Optimal control of large fluctuations

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We consider the problem of optimal control of large fluctuations. Our approach is based on the concept of the optimal fluctuational path along which the system is most likely to move when it fluctuates to a given state. Optimal control requires double optimization: over realizations of the control field and fluctuational paths. We formulate the appropriate variational problem. Using a white-noise-driven dynamical system as an example, we show that even comparatively weak control fields, if applied in an optimal way, can exponentially strongly reduce the probability of an undesirable fluctuation or increase the probability of a desirable one. Explicit expressions are obtained for the cases of control by a spatially uniform time-dependent field and by a stationary nonuniform field. We show that, in the problem of control, there generically occur singularities related to topological singularities found in the problem of large fluctuations. [S1063-651X(97)09203-9]

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I. INTRODUCTION

Large infrequent fluctuations play a key role in a broad range of physical processes, from cosmology and nucleation at phase transitions to earthquakes and mutations in DNA sequences. They are also of crucial importance for engineering as they are often responsible for failures of systems and devices. Therefore control of large fluctuations is a challenging and fundamental problem. Despite numerous efforts no generally accepted principles have been found that describe the probabilities of large fluctuations in systems away from thermal equilibrium [1], which include lasers and electronic devices, electron traps used in fundamental measurements [2], pattern forming systems [3], biological systems, and systems studied in engineering. At the same time there is an emerging understanding that not only is the problem of fundamental importance, but that large fluctuations can sometimes play a creative role: they can strongly enhance a signal in a nonlinear system and improve signal processing through stochastic resonance [4]; they can also give rise to a unidirectional current in spatially periodic structures (ratchets) [5].

Recently a very substantial progress has been made in understanding large fluctuations by combining the physical picture of the fluctuations with the path-integral technique and the results of nonlinear dynamics and catastrophe theory [6–8] and the modern approach to the problem is based on the optimal path concept. An optimal path is the path along which the system moves, with overwhelming probability, when it fluctuates from the vicinity of the stable state (where it spends most of its time) to a given state. Optimal paths are real physical objects: they have been experimentally observed [9]. In the theory of large fluctuations, the pattern of optimal paths plays a role similar to that of the phase portrait in nonlinear dynamics.

In this paper we consider the problem of controlling large fluctuations in an optimal way. The theory of optimal control has been substantially developed recently, and the results have been applied to controlling various physical phenomena [10] (see Ref. [11] for a review). In our analysis we combine the results for large fluctuations with the ideas and techniques of the modern theory of optimal control. In Sec. II we provide a general variational formulation of the problem using a white-noise-driven system as an example. In Sec. III we consider optimal control by comparatively weak fields. Explicit expressions for exponentially strong change of the fluctuation probability by a spatially uniform time-dependent control field and by a stationary field optimally configured in space are discussed in Sec. IV. Section V contains concluding remarks.

II. GENERAL FORMULATION

The problem of optimal control of fluctuations can be formulated in the following way: how to obtain a maximal increase or decrease of the probability of a fluctuation to a given target state (or switching between coexisting stable states) by driving the system with an external field $\mathbf{E}(\mathbf{r}, t)$, for a minimal value of a certain penalty functional $F[\mathbf{E}]$. The form of this functional depends on the specific problem [12]; e.g., in the case of control by electromagnetic field it can be the total energy in a pulse.

A comparatively simple and powerful approach to optimal control of large fluctuations is based on the idea of double optimization: one may consider optimal control of the optimal (most probable) fluctuations. It has been shown theoretically and demonstrated in the experiment [9] that, in a large fluctuation, the probability distribution of moving to a given state along different paths often peaks exponentially sharply at the optimal fluctuational path. Therefore the problem of control is naturally reduced to affecting the motion along this path and/or changing the path, and even a small control field may produce strong effect on the fluctuations.

To illustrate this approach we shall consider the most simple but nontrivial and important problem: control of large fluctuations in a dynamical system driven by white Gaussian noise $\mathbf{f}(t)$. The equation of motion of the system is of the form

$$\dot{\mathbf{r}} = \mathbf{K}(\mathbf{r}; \mathbf{E}) + \mathbf{f}(t), \quad \langle f_m(t)f_m(t') \rangle = D \delta_{mm} \delta(t-t'). \quad (1)$$

Here $\mathbf{r}$ may be considered as a coordinate of the system (e.g., the position vector of a Brownian particle), and $\mathbf{K}$ is the
regular force that drives the system in the absence of the noise \( f(t) \). The force \( K \) depends on the control field \( E = E(r; t) \). We assume that \( K \) depends on time only in terms of the field \( E \); generalization to the case where \( K \) periodically depends on time even for \( E = 0 \) will be considered elsewhere. Various phenomenological and microscopic models described by Eq. (1) were discussed in [13].

The probability density \( P(r) \) of a large fluctuation to a point \( r \) far away from the stable state is known to display activation dependence on the noise intensity \( D \) (in the simple case of thermal equilibrium systems \( D \approx T \), where \( T \) is temperature):

\[
P(r) \approx \exp[-S(r)/D].
\]

In thermal equilibrium systems the “activation energy” \( S(r) \) is given by the appropriate free energy for the fluctuation to the point \( r \). In the general case it is given by the minimal value of a certain functional. For model (1) this functional is of the form [14]

\[
S[\tilde{r}; E] = \frac{1}{2} \int dt [\dot{\tilde{r}} - K(\tilde{r}; E)]^2, \quad S(r) = \{\min S[\tilde{r}; E]\}_{\tilde{r}(t)}.
\]

The minimum in Eq. (3) is taken over the paths \( r(t) \).

Equation (2) also applies to the probability of escape from a metastable state. With an appropriately modified functional \( S[\tilde{r}; E] \), it holds for systems driven by a nonwhite (color) Gaussian noise (see [15] for a review), as well as for birth-death processes (in the latter case \( D \) should be redefined) [16,7b].

For weak noise intensity \( D \), even small variations in the control field \( E \) can lead to a change in the activation energy \( S \) which greatly exceeds \( D \), and thus to a very strong change of the probability \( P \). In the problem of optimal control of the fluctuations it is advantageous therefore to analyze the activation energy \( S \) as a yield of the control processes. This provides a unified approach to a broad class of problems.

Effectiveness of control is determined by the penalty functional \( F[E(r, t)] \) for the control field: a desired effect should be achieved at a minimal “price.” This price is determined by the value of \( F \). We assume \( F \) to be quadratic in the field \( E \) (cf. [12]):

\[
F[E(r, t)] = \frac{1}{2} \{E, \tilde{M}E\}
\]

\[
= \frac{1}{2} \int dr dr' \int dt dt' \sum_{n, m} E_n(r, t) \times M_{nm}(r, r'; t, t') E_m(r', t'),
\]

where \( \tilde{M} \) is a positive definite Hermitian operator.

For a given realization of the field \( E(r, t) \), the probability density \( P(r) \) for the system to reach a point \( r \) is determined by the minimum of the functional \( S[\tilde{r}; E] \). Therefore optimal control of large fluctuations is described by the solution of the following variational problem:

\[
\delta R[\tilde{r}; E] = 0, \quad R[\tilde{r}; E] = S[\tilde{r}; E] + \lambda (F[\tilde{E}] - F).
\]

Here \( \lambda \) is the Lagrange multiplier which allows for the fact that realizations of the field \( E(r, t) \) provide a given value \( F \) to the penalty functional \( F \) (cf. [17]). The minimum is taken with respect to the paths \( r(t) \) along which the system moves to a given target state \( r_f \), and over realizations of the control field \( E(r, t) \). The boundary conditions for the extreme paths \( r(t) \) which arrive at the state \( r_f \) at a given instant \( t_f \) follow from the fact that, prior to the large fluctuation, the system spends a long time fluctuating about the attractor \( r_a \), so that

\[
r(t) \to r_a \quad \text{for} \quad t \to -\infty, \quad r(t_f) = r_f.
\]

The overall result of the control processes is the optimal field \( E_{opt}(r, t) \), the optimal path \( r_{opt}(t) \) which is the most probable path to a state \( r_f \) for the corresponding field realization, and also the optimal activation energy of the fluctuation to the point \( r_f \):

\[
R_{opt}(r_f, F) = S[r_{opt}(t), E_{opt}(r, t)]
\]

We emphasize that, depending on the sign of the Lagrange multiplier \( \lambda \) in Eq. (5), the value of \( R_{opt} \) may be minimal or maximal, for a given value of the penalty functional \( F \). These two cases correspond, respectively, to the optimal enhancement or suppression of fluctuations to a given point \( r_f \) by the control field (see Sec. III). The possibility of controlling fluctuations and cooperating with fluctuations in controlling the dynamics of a system was considered recently by Vugmeister and Rabitz [18] using the traditional formalism of optimal control theory in terms of target cost functional. Explicit results were obtained for a one-variable linear system.

The activation energy \( R_{opt}(r, F) \) might be expected to be a smooth function of the state of the system \( r_f \). However, this is not always the case. In fact, \( R_{opt} \) has generic singularities. Their occurrence is a consequence of the occurrence of caustics in the sets of extreme paths for variational problems of type (5). However, in contrast to extreme paths in quantum mechanics and optics, optimal fluctuational paths do not encounter caustics. This is related to the fact that optimal fluctuational paths describe a non-negative quantity, the probability density to reach a given state.

Generic singularities of the set of optimal paths are switchings [8]: when the final point of the path \( r_f \) changes (by a small but finite distance, for finite \( D \)), the path \( r_{opt} \) changes discontinuously, to a totally different solution of problem (3) which provides the absolute minimum of \( S(r_f) \) for a given \( E(r, t) \) (not just an extremum). Switchings of optimal paths have been recently observed in experiment [9](b).

The effect of switching occurs also in optimal trajectories of the control field \( E_{opt}(r, t) \) [19], as illustrated in Sec. IV for the case of comparatively weak control fields. The general analysis of the singularities of the pattern of optimal realizations of a control field is based on the results of the theory of Lagrangian manifolds and catastrophe theory and will be given elsewhere.

**III. CONTROL BY A WEAK FIELD**

A simple explicit solution of the problem of optimal control may be obtained in the important case where the controlling field \( E(r, t) \) is weak compared to the driving force \( K \)
away from the fixed points of the system (where \( K = 0 \)). In this case we write the force \( K \) in Eq. (1) as a superposition of the force \( K^{(0)} \) in the absence of the control field and the control field itself,

\[
K(r; E) = K^{(0)}(r) + E(r, t).
\] (8)

It is well known from variational calculus that, to the first order in the field \( E \), the expression for the activation energy \( S(r) \) (3) can be evaluated along the optimal fluctuational trajectory \( r^{(0)}_\text{opt}(t) \) in the absence of the control field:

\[
S(r) \approx S[r^{(0)}_\text{opt}(t); E(r^{(0)}_\text{opt}(t), t)] = S^{(0)}(r) - \int dt f^{(0)}_\text{opt}(t) \cdot E(r^{(0)}_\text{opt}(t), t),
\] (9)

\[
S^{(0)}(r) = S[r^{(0)}_\text{opt}(t); 0], \quad f^{(0)}_\text{opt}(t) = r^{(0)}_\text{opt} - K^{(0)}(r^{(0)}_\text{opt}).
\]

It is straightforward now to perform optimization over the field \( E \) with the penalty functional (4). If the integral operator \( \hat{M} \) in Eq. (4) has a reciprocal operator \( \hat{M}^{-1} \), the formal solution of the variational problems (5) and (9) for the optimal field can be written as

\[
E^{(0)}_\text{opt}(r, t) = \lambda^{-1} \hat{M}^{-1} \varphi(r, t), \quad \varphi(r, t) = f^{(0)}_\text{opt}(t) \delta(r - r^{(0)}_\text{opt}(t)).
\] (10)

[the function \( \varphi(r, t) \) is equal to zero for \( t \) lying outside the interval where the system moves to the target state along the optimal path \( r^{(0)}_\text{opt}(t) \)].

Substituting solution (10) into the expression for the functional \( F \) (4), and setting the value of the functional equal to a given value \( \mathcal{F} \), we obtain two values of the Lagrange multiplier \( \lambda \), with opposite signs, and the final expression for the increment of the activation energy of the optimal fluctuation (7) takes on the form

\[
R^{(0)}_\text{opt}(r_f, F) = S^{(0)}(r_f) \pm \Delta S, \quad \Delta S = (2 \mathcal{F})^{1/2} \varphi \hat{M}^{-1} \varphi^{1/2}.
\] (11)

It is seen from Eq. (11) that indeed, even for a weak control field \( E \), the field-induced change of the exponent \( -R^{(0)}_\text{opt}/D \) in the expression for the probability of fluctuations to a given state \( r_f \) can greatly exceed unity for \( \mathcal{F}^{1/2} \gg D \). This means that even a weak control field may give rise to an exponentially strong decrease or increase [for the plus or minus signs in Eq. (11), respectively] of the fluctuation probability.

IV. RESULTS FOR SPECIAL TYPES OF A CONTROL FIELD

A. Coordinate-independent field

The general expression (11) for the change of the activation energy of a large fluctuation due to a weak control field is simplified for special types of control. We shall start with the analysis of the case where the control field \( E \) is independent of the coordinates of the system, so that the penalty functional can be written as

\[
F[E] = \frac{1}{2} \int_{t_i}^{t_f} E^2(t) dt.
\] (12)

In the case of control by a laser field, form (12) corresponds to optimization over the total energy of a radiation pulse, for a given spatial distribution of the radiation, and the instants \( t_i \) and \( t_f \) correspond to the beginning and end of the pulse.

It follows from Eqs. (10) and (11) that the optimal realization of the control field and the correction to the activation energy are of the forms

\[
E^{(0)}_\text{opt}(t) = \mp (2 \mathcal{F})^{1/2} f^{(0)}_\text{opt}(t) \left[ \int_{t_i}^{t_f} dt f^{(0)}_\text{opt}(t) \right]^{-1/2},
\]

\[
\Delta S = (2 \mathcal{F})^{1/2} \left[ \int_{t_i}^{t_f} dt f^{(0)}_\text{opt}(t) \right]^{1/2}.
\] (13)

Here, the sign in the expression for \( E^{(0)}_\text{opt}(t) \) is opposite to the sign of the correction to \( S^{(0)} \) in the expression for \( \Delta S \) for the activation energy of the fluctuation \( R^{(0)}_\text{opt} \); the sign + in Eq. (13) corresponds to the decrease of \( R^{(0)}_\text{opt} \) by the optimal control field (13).

In deriving Eqs. (13), we assumed that \( t_f \) is the instant of time at which the system arrives at a target state \( r_f \). It is clear that, for a time-dependent control field, a natural goal would be to bring the system to a given point by the end of the pulse, i.e., just for \( t = t_f \). Respectively, the optimal force \( f^{(0)}_\text{opt}(t) \) should be evaluated for the optimal fluctuation in which the system arrives to \( r_f \) at the instant \( t_f \).

Controlling switching probability

Special consideration is required in the problem of optimal control of switching from a metastable state. In this case, a natural formulation would be to ask what is the most appropriate temporal shape of a pulse of the control field which, for the penalty functional of form (12), results in the most probable switching of the system? For systems driven by Gaussian noise, the probability of switching is determined, to logarithmic accuracy, by the probability to reach an unstable stationary state (or an unstable limit cycle) on the boundary of the basin of attraction to a stable state from which the system escapes [15], and this unstable state is reached for \( t_f \to \infty \) in Eq. (6). The corresponding path in the absence of the control field \( r^{(0)}_\text{opt}(t) = r^{(0)}_\text{opt}(t - t_0) \) is an instanton: the system moves extremely slowly near the stable state, then it makes a “leap” to the vicinity of the unstable state where its motion again becomes infinitely slow. The duration of the leap is of the order of the relaxation time, and by \( t_0 \) we denoted an instant of time somewhere in the middle of the leap (e.g., where the force \( f^{(0)}_\text{opt} \) is maximal). The activation energy of escape is independent of \( t_0 \); this is the well-known translational invariance of instanton solutions.

In the problem of control of the escape rate, the shape of the pulse of the control field

\[
E^{(0)}_\text{opt}(t) = f^{(0)}_\text{opt}(t) = \tilde{f}^{(0)}_\text{opt}(t - t_0)
\] (14)
should be found for the optimal time $t_0$, with respect to the beginning $t_i$ and the end $t_f$ of the field pulse. The corresponding condition reads

$$\tilde{r}_{opt}(t_f - t_0) = \tilde{r}_{opt}(t_i - t_0)$$  \hspace{1cm} (15)

The field-induced change in the activation energy of the escape rate is then given by Eq. (13) with the integral $f_{opt}^{r_f} dt \tilde{r}_{opt}(t-t_0)$ evaluated for the corresponding $t_0$. Eq. (15) is the condition for this integral to be maximal with respect to $t_0$.

We note that, in the general case, the algebraic equation (15) may have several roots, and it is necessary to take the root which provides a global maximum to the above integral. Switching from one root to another is a sort of a critical phenomenon in the problem of control, which is to some extent similar to a first order phase transition.

Equations (13)–(15) provide an explicit solution of the problem of optimal control of the escape rates. They also make it possible to investigate how the effectiveness of the control, which is determined by the value of $\Delta S$, Eq. (13), depends on specific features of the system dynamics. It is clear from Eq. (13) that, for the penalty functional of the form (12), the modulation of the escape rate increases with the increasing duration of a pulse $t_f - t_i$, for a given value of $\mathcal{F}$. This dependence saturates when the duration of the pulse noticeably exceeds the relaxation time of the system. For a simple model this dependence is shown in Fig. 1.

B. Optimal control by a stationary field

We shall now investigate the case where the control field $E(r)$ is time independent. We limit ourselves to the most simple case of an “isotropic” control field where the matrix $M_{nm}$ in Eq. (4) is proportional to a unit matrix, and we assume that this matrix depends only on the difference of the spatial arguments $r - r'$. In this case the penalty functional becomes

$$F[E(r)] = \frac{1}{2} \int dr dr' M(r-r') E(r) \cdot E(r')$$  \hspace{1cm} (16)

[again, one may think of the penalty functional (16) as of the energy of an electric field].

Variation over the control field $E$ in functionals (5), (9), and (16) can be conveniently performed in the Fourier representation. The formal solution (10) can then be written in the explicit form as

$$E_{opt}(r) = \lambda^{-1} \int_{-\infty}^{0} dt \int \frac{d\mathbf{k}}{(2\pi)^2} M^{-1}_{\mathbf{k}} f_{opt}(t) \times \exp(i\mathbf{k} \cdot \mathbf{r} - r_{opt}(t)) \] , \hspace{1cm} (17)

$$M_{\mathbf{k}} = \int dr M(r) \exp(-i\mathbf{k} \cdot \mathbf{r}) .$$

Here $d$ is the number of components of the vector $r$. We have assumed that the system moves along the optimal path $r_{opt}(t)$ with the time origin chosen in such a way that it arrives at the target state for $t_f = 0$. In the problem of escape, integration over time in Eq. (17) should be performed from $-\infty$ to $\infty$.

With account taken of Eq. (17), expression (11) for the change of the activation energy due to the control field becomes

$$\Delta S = (2\mathcal{F})^{1/2} \int_{-\infty}^{0} dt \int dt' \int \frac{d\mathbf{k}}{(2\pi)^2} M^{-1}_{\mathbf{k}} \times f_{opt}(t) \cdot f_{opt}(t') \exp(i\mathbf{k} [r_{opt}(t) - r_{opt}(t')]) \] , \hspace{1cm} (18)

It is interesting to analyze the form of the control field as given by Eq. (17) in an important case where the effective correlation length $l_c$ of the field is small compared to the characteristic length of the optimal trajectory, in particular with the distance from the attractor to the target state. The reciprocal length $l_c^{-1}$ characterizes the range of $\mathbf{k}$ over which the function $M_{\mathbf{k}}$ varies.

It follows from Eq. (17) that, for small $l_c$, the field $E_{opt}(r)$ peaks sharply on the optimal path $r_{opt}(t)$ along which the system moves to a given target state in the absence of the control field. This is in agreement with simple qualitative arguments that the effect on fluctuations would be expected to be most pronounced if the control field is concentrated on the optimal path. Equation (17) shows also how the field should be distributed along the optimal path. The width of the tube of the control field is determined by the correlation length $l_c$, for $l_c$ greatly exceeding the width of the tube of the fluctuational paths $\sim D^{1/2}$.

Spatial location of the optimal control field for fluctuations to different target points $r_j$ is illustrated in Fig. 2. In this figure, dashed lines are caustics in the pattern of extreme fluctuational paths. The occurrence of caustics is a generic feature of the solutions of the variational problems (5) and (6) for systems away from thermal equilibrium. Caustics...
To the lowest approximation in the amplitude of the control field, the optimal field is located along the optimal fluctuational paths in the absence of the field. Therefore the switching line for the fluctuational paths also separates the areas in which the optimal control field has a different spatial structure, as shown in Fig. 2. For higher fields the shape of the optimal paths depends on the field. However, the topological structure of singularities in the pattern of the control field remains the same.

V. CONCLUSIONS

It follows from the results of the present paper that even a weak control field may exponentially strongly affect the probability of a large fluctuation to a given target state, as well as the probability of escape from a metastable state. Depending on the goal, fluctuation probabilities can be increased or decreased. The optimal control field can be found from a variational problem. This same problem also describes optimal fluctuational paths in the presence of the control field. In fact, this problem provides mutually interrelated optimal realizations of the control field and noise that, acting together, bring the system to a given state. The solution of this problem can be obtained numerically in the general case. For an arbitrary nonlinear fluctuating system we have found this solution in an explicit form in the case of a comparatively weak control field.

The optimal control field depends on the type of the penalty functional and on the features of the system dynamics. The optimal form of the field in space, as well as the shape of the field pulse, differ dramatically for target states which are close to each other in the state space of the system but lie on the opposite sides of the switching lines (hypersurfaces); the positions of the switching lines are given by the solution of the variational problem for fluctuational paths and control field.

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[7] (a) V. A. Chinarov, M. I. Dykman, and V. N. Smelyanskiy, Phys. Rev. E 47, 2448 (1993); (b) M. I. Dykman, E. Mori, J.

FIG. 2. Generic singularities of the pattern of the optimal time-independent control field E in systems with two dynamical variables x and y. Smearred lines show schematically the field configurations for optimal control of fluctuations of the system. The target states are at the ends of the field tubes (the stable state of the system is at the origin). For comparatively small E, the tubes are centered at the optimal fluctuational trajectories for E = 0. The width of the tubes is determined by the correlation length of the field. The location of the control field changes nearly discontinuously if the target state crosses the switching line, which is shown by a bold line; for points close to the switching line, two geometries of the control field are nearly equally effective. Dashed line show caustics in the pattern of the extreme paths of the variational problem (5) and (6).


