Cooperating with nonequilibrium fluctuations through their optimal control

B. E. Vugmeister and H. Rabitz
Department of Chemistry, Princeton University, Princeton, New Jersey 08544
(Received 25 October 1996)

The task of fluctuation control in stochastic systems is reformulated as an optimal control problem. We show that it is possible to design an external control field that works cooperatively with system fluctuations to achieve a desired physical objective. The proposed approach is illustrated with one-dimensional Brownian motion as a simple model. [S1063-651X(97)09403-8]

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

I. INTRODUCTION

Optimal control theory, originally developed for engineering problems, has been applied recently to address the control of various phenomena in physics and chemistry including magnetic resonance selective excitations [1], crystal lattice vibrations [2], population inversion [3], selective chemical reactions [4,5], birefringence of liquid crystals [6], etc. (see Ref. [7] for a review). In these phenomena an applied external field is used as a control variable.

In recent experimental and theoretical studies [8,9] of large nonequilibrium fluctuations driven by random fields in the form of Gaussian noise, it has been shown that the probability distribution of fluctuations peaks sharply for the most probable *optimal* path for the fluctuation trajectory. This observation opens a broad area of research in the field of large fluctuations in terms of optimal control theory. That is, can we design controls that optimally work in cooperation with natural fluctuations to better achieve a desired physical objective?

In the present paper we show that the task of control in the presence of nonequilibrium fluctuations can be formulated as a problem in optimal control theory. This approach allows one to use the powerful mathematical and numerical techniques developed in that field [10]. To demonstrate the basic formalism, we apply it to the case of simple linear Brownian motion for which analytical results can be obtained.

II. OPTIMAL CONTROL FORMALISM

In the conventional formulation of optimal control theory one is interested in determining the temporal form of the external control field that steers the system to the vicinity of a given point in the phase space often at given moment of time. In order to be specific and illustrate the main ideas, we will consider a simple formulation of optimal control theory. We assume that the system is described by an equation of motion with one degree of freedom,

$$\frac{dx}{dt}=F(x,E), \tag{1}$$

where $E(t)$ is the external control field, and $F(x,E)$ acts as the total force that drives the system. In order to find the optimal external field $E(t)$ that steers the system to the vicinity of a desired target point x_g at the target time t_g (starting at point x_0 at $t=0$), one minimizes the cost functional

$$J_E=\tfrac{1}{2}k(x(t_g)-x_g)^2+\int_0^{t_g}dt\lambda(t)\left(\frac{dx}{dt}-F(x,E)\right)+\tfrac{1}{2}\chi\left[\int_0^{t_g}dtE(t)^2-U\right]. \tag{2}$$

The first term in Eq. (2) corresponds to the desired goal of reaching the point x_g at time $t=t_g$. $\lambda(t)$ is a Largange multiplier function that assures that the optimal solution is constrained to satisfy Eq. (1). The Lagrange multiplier χ assures that the total energy of the field is fixed at the value U [11,12],

$$\tfrac{1}{2}\int_0^{t_g}dt\ E(t)^2=U. \tag{3}$$

The temporal form of the optimal control field can be found by minimization of J_E with respect to $x(t)$, $\lambda(t)$, χ, and $E(t)$, and solving the corresponding Euler-Lagrange equations.

In order to investigate the role of fluctuations in the model described by Eq. (1), we introduce the random field (force) $f(t)$ which we choose to be Gaussian white noise. Assuming that the intensity of the random field is sufficiently small, we may rewrite Eq. (1) as

$$\frac{dx}{dt}=F(x,E)+f(t), \tag{4}$$

with

$$\langle f(t)f(t')\rangle=D\delta(t-t'), \tag{5}$$

where D is the characteristic noise intensity. The probability $P[f(t)]$ of the realization of a particular random field trajectory is given by [13]

$$P[f(t)]\propto\exp\left[-\frac{1}{2D}\int dtf(t)^2\right]. \tag{6}$$

One can see from Eq. (6) that the probability P reaches its maximum for the most probable random field which minimizes the integral $\int dt\ f(t)^2$ under the constraint that the equation of motion, Eq. (4), is satisfied. Such a constraint leads to a nonzero value of the most probable random field, which, according to Eq. (6), would be equal to zero without constraints. We will call the most probable random field $f(t)$ as the *optimal random field* $f_{\rm opt}(t)$ to distinguish it from the *optimal control field* $E_{\rm opt}(t)$.

The optimal control field $E_{\rm opt}$ cooperating with the optimal random field $f_{\rm opt}(t)$ determines the particular fluctuation trajectory $x(t)$, called optimal trajectory or optimal fluctuation. The probability of an optimal fluctuation is equal to the probability of the realization of the optimal random field. In order to find the optimal trajectory of the system leading to point x_g it has been proposed [8] to minimize $\int dt\ f(t)^2$ under the constraint that the equation of motion, Eq. (4), with boundary conditions $x(0)=x_0, x(t_g)=x_g$ be satisfied. However, a full formulation of this problem with the control field has not been implemented, as discussed below.

Rather than imposing the hard demand that $x(t_g)=x_g$, one can use optimal control theory by introducing the target functional [i.e., $\frac{1}{2}k(x(t_g)-x_g)^2$] for the model (4) that determines the boundary conditions for the Lagrange multiplier function, and permits finding $x(t_g)$ self-consistently. We seek the fluctuation path that approachs the point x_g in an optimal manner, corresponding to the minimization of the functional

$$J_{f,E}=\tfrac{1}{2}k(x(t_g)-x_g)^2+\tfrac{1}{2}\int_0^{t_g}dt\ f(t)^2+\int_0^{t_g}dt\lambda(t)\left(\frac{dx}{dt}-F(x,E)-f(t)\right)+\tfrac{1}{2}\chi\left[\int_0^{t_g}dtE(t)^2-U\right]. \tag{7}$$

Thus we seek the best control $E(t)$ that can cooperatively work with the optimal random fluctuation $f(t)$ of minimal norm in order to meet the objective $x(t_g)=x_g$. It is apparent that $x(t_g)$ will be driven closer to x_g as k increases. The variation of the functional $J_{f,E}$ yields

$$\delta J_{f,E}=k(x(t_g)-x_g)\delta x(t_g)+\int_0^{t_g}dt\ f(t)\delta f(t)+\int_0^{t_g}dt\lambda(t)\times\left(\frac{\partial\delta x}{\partial t}-\frac{\partial F}{\partial x}\delta x(t)-\frac{\partial F}{\partial E}\delta E(t)-\delta f(t)\right)+\chi\int_0^{t_g}E\,\delta E(t). \tag{8}$$

Assuming $\delta J_{f,E}=0$, and integrating by parts,

$$\int_0^{t_g}dt\lambda(t)\frac{\partial\delta x}{\partial t}=\lambda\,\delta x|_0^{t_g}-\int_0^{t_g}dt\frac{\partial\lambda}{\partial t}\delta x, \tag{9}$$

we obtain the following equations [along with Eqs. (3) and (4)]:

$$f(t)=\lambda(t), \tag{10}$$

$$\frac{\partial\lambda}{\partial t}=\lambda\frac{\partial F}{\partial x}, \tag{11}$$

$$\lambda(t_g)=k(x_g-x(t_g)), \tag{12}$$

$$\chi E(t)=\frac{\partial F(x,E)}{\partial E}\lambda(t). \tag{13}$$

The following minimization algorithm may be adopted [11] to solve Eqs. (3), (4), and (11)–(13).

(1) Make an initial guess for the field $E(t)$ consistent with Eq. (3), and set $f=0$.

(2) Integrate the equation of motion, Eq. (4), with the initial condition.

(3) With the resultant time evolution of $x(t)$, apply the boundary condition, Eq. (12), and integrate Eq. (11).

(4) With the resultant time evolution of $x(t)$ and $\lambda(t)$ calculate $E(t)$ from Eq. (13) while adjusting the Lagrange multiplier χ to satisfy Eq. (3).

(5) Use the control field $E(t)$ and ''random'' field $f(t)$ from Eq. (10) and repeat steps (2)–(4) until a convergent solution is obtained.

Recently Smelyanskiy and Dykman [14] considered the optimal control of large fluctuation using a different formalism without the target term in the cost functional. Explicit results were obtained with perturbation theory with respect to control field. The present approach utilizing optimal control theory allows one to go beyond the perturbation theory in a convenient way.

III. LINEAR BROWNIAN MOTION

In order to illustrate the formalism above, we consider linear Brownian motion that corresponds the replacement of $F(x,E)$ in Eq. (4) by

$$F(x,E)=-\gamma x+E \tag{14}$$

This simple case allows for the analytical solution for the temporal form of the external optimal field and for the probability of the optimal fluctuations.

Equations (11) and (13) reduce to

$$\frac{\partial\lambda}{\partial t}=\gamma\lambda, \tag{15}$$

$$E(t)=\frac{\lambda(t)}{\chi}. \tag{16}$$

We obtain

$$x(t)=\frac{1}{2\gamma}(e^{\gamma t}-e^{-\gamma t})\left[k(x_g-x(t_g))e^{-\gamma t_g}\pm\left(\frac{2\gamma U}{e^{2\gamma t_g}-1}\right)^{1/2}\right], \tag{17}$$

$$E_{\rm opt}(t)=\pm\left(\frac{2\gamma U}{e^{2\gamma t_g}-1}\right)^{1/2}e^{\gamma t}, \tag{18}$$

$$f_{\rm opt}(t)=k(x_g-x(t_g))e^{\gamma t}. \tag{19}$$

The value of $x(t_g)$ should be obtained self-consistently from Eq. (17) by setting $t=t_g$

One can see from Eqs. (18) and (19) that the shape of the external optimal field $E_{\rm opt}(t)$ coincides exactly with the shape of random field $f_{\rm opt}(t)$. The positive growth of these functions with larger values of γ is natural as γ acts as damping rate in Eq. (14), and both the control field and random field must work cooperatively to overcome the damping to achieve $x(t_g)\approx x_g$. When obtaining $E_{\rm opt}(t)$ in Eq. (18), we used Eq. (3) in order to find χ, and the two possible solutions for χ correspond to two different fields $E_{\rm opt}$ differing only in sign. The positive value of $E_{\rm opt}$ corresponds to the external field that drives the system in the same direction as $f_{\rm opt}$. It is apparent that such a control field decreases the energy of the random field required to achieve the value $x(t_g)=x_g$. Indeed, we obtain (choosing, for simplicity, $k\gg 1$)

$$\frac{1}{2}\int_0^{t_g} dt\ f_{\rm opt}(t)^2=\frac{\gamma(x_g\mp\tilde{x})^2}{1-e^{-2\gamma t_g}}, \tag{20}$$

where

$$\tilde{x}=\frac{1}{2\gamma}[2\gamma U(1-e^{-2\gamma t_g})]^{1/2}. \tag{21}$$

Equation (20) shows that the energy of the random field utilized to aid in steering the system to point $x_g>0$ is diminished if $E_{\rm opt}>0$. The converse situation $E_{\rm opt}<0$ would result in an indesirable increase of the energy of $f_{\rm opt}$. Such a situation, known as a *mini-max* solution, has been discussed recently [12] in the study of control in the presence of disturbances, with fixed energy. The latter work sought the best control in the presence of the worst possible disturbances with fixed energy as a means of assuring a robust control with the fluctuations having a minimal effect on the outcome. In contrast, the present work seeks the best control field with fixed energy that can cooperatively work with disturbances (fluctuations) to optimally achieve the objective. Thus uncontrolled disturbances can be beneficial if we treat them properly.

Finally, using Eqs. (6) and (20), we represent the transition probability to reach the point x_g at $t=t_g$ starting from $x_0=0$ at $t=0$ as

$$P(x_0,0;x_g,t_g)=P[f_{\rm opt}(t)]\propto\exp\left[-\frac{\gamma}{D}\frac{(x_g\mp\tilde{x})^2}{(1-e^{-2\gamma t_g})}\right]. \tag{22}$$

One can see from Eq. (22) that the meaning of $\tilde{x}$ can be given as the shift of the most probable value of x_g due to cooperation between the optimal control field $E_{\rm opt}(t)$ and optimal random field $f_{\rm opt}(t)$. For $\gamma t_g\gg 1$ this shift is seen to approach the time independent value $(U/2\gamma)^{1/2}$ from Eq. (21). As seen from Eq. (22), the control field increases the transition probability of approaching the target x_g.

We emphasize that at $U=0$ (i.e., $E=0$), Eq. (22) coincides with the exact results for the nonequilibrium transition probability for linear Brownian motion. There are two possible reasons for such a coincidence. First, the probability distribution over the paths peaks sharply at the most probable optimal path. Such an explanation, that is appropriate for large occasional fluctuations, has been given in Refs. [8,9]. On the other hand, in linear systems the distribution of different paths is Gaussian due to the character of the random force $f(t)$. In this situation the most probable transition probability coincides with the observable average transition probability apparently due to the symmetrical form of the Gaussian distribution of the different paths, rather than narrow path distribution. This aspect has not been given enough attention in previous analyses of optimal fluctuations.

IV. CONCLUSION

In conclusion we have shown that the analysis of nonequilibrium fluctuations in stochastic systems can be attractively formulated in terms of conventional optimal control theory as a problem of finding the external control field that increase the probability for the system to reach the target state. The full exploration of this observation should open up dynamical controls that may *work cooperatively with* system fluctuations.

ACKNOWLEDGMENTS

The authors acknowledge support from the Office of Naval Research and the National Science Foundation. We are thankful to M. I. Dykman and V. N. Smelyanskiy for the communication of their results before publication, and for useful stimulating discussions.

[1] S. Conolly, D. Nishimura, and A. Macovski, IEEE Med. Im. **5**,106 (1986); W. S. Warren and M. S. Silver, Adv. Magn. Res. **12**, 247 (1988).
[2] A. M. Weiner, D. E. Leaird, G. P. Wiederrecht, and K. A. Nelson, Science **247**, 1317 (1990).
[3] J. S. Melinger, A. Hariharan, S. R. Gandhi, and W. S. Warren, J. Chem. Phys. **95**, 2210 (1991).
[4] J. Botina, H. Rabitz, and N. Rahman, J. Chem. Phys. **104**, 4031 (1996).
[5] P. Gross, D. Neuhauser, and H. Rabitz, J. Chem. Phys. **94**, 1158 (1991); D. J. Tannor and S. A. Rice, Adv. Chem. Phys. **70**, 441 (1988).
[6] B. E. Vugmeister, J. Botina, and H. Rabitz, Ferroelectrics (to be published).
[7] W. S. Waren, H. Rabitz, and M. A. Dahleh, Science **259**, 1581 (1993).
[8] M. I. Dykman, Phys. Rev. A **42**, 2020 (1990).
[9] M. I. Dykman, P. V. E. McClintock, V. N. Smelyanskiy, N. D. Stein, and N. G. Stocks, Phys. Rev. Lett. **68**, 2718 (1992).
[10] A. E. Bryson and Yu-Chi Ho, *Applied Optimal Control* (Hemisphere, New York, 1975).
[11] R. Kosloff, S. A. Rice, P. Gaspard, S. Tersigni, and D. J. Tannor, Chem. Phys. **139**, 201 (1989).
[12] J. G. B. Beumee and H. Rabitz, J. Chem. Phys. **97**, 1353 (1992).
[13] R. P. Feynman and A. R. Hibbs, *Quantum Mechanics and Path Integrals* (McGraw-Hill, New York, 1965).
[14] V. N. Smelyanskiy and M. I. Dykman, Phys. Rev. E **55**, 2516 (1997).