

The optimal path then corresponds to the deterministic trajectory arriving at the observation time t_f to the point x_f after having passed through x at some previous time $t<t_f$. The dispersion $\sigma(t;x_f)$ satisfies the evolution equation

$$\dot{\sigma}(t;x_f)=2U''(x)\sigma(t;x_f)-1, \tag{5}$$

with the ''final'' condition $\sigma(t=t_f;x_f)=0$, and where $x=x_{\mathrm{opt}}(t;x_f)$. If the variable t is eliminated between both evolution equations, we can write

$$\sigma(t;x_f)\equiv\sigma(x_{\mathrm{opt}}(t;x_f);x_f),$$
$$\sigma(x;x_f)=[U'(x)]^2\int_x^{x_f}dy[U'(y)]^{-3}. \tag{6}$$

Notice that because of the conditions mentioned above, $U'(y)\neq0$ for any point inside the integration interval. If the potential $U(x)$ has several stable points, the dispersion

$\sigma(x;x_f)$ shows a nonmonotonous behavior when x_f lies near an unstable point $x_{\rm un}$, where the potential presents a local maximum. The nonmonotony is more pronounced as x_f gets closer to the instability point. Dykman *et al.* [5] also carried out analog experiments to analyze the dynamics of large fluctuations. Although the analytical description matches the experimental findings at a qualitative level, there are some discrepancies which deserve further attention.

The formulation of the theory requires the strength of the noise to be sufficiently small compared to the deterministic force acting on the system during the duration of the fluctuation. If the end point x_f is very far from the stable point, the probability of such a fluctuation is very small and very difficult to observe experimentally. Thus, to observe these large fluctuations, one is forced to use in the analog experiments noise intensities which are not sufficiently small. Then finite size effects in the experimental observations have to be taken into account when comparing with the theoretical predictions [5,9]. It seems desirable to have numerical results obtained in the limit of very small noise strengths, with which the ideas of the optimal path could be tested. This is one of the motivations of the present work.

The pre-history probability density can also be expressed in terms of ratio of transition probabilities as [5,8]

$$p_h(x,t;x_f,t_f)=\left(\frac{P_3(x_i,t_i;x,t;x_f,t_f)}{P_2(x_i,t_i;x_f,t_f)}\right)_{t_i\to-\infty}, \qquad (7)$$

where $P_2(x_i,t_i;x_f,t_f)$ and $P_3(x_i,t_i;x,t;x_f,t_f)$ are, respectively, the two- and three-time joint probability densities for times $t_i<t<t_f$, of the stochastic process $x(t)$, and where the particularization for $t_i\to-\infty$ indicates that the system was prepared in some state x_i in the far past and then, at any finite time like t or t_f, we will find it at equilibrium. Expressing the joint probability densities P_2 and P_3 for a stationary Markov process in terms of conditional probability densities, we can write

$$p_h(x,t;x_f,t_f)=\frac{P_1^{\rm eq}(x)}{P_1^{\rm eq}(x_f)}w_{1|1}(x_f,t_f-t|x), \qquad (8)$$

where $P_1^{\rm eq}$ represents the one-time equilibrium distribution and $w_{1|1}(x_f,t_f-t|x)$ the conditional probability density for the system to reach the value x_f at time t_f-t if it was at x initially. Furthermore, if the system satisfies the detailed balance condition [10]

$$P_1^{\rm eq}(x)w_{1|1}(x_f,t_f-t|x)=w_{1|1}(x,t_f-t|x_f)P_1^{\rm eq}(x_f), \qquad (9)$$

we can immediately write

$$p_h(x,t;x_f,t_f)=w_{1|1}(x,|t-t_f||x_f)(t<t_f) \qquad (10)$$

which shows that for Markov systems with detailed balance, the prehistory distribution for times t prior to the final observation time $t=t_f$ can be found from a knowledge of the *forward* conditional probability density $w_{1|1}(x,|t-t_f||x_f)$. As this function satisfies a Fokker-Planck equation, any of the proposed approximation schemes (cumulant expansion [11], van Kampen's noise strength expansion [12], etc.) which provide a good description of the conditional probability during the time range of interest (i.e., times smaller than the jump time between stable points) can be used to construct the prehistory distribution. In this work, we will make use of the above relation to develop an efficient and reliable numerical solution.

A way to proceed to compute the prehistory distribution from the Langevin equation is to generate very many stochastic trajectories, starting from a set of initial values distributed according to the equilibrium distribution. Then the prehistory distribution is constructed by registering the paths that pass through x at times t before reaching the desired end point x_f at t_f. This direct procedure is practical as long as the end point is not too far from the stable point. If the fluctuation is very large, one faces the same kind of troubles as in the analog experiments. That is, the observation of large fluctuations for small noise strengths requires the generation of an exceedingly large number of trajectories. On the other hand, if the noise intensity used in the simulation is increased so that the probability of observing a large fluctuation is large enough, the limits of applicability of the analytical theory are violated. The noise term and the systematic force are then of comparable strength when a trajectory gets close to an unstable point $x_{\rm un}$, and finite noise effects have to be taken into consideration.

The property mentioned above, Eq. (10), can be used to implement the simulation for the observation of large-amplitude fluctuations with a small enough noise strength. Instead of waiting for the system to reach the end point, we start the evolution from an initial state located at the end point x_f. Then, we generate trajectories starting from x_f at $t_f=0$, and let the system evolve in time. The construction of the prehistory distribution from the stochastic trajectories is straightforward. The noise intensity D is chosen such that

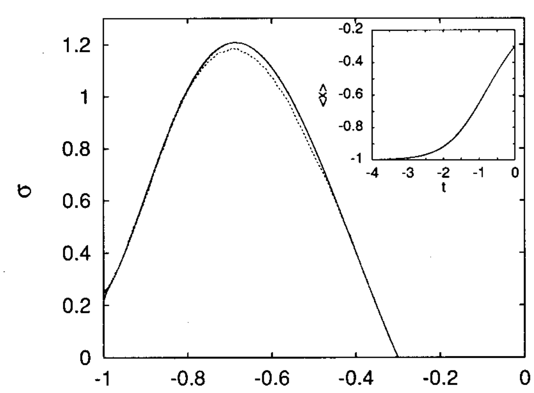

FIG. 1. Dispersion parameter of the prehistory distribution as a function of $\langle x\rangle$. The dotted line represents the numerical results for $D=0.002$ and $x_f=-0.3$. The solid line corresponds to the analytical results. Inset: the optimal path. The numerical results and those predicted by Eq. (4) are identical within the scale of the plot.

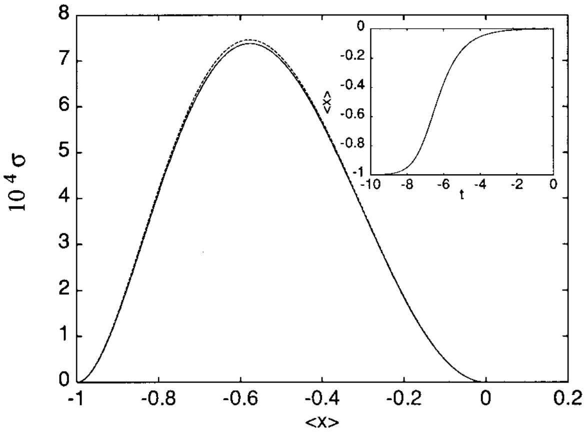

FIG. 2. The same as in Fig. 1, but for a fluctuation with end point much closer to the unstable point, i.e., $x_f = -0.001$ and $D = 10^{-8}$.

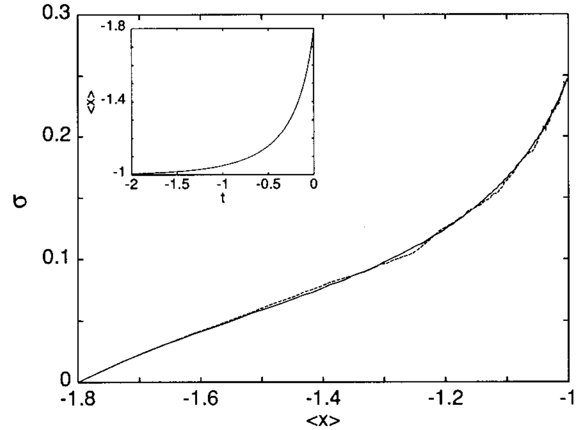

FIG. 3. The same as in Fig. 1, but for a fluctuation with end point, $x_f = -1.8$ and $D = 10^{-4}$.

$|x_{\rm un} - x_f| > D^{1/2}$. This condition guarantees the validity of the optimal path approximation during the time evolution of interest (i.e., times smaller than the transition times). Thus a comparison between theory and simulations is feasible without any finite size noise corrections. It should be pointed out that our procedure allows us to analyze the problem with very little computational effort. A few thousand trajectories provide good enough statistics for the averages.

Following a standard procedure [13], we numerically integrated the Langevin equation for the symmetric bistable potential $U(x) = -x^2/2 + x^4/4$ considered in [5]. The time behavior of the average position $\langle x \rangle$ corresponds to optimal path satisfying Eq. (4). The dispersion parameter σ defined as $\sigma = (\langle x^2 \rangle - (\langle x \rangle)^2)/D$ is to be compared with $\sigma(x;x_f)$ obtained with the optimal path method, Eq. (6).

In Fig. 1, we plot the behavior of the dispersion parameter vs $\langle x \rangle$, as well as (see the inset) the time evolution of the average for a noise strength $D = 0.002$ and $x_f = -0.3$. The time evolution of this last quantity obtained in the numerical solution is indistinguishable from the optimal path. It is interesting to note that the finite jump in the average position near $t = 0$ observed in the analog experiments (see the inset in Fig. 1 of [5]) is not present here, as this is a finite D effect. The nonmonotonous behavior of the dispersion parameter is also clearly seen. The agreement between the numerical results (dotted line) and the analytical approximation (solid line) is excellent. In Fig. 2, we present the results for a case where the end point x_f is much closer to the unstable point $x_{\rm un} = 0$. The noise strength has to be very small in order to satisfy the conditions under which the optimal path approach to the prehistory problem is formulated. In particular, one has to guarantee that the strength of the stochastic force is small compared to that of the systematic term in the Langevin equation. If this condition is violated, the probability of trajectories crossing the unstable point is not negligible, and, consequently, there will be paths arriving at point x_f after crossing the unstable point. These paths are not contemplated in the formulation of the prehistory problem. The inset again shows the time behavior of the average position. Notice that the time scale of the evolution is now longer than in the previous case. Also, when the optimal path is near the unstable point, it remains in that neighborhood for a long time. The nonmonotony of the dispersion parameter is also more pronounced, as expected from the predictions of the optimal path theory.

The condition for nonmonotony of the dispersion can be obtained by requiring that, in the interval of values of x considered, the dispersion has a maximum. Then it follows from Eq. (6), that, in order to observe a maximum, there must be a solution of the equation

$$\sigma(x;x_f) = \frac{1}{2U''(x)} \tag{11}$$

for some value x in the interval $(x_{\rm st}, x_f)$. For the symmetric monostable potential $U(x) = x^2/2 + x^4/4$, there is no solution of Eq. (11) for any end point.Thus, the dispersion is always monotonous. This is also the case for the bistable potential if the end point $x_f < x_{\rm st}$. In Fig. 3, we show the behavior for these types of final conditions ($x_f = -1.8$, $D = 10^{-4}$). In contrast with the previous cases, the average very quickly reaches its steady value, and the dispersion shows a monotonic behavior. Thus the monotony or nonmonotony of the dispersion is related to the condition given in Eq. (11). In particular, the behavior of the dispersion can be nonmonotonous for asymmetric monostable potentials. We are presently carrying out a more extensive analysis of this feature for potentials other than the ones considered here.

In conclusion, we believe that our calculation provides an adequate numerical test to the ideas of the optimal path. The procedure followed here relies in the use of the properties of Markov processes supporting detailed balance. We have also explored the influence on the dynamics of the location of x_f with respect to the singular point(s) of the potential during the time scale appropriate for the pre-history distribution.

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