

## Nonstationary optimal paths and tails of prehistory probability density in multistable stochastic systems

B. E. Vugmeister, J. Botina, and H. Rabitz

*Department of Chemistry, Princeton University, Princeton, New Jersey 08544*

(Received 8 January 1997)

The tails of prehistory probability density in nonlinear multistable stochastic systems driven by white Gaussian noise, which has been a subject of recent study, are analyzed by employing the concepts of nonstationary optimal fluctuations. Results of numerical simulations show that the prehistory probability density is non-Gaussian and highly asymmetrical, and that it is an essential feature of noise driven fluctuations in nonlinear systems. We also show that in systems with detailed balance the prehistory probability density is the conventional transition probability that obeys the backward Kolmogorov equation. [S1063-651X(97)11705-6]

PACS number(s): 05.40.+j, 02.50.-r, 05.20.-y

### I. INTRODUCTION

Recent theoretical and experimental studies [1,2] of large fluctuations in stochastic systems driven by white Gaussian noise have shown that, among the different fluctuation paths of the system, the most probable *optimal* fluctuation path plays a crucial role. This is true for large output fluctuations, since the probability of encountering such fluctuations peaks sharply at the deterministic optimal fluctuation trajectory driven by an optimal realization from the random noise bath.

The most probable fluctuation path, which we will call the stationary optimal path (SOP), is the optimal trajectory  $x_{\text{opt}}^s(t; t_f, x_f)$  that brings the system to a given point  $x_f$  of the phase space at instant  $t_f$  from the vicinity of the initial attractor  $x_{\text{eq}}$ , where the system has been fluctuating for a long period of time prior to reaching the point  $x_f$ . The concept of SOP can be traced back to the work of Onsager and Machlup [3] and has been further widely used (see, e.g., Refs. [4–10]).

In particular, the SOP determines the quasistationary probability density  $P^{\text{eq}}(x_f)$ , referenced to the local equilibrium point  $x_{\text{eq}}$ , a system located at point  $x_f$  under the condition that it never left the region of attraction to  $x_{\text{eq}}$ . Another quantity of interest is the transition probability density  $P(x_f, t_f; x_0, t_0)$  for the system to be at point  $x_f$  at  $t_f$ , given that it was at  $x_0$  at time  $t_0$ . It follows that  $P(x_f, t_f; x_0, t_0) \rightarrow P^{\text{eq}}(x_f)$  for  $t_0 \rightarrow -\infty$ , provided that  $x_0$  belongs to the domain of attraction to  $x_{\text{eq}}$ .

The distribution of different paths for a nonlinear double well potential has been investigated [1,2] through consideration of the so called *prehistory* probability density  $P_h(x_f, t_f; x_0, t_0)$ ; that is a conditional probability that the system will be brought to the final point  $x_f$  at  $t_f$  from the vicinity of the equilibrium position  $x_{\text{eq}}$  via the point  $x_0$  at the intermediate instant  $t_0$ . Using the fact that the prehistory probability density reaches its maximum on the SOP ending at  $x_f$ , then  $\ln P_h(x_f, t_f; x_0, t_0)$  has been represented as a power series with respect to the deviation of  $x_0$  from the optimal path. The first term in this series is responsible for the Gaussian behavior of the  $P_h(x_f, t_f; x_0, t_0)$  near its maximum. It is apparent that the validity of the power series expansion re-

quires that the deviation of  $x_0$  from the SOP be sufficiently small.

Until now, to our knowledge, there have been no attempts to calculate the prehistory probability density outside of the Gaussian domain. The region where one can observe the deviation of  $P_h(x_f, t_f; x_0, t_0)$  from the universal Gaussian form is most interesting, since it reflects the specificity of the particular system.

Motivated by the fact that the deviation of  $P_h(x_f, t_f; x_0, t_0)$  from the Gaussian form has been observed in experiments [1], in this paper we performed an analysis of the prehistory probability density for a broad range of initial positions  $x_0$  outside the vicinity of the SOP. This approach is based on the calculation of ‘‘nonstationary optimal paths,’’ which we call the nonstationary optimal trajectories that maximize the value of the transition probability considered as a functional of different paths starting at point  $x_0$  at time  $t_0$  and ending at point  $x_f$  at time  $t_f$ . We will show below that the nonstationary optimal path formalism naturally allows for a calculation of the highly non-Gaussian tails of the prehistory probability density appearing in nonlinear systems.

### II. NONSTATIONARY OPTIMAL PATHS IN NONLINEAR SYSTEMS

We will consider a one dimensional stochastic system, as this has been the subject of modeling in analog experiments [1] described by the equation (dimensionless units)

$$\dot{x} = -U'(x) + f(t), \quad (1)$$

where  $U'(x)$  is the deterministic force induced by the nonlinear double well potential

$$U(x) = -\frac{1}{2}x^2 + \frac{1}{4}x^4, \quad (2)$$

and  $f(t)$  is random Gaussian white noise with the correlation function

$$\langle f(t)f(t') \rangle = D\delta(t-t'). \quad (3)$$

In order to calculate the transition probabilities we make use of Feynman’s notion [11] of relating the probability functional  $\Phi[x(t)]$  of the system output fluctuations and the probability functional  $P[f(t)]$  of the input noise. For Gaussian noise the probability functional  $P[f(t)]$  is given by

$$P[f(t)] \propto \exp\left[-\frac{1}{2D} \int_{t_0}^{t_f} dt f(t)^2\right]. \quad (4)$$

One can see from Eq. (4) that  $P[f(t)]$ , and hence  $\Phi[x(t)]$ , reaches its maximum for the most probable *optimal* random field  $f_{\text{opt}}$ , introduced in Ref. [5], which minimizes the integral  $\int dt f(t)^2$  under the constraint that the equation of motion, Eq. (1), is satisfied and  $x(t_0)=x_0$ ,  $x(t_f)=x_f$ . Such a constraint leads to a nonzero value of the optimal noise field  $f_{\text{opt}}(t)$ , which would be zero without constraints. We will assume that points  $x_0$  and  $x_f$  belong to the region of attraction of the same attractor, including any small vicinity of the separatrix.

The optimal transition probability is given by the most favorable realization of noise which brings the system from point  $(x_0, t_0)$  to point  $(x_f, t_f)$ , i.e.,

$$P(x_f, t_f; x_0, t_0) \propto \exp\left[-\frac{1}{2D} \int_{t_0}^{t_f} dt f_{\text{opt}}(t)^2\right]. \quad (5)$$

In order to find the quasistationary probability distribution  $P^{\text{eq}}(x_f)$ , one should take the limit in Eq. (5),  $x_0 \rightarrow x_{\text{eq}}$ ,  $t_0 \rightarrow -\infty$ . The corresponding optimal trajectory is a SOP, and the corresponding optimal field is a quasistationary optimal field  $f_{\text{opt}}^s(t)$ . We have

$$P^{\text{eq}}(x_f) \propto \exp\left[-\frac{1}{2D} \int_{-\infty}^{t_f} dt f_{\text{opt}}^s(t)^2\right]. \quad (6)$$

Following Ref. [5], we replace  $f(t)$  in Eq. (5) by its form given by the equation of motion, Eq. (1). We obtain

$$P(x_f, t_f; x_0, t_0) \propto \exp\left[-\frac{S}{2D}\right], \quad (7)$$

where  $S$  is the action integral

$$S = \frac{1}{2} \int_{t_0}^{t_f} dt [\dot{x} + U'(x)]^2. \quad (8)$$

Note that, in the case of white noise, Eq. (7) can be obtained also from the corresponding Fokker-Plank equation with the use of WKB approximation [12]. The validity of Eqs. (5) and (8) corresponds to the limit of low noise intensity for which  $S/D \gg 1$ .

Variation of the resulting action integral gives rise to effective dynamics described by the Hamiltonian

$$H = \frac{1}{2} \dot{x}^2 - \frac{1}{2} U'(x)^2 \quad (9)$$

and equation of motion

$$\ddot{x} - U'(x)U''(x) = 0, \quad (10)$$

with boundary condition

$$x(t_0) = x_0, \quad x(t_f) = x_f. \quad (11)$$

Equation (10) is the Euler-Lagrange equation for the functional, Eq. (8).

The solution of Eqs. (10) and (11) represents the nonstationary optimal path  $x_{\text{opt}}(t)$  between points  $(x_0, t_0)$  and

$(x_f, t_f)$  corresponding to finite energy in Eq. (9). The SOP  $x_{\text{opt}}^s(t; x_f, t_f)$  ending at point  $x_f$  at  $t_f$  represents a partial solution of Eq. (10) that satisfies the first order differential equation

$$\frac{dx_{\text{opt}}^s}{dt} = U'(x_{\text{opt}}^s), \quad (12)$$

with boundary conditions

$$x(t_f) = x_f, \quad x(-\infty) = x_{\text{eq}}. \quad (13)$$

The solution of Eqs. (12) and (13) with  $x_{\text{eq}} = -1$  for the double well potential given by Eq. (2) is the *instanton* solution [13]

$$x_{\text{opt}}^s(t) = -\frac{1}{\sqrt{1 + C \exp[2t]}}, \quad f_{\text{opt}}^s(t) = \frac{2C \exp[2t]}{\sqrt{(1 + C \exp[2t])^3}}, \quad (14)$$

where the constant  $C$  determines the value  $x_{\text{opt}}^s(t_f) = x_f$ . The other partial solution of the second order differential equation [Eq. (10)] satisfies the equation  $dx/dt = -U'(x)$ , that is the equation of motion [Eq. (10)] without noise. Note that in the general case with a nonlinear dependence of  $U'(x)$  on  $x$ , the solution of Eq. (10) cannot be presented as a linear combination of the partial solutions.

The nonstationary optimal paths for the potential given by Eq. (2) have been found by numerical integration of Eq. (10), subject to boundary conditions, Eq. (11). The two point boundary value problem has been reexpressed by considering the problem with initial conditions  $x(t_0) = x_0$  and  $\dot{x}(t_0) = v_0$ . A minimization procedure has been employed in order to find the best value of the initial velocity  $v_0$  to reach the target point  $x_f$  at  $t_f$ . As a test for the calculations, the energy conservation law in Eq. (9) has been verified for each trajectory obtained.

In Figs. 1(a) and 2(a), we illustrate the typical nonstationary optimal paths corresponding to  $x_f = -0.1$  for different values of  $x_0$  and  $\tau = t_f - t_0$ . For comparison we show also the SOP, given by Eq. (14) [for  $x_f = -0.1$ , the constant  $C = 99$  in Eq. (14)]. As one can see from Fig. 2(a), the essential feature of the nonstationary optimal trajectories starting at  $x_0 < 0$  is the possibility of a sign change of the velocity  $\dot{x}(t)$  at an intermediate point of the trajectory. For small values of  $\tau$ , nonstationary optimal trajectories deviate significantly from the SOP, whereas for asymptotically large  $\tau$  they rapidly approach the SOP independently of the initial point  $x_0$ . This behavior can also be understood from the exact solution of Eq. (10) for the harmonic potential presented in Sec. III.

With the use of Eq. (1) and the known temporal form of the nonstationary trajectories, one can reproduce the corresponding values of the optimal noise field. The values of  $f_{\text{opt}}(t)$  for the trajectories shown in Figs. 1(a) and 2(a) are presented in Figs. 1(b) and 2(b). In the next section the approach above will be used for the calculation of the prehistory probability density for a broad range of initial positions  $x_0$ .

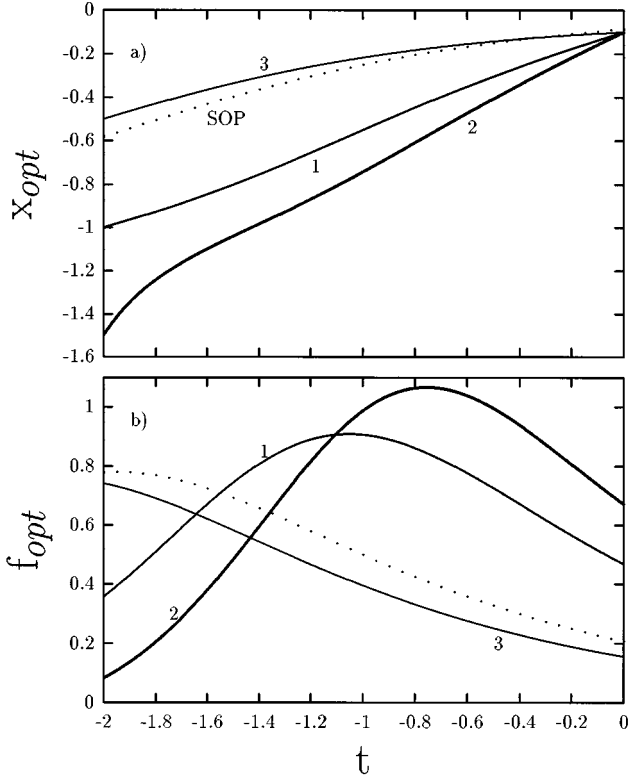


FIG. 1. The nonstationary optimal path (a) and optimal field (b) for the nonlinear potential Eq. (2) and  $\tau=2$  corresponding to the final point  $x_f = -0.1$  and initial points  $x_0 = -1$  (1),  $-1.5$  (2), and  $-0.5$  (3). The dotted lines show the stationary optimal path and the corresponding optimal field.

### III. PREHISTORY PROBABILITY DENSITY

The prehistory probability density is given by [1]

$$P_h(x_f, t_f; x_0, t_0) \propto \exp \left[ -\frac{1}{D} \left( \int_{-\infty}^{t_f} dt f_{\text{opt}}(t, x_0, x_f)^2 - \int_{-\infty}^{t_f} dt f_{\text{opt}}^s(t, x_f)^2 \right) \right], \quad (15)$$

where the optimal noise field  $f(t, x_0, x_f)$  induces the nonstationary optimal trajectory which starts at  $x_{\text{eq}}$  at  $t = -\infty$ , passes point  $x_0$  at  $t_0$ , and reaches point  $x_f$  at  $t_f$ ;  $f_{\text{opt}}^s$  is the stationary optimal field that induces the SOP ending at point  $x_f$  at  $t_f$ . Thus we may write

$$\int_{-\infty}^{t_f} dt f_{\text{opt}}(t, x_0, x_f)^2 = \int_{-\infty}^{t_0} dt f_{\text{opt}}^s(t, x_0)^2 + \int_{t_0}^{t_f} dt f_{\text{opt}}(t, x_0, x_f)^2, \quad (16)$$

and with Eqs. (15) and (16), we arrive at

$$P_h(x_f, t_f; x_0, t_0) = \frac{P^{\text{eq}}(x_0) P(x_f, t_f; x_0, t_0)}{P^{\text{eq}}(x_f)}. \quad (17)$$

The difference between  $P_h(x_f, t_f; x_0, t_0)$  and  $P(x_f, t_f; x_0, t_0)$  is that  $P_h(x_f, t_f; x_0, t_0)$  satisfies the normal-

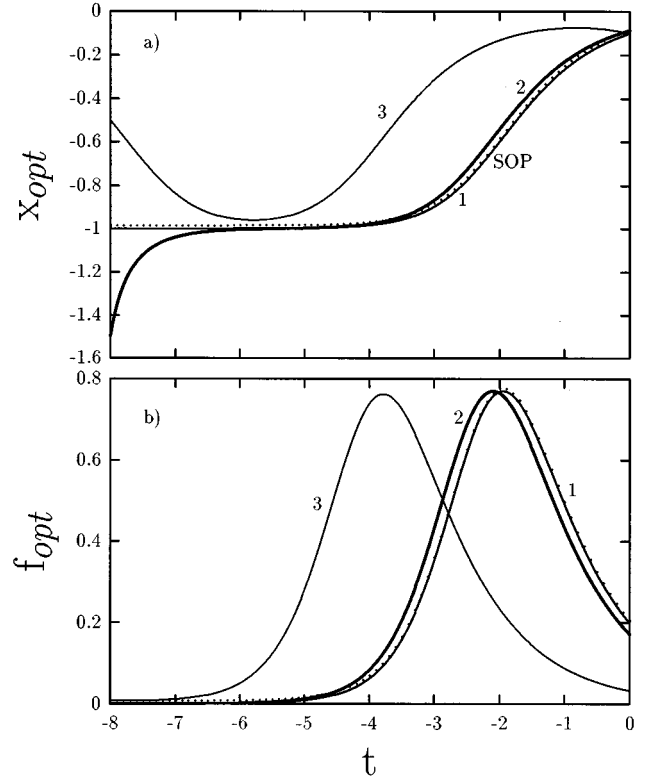


FIG. 2. The nonstationary optimal path (a) and optimal field (b) for the nonlinear potential Eq. (2) and  $\tau=8$  corresponding to the final point  $x_f = -0.1$  and initial points  $x_0 = -1$  (1),  $-1.5$  (2), and  $-0.5$  (3). The dotted lines show the stationary optimal path and the corresponding optimal field.

ization condition with respect to initial points  $x_0$  [ $\int dx_0 P_h(x_f, t_f; x_0, t_0) = 1$ ] whereas  $P(x_f, t_f; x_0, t_0)$  satisfies the analogous normalization condition with respect to final points  $x_f$ . Equation (15) shows that if  $x_0$  belongs to the stationary optimal path ending at  $x_f$ , then both integrals in Eq. (15) are equal and cancel, meaning that  $P_h(x_f, t_f; x_0, t_0)$  reaches its maximum on the stationary optimal path [1].

It follows from Eq. (17) that  $P^{\text{eq}}(x_f)$  given by Eqs. (6), (1), and (14) satisfies the principle of detailed balance

$$\frac{P^{\text{eq}}(x_f)}{P^{\text{eq}}(x_0)} = \exp \left[ -\frac{1}{D} [U(x_f) - U(x_0)] \right], \quad (18)$$

and  $P(x_f, t_f; x_0, t_0)$  is the conventional transition probability that obeys the forward Kolmogorov equation [14] due to the white character of the noise. Then the prehistory probability density should obey the backward Kolmogorov equation and, in fact, does not depend on the prehistory. Below we will illustrate this conclusion, which is a consequence of the chosen quasiequilibrium value of the initial distribution, on the model system with a quasiharmonic potential. In the general case the prehistory probability density does depend on prehistory in multistable stochastic systems. Note also that, being consistent with the concept of optimal fluctuation, we assume that  $U(x_f) > U(x_0)$  (a particle is ‘‘climbing uphill’’), resulting in occasional fluctuations described by the prehistory probability density.

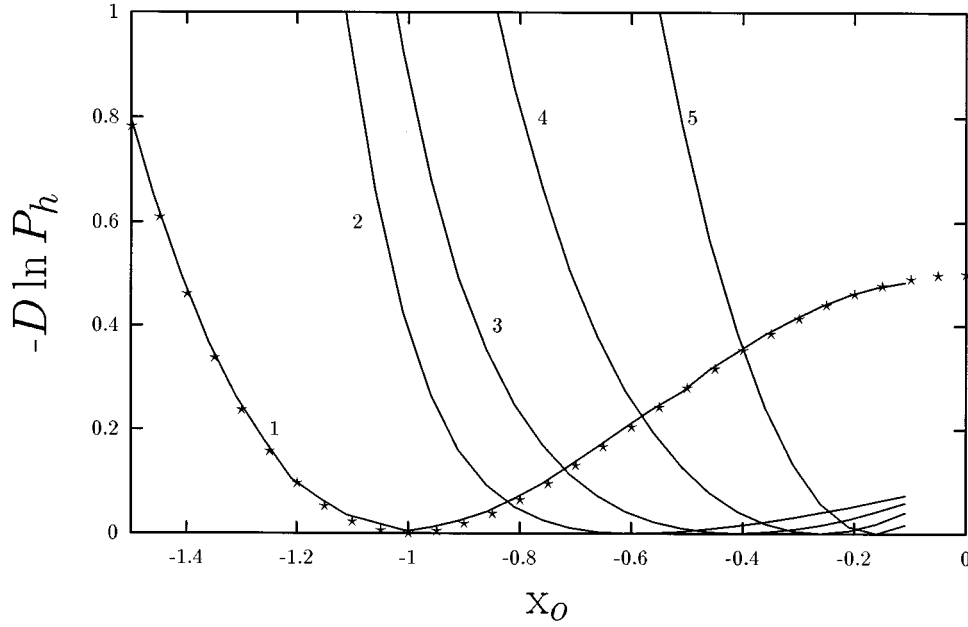


FIG. 3. The activation energy of the prehistory probability density for  $x_f = -0.1$  as a function of initial position  $x_0$ : (1)  $\tau=8$ , (2)  $\tau=2$ , (3)  $\tau=1.5$ , (4)  $\tau=1$ , and (5)  $\tau=0.5$ . The data for curves 2–5 are multiplied by ten. Stars represent the values of  $2[U(x_0) - U(x_{\text{eq}})]$ , and confirm that quasiequilibrium distribution takes place for large  $\tau$ .

In Refs. [1,2] the partial solution [Eq. (12)] has been used for the evaluation of the prehistory probability density based on the iterative solution of Eq. (10) near the SOP implying that the values of  $[x_0 - x_{\text{opt}}^s(t_0; x_f, t_f)]$  are not too large. We stress, however, that using the formalism above, the prehistory probability density as well as the transition probabilities can be evaluated without the limitation on the values of  $[x_0 - x_{\text{opt}}^s(t_0; x_f, t_f)]$ .

Prior to concentrating on the results of numerical calculations for the case of the nonlinear potential [Eq. (2)], we will present for illustration the simple expressions for  $P(x_f, t_f; x_0, t_0)$  and  $P_h(x_f, t_f; x_0, t_0)$  with the quasiharmonic potential of the form

$$U(x) = \begin{cases} \frac{1}{2} x^2, & x \leq 1 \\ \frac{1}{2} (x-2)^2, & x > 1. \end{cases} \quad (19)$$

In this case the solution of Eq. (10) can be obtained analytically. We have, in the domain of attraction at  $x_{\text{eq}}=0$ ,

$$x_{\text{opt}}(t) = \frac{1}{e^{t_f-t_0} - e^{t_0-t_f}} [e^t (x_f e^{-t_0} - x_0 e^{-t_f}) + e^{-t} (x_0 e^{t_f} - x_f e^{t_0})], \quad x < 1, \quad (20)$$

where  $x_{\text{opt}}(t)$  is the nonstationary optimal path.

The optimal noise field is of the form

$$f_{\text{opt}}(t) = \frac{2e^t}{e^{t_f-t_0} - e^{t_0-t_f}} (x_f e^{-t_0} - x_0 e^{-t_f}). \quad (21)$$

Note that the two terms in Eq. (20) proportional to  $e^t$  and  $e^{-t}$ , respectively, represent the two partial solutions of Eq. (10). Only the partial solution proportional to  $e^t$ , which reaches a finite limit at  $t_0 \rightarrow -\infty$ , contributes to the SOP. In

fact, for  $t_0 \rightarrow -\infty$ , it follows from Eq. (20) that  $x_{\text{opt}}(t) = x_{\text{opt}}^s(t; x_f, t_f) = x_f e^{t-t_f}$  [3].

From Eqs. (5) and (17), we obtain

$$P(x_f, t_f; x_0, t_0) \propto \exp \left[ -\frac{1}{D} \frac{(x_f - x_0 e^{-(t_f-t_0)})^2}{1 - e^{-2(t_f-t_0)}} \right], \quad (22)$$

$$P_h(x_f, t_f; x_0, t_0) \propto \exp \left[ -\frac{1}{D} \frac{(x_0 - x_f e^{-(t_f-t_0)})^2}{1 - e^{-2(t_f-t_0)}} \right]. \quad (23)$$

One can see from Eqs. (22) and (23) that in the case of the quasiharmonic potential the nonstationary optimal path approach reproduces the exact results for the transition probability and the prehistory probability density in linear stochastic systems with Gaussian noise. Note that the prehistory probability density given by Eq. (23) obeys the backward Kolmogorov equation [14].

The prehistory probability density for the nonlinear potential given by Eq. (2) has been calculated numerically with the use of Eq. (15). Precaution is required, however, since near the SOP the exponent in Eq. (15) becomes the small difference of large numbers. In order to improve the accuracy of the calculations, we may represent the exponent of  $P_h(x_f, t_f; x_0, t_0)$  in the form

$$\int_{-\infty}^{t_f} dt [f_{\text{opt}}^s(t, x_0)^2 - f_{\text{opt}}^s(t, x_f)^2] + \int_{t_0}^{t_f} dt [f_{\text{opt}}(t, x_0, x_f)^2 - f_{\text{opt}}^s(t, x_f)^2]. \quad (24)$$

One can see from Eq. (24) that if  $x_0$  belongs to the stationary optimal path ending at point  $x_f$  at  $t_f$ , then both integrands in

Eq. (24) vanish. The calculated values of  $-D \ln P_h(-0.1, 0; x_0, -\tau)$  are presented in Fig. 3. It is seen that the parabolic character of the curves, and hence the Gaussian character of prehistory probability density, takes place only in a small region in the vicinity of SOP where the prehistory probability density reaches its maximum. In general, the function  $P_h(x_f, t_f; x_0, t_0)$  is highly asymmetrical, and that is the essential feature of the path distribution in nonlinear systems.

#### IV. CONCLUSION

We have shown that the concept of a nonstationary optimal path is an adequate approach for the analysis of transition probabilities and prehistory probability density in noise driven systems. The concept allows one to analyze the optimal path distribution outside of the immediate vicinity of the stationary optimal path. The observed highly asymmetrical shape of the prehistory probability density is the essential feature of the fluctuations in nonlinear noise driven systems.

We hope that this observation will stimulate additional experiments on the analysis of optimal path distributions in nonlinear systems.

The nonstationary optimal path approach for the analysis of fluctuations in stochastic systems should be especially useful for exploring the possibilities of control of fluctuations by an external field. It has been shown recently [15,16] that an optimal control field with a finite time duration can naturally cooperate with the nonstationary optimal noise such that its temporal form coincides with the temporal form of the optimal fluctuations.

#### ACKNOWLEDGMENTS

We are thankful to M. I. Dykman, R. S. Maier, M. Marder, and V. N. Smelyanskiy for the useful discussions of the results of the paper. The authors acknowledge support from the Office of Naval Research and National Science Foundation.

- 
- [1] M. I. Dykman, P. V. E. McClintock, V. N. Smelyanskiy, N. D. Stein, and N. G. Stocks, *Phys. Rev. Lett.* **68**, 2718 (1992).
  - [2] M. I. Dykman, D. G. Luchinckiy, P. V. E. McClintock, and V. N. Smelyanskiy, *Phys. Rev. Lett.* **77**, 5229 (1996).
  - [3] L. Onsager and S. Machlup, *Phys. Rev.* **91**, 1505 (1953); **91**, 1512 (1953).
  - [4] A. D. Wentzell and M. I. Freidlin, *Russ. Math. Surveys* **25**, 1 (1970); M. I. Freidlin and A. D. Wentzell, *Random Perturbations of Dynamical Systems* (Springer-Verlag, New York, 1984).
  - [5] M. I. Dykman and M. A. Krivoglaz, *Zh. Eksp. Teor. Fiz.* **77**, 60 (1979) [*Sov. Phys. JETP* **50**, 30 (1979)]; M. I. Dykman, *Phys. Rev. A* **42**, 2020 (1990).
  - [6] M. Marder, *Phys. Rev. Lett.* **74**, 4547 (1995); *Phys. Rev. E* **54**, 3442 (1996).
  - [7] A. J. Bray and A. J. McKane, *Phys. Rev. Lett.* **62**, 493 (1987).
  - [8] R. S. Maier and D. L. Stein, *Phys. Rev. Lett.* **69**, 3691 (1992); **71**, 1783 (1993); **77**, 4861 (1996); *J. Stat. Phys.* **83**, 291 (1996).
  - [9] T. Naeh, M. M. Klosek, B. J. Matkowsky, and Z. Schuss, *SIAM J. Appl. Math.* **50**, 595 (1990).
  - [10] R. Olender and R. Elber, *J. Chem. Phys.* **105**, 9299 (1996).
  - [11] R. P. Feynman and A. R. Hibbs, *Quantum Mechanics and Path Integrals* (McGraw-Hill, New York, 1965).
  - [12] E. Ben-Jacob, D. J. Bergman, B. J. Matkowsky, and Z. Schuss, *Phys. Rev. A* **26**, 2805 (1982).
  - [13] R. Rajaraman, *Solitons and Instantons* (North-Holland, Amsterdam, 1982).
  - [14] G. Gardiner, *Handbook of Stochastic Methods* (Springer-Verlag, Berlin, 1985).
  - [15] B. E. Vugmeister and H. Rabitz, *Phys. Rev. E* **55**, 2522 (1997).
  - [16] V. N. Smelyanskiy and M. I. Dykman, *Phys. Rev. E* **55**, 2516 (1997).