Upper bound for the time derivative of entropy for nonequilibrium stochastic processes

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We have shown how the intrinsic properties of a noise process can set an upper bound for the time derivative of entropy in a nonequilibrium system. The interplay of dissipation and the properties of noise processes driving the dynamical systems in presence and absence of external forces, reveals some interesting extremal nature of the upper bound.

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I. INTRODUCTION

A consequence of the second law of thermodynamics is that the rate of change of entropy with time for a nonequilibrium stochastic process is always positive. While in traditional classical thermodynamics, the specific nature of a stochastic process is irrelevant, this may play an important role in understanding the connection between the phase space of a dynamical system and the related thermodynamically inspired quantities such as entropy production, flux, etc. The relationship has recently been explored by a number of authors [1–13]. The object of the present paper is to address a related issue.

In what follows we shall be concerned with the dissipative dynamical systems that are thermodynamically open [14] in the sense that they can be described by classical stochastic processes with the help of the standard Langevin equations. When a dynamical system is driven by a noise process, e.g, color [15] or cross-correlated processes [16,17], the nature of the noise processes may influence the dynamical system through the appropriate modification of the phase space structure of the overall system. In view of the immediate connection between information entropy and probability distribution function of the phase space variables, it is worthwhile to enquire about the imprints of the nature of noise on entropy. Our specific aim in this paper is to show how the properties of the noise processes can set an upper bound on the rate of entropy change in a nonequlibrium system. By directly extending our earlier treatment on a related problem [11] we have examined some interesting extremal properties of this bound.

The outline of the paper is as follows: In Sec. II we introduce the Fokker-Planck description of a dynamical system driven by two different kinds of stochastic processes (e.g, color and cross correlated) and an upper bound for the rate of entropy change based on this formulation. We illustrate the result in Sec. III for the two specific cases. The paper is concluded in Sec. IV.

II. THE FOKKER-PLANCK DESCRIPTION OF NOISE PROCESSES AND UPPER BOUND FOR THE RATE OF ENTROPY CHANGE

We consider a dynamical system driven by the external Ornstein-Uhlenbeck noise processes. The relevant Langevin equations of motion can be written as

$$\dot{x}_i = F_i^0(\{x_i\}) + \eta_i , \quad i=1,\ldots,N, \tag{1}$$

where N is the dimension of the phase space. $F_i^0(x)$ corresponds to the dissipative term as well as the external applied deterministic force, if any. The second term η_i in Eq. (1) refers to an external, Gaussian, color noise for the ith component of x.

The Fokker-Planck equation corresponding to Langevin Eq. (1) in the extended phase space can be written as [for details, see Ref. [11]]

$$\frac{\partial \rho(X,t)}{\partial t} = -\sum_{i=1}^{2N} \frac{\partial}{\partial X_i}(F_i \rho) + \sum_{i=1}^{2N} D_i \frac{\partial^2 \rho}{\partial X_i^2}, \tag{2}$$

where

$$X_i = \begin{cases} x_i & \text{for } i=1,\ldots,N \\ \eta_i & \text{for } i=N+1,\ldots,2N, \end{cases}$$

F_i and D_i are drift and diffusion coefficients, respectively, and have their usual significance as discussed in Ref. [11]. $\rho(X,t)$ is the extended phase space probability distribution function.

As a second example we consider a dynamical system driven by both additive and multiplicative noise processes η_i and ζ_i, respectively. The Langevin equation for this process, in general, can be written as

$$\dot{X}_i = L_i(\{X_i\},t) + g_i(X_i)\zeta_i + \eta_i , \quad i=1,\ldots,N, \tag{3}$$

where L_i contains the dissipative term as well as the external applied deterministic force, if any. $g_i(X_i)$ is the coupling between the system and the multiplicative processes ζ_i. ζ_i, and η_i are white, Gaussian noise processes with the following correlation between them:

$$\langle \zeta_i(t)\eta_j(t')\rangle = \langle \zeta_i(t')\eta_j(t)\rangle = 2\lambda_{ij}\sqrt{D'_{ij}\alpha_{ij}}\,\delta(t-t')\,\delta_{ij}, \tag{4}$$

where D'_{ij} and α_{ij} correspond to the strength of multiplicative and additive noises, respectively and λ represents the cross correlation between them with the limit $0 \leqslant \lambda \leqslant 1$.

The Fokker-Planck equation corresponding to Langevin Eq. (3) can be written as

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$$\frac{\partial \rho(X,t)}{\partial t} = -\sum_{i=1}^{N} \frac{\partial}{\partial X_i}(F_i \rho) + \sum_{i=1}^{N} D_i \frac{\partial^2 \rho}{\partial X_i^2}. \tag{5}$$

Again F_i and D_i are drift and diffusion coefficient, respectively, and have same significance as in the Eqs. (11)–(13) of Ref. [11].

The Fokker-Planck Eqs. (2) or (5) can be rearranged into the general form of continuity equation

$$\frac{\partial \rho(X,t)}{\partial t} = -\nabla_X \cdot j \tag{6}$$

where j denotes the current and ∇_X term the phase space divergence. The ith component of j can be written as

$$j_i = F_i \rho - D_i \frac{\partial \rho}{\partial X_i}. \tag{7}$$

Using Eq. (6) we are now in a position to define the upper bound for the rate of evolution of entropy. In the microscopic picture, the Shannon form of the entropy is connected to the probability density function $\rho(X,t)$ as

$$S = -\int dX \rho(X,t) \ln \rho(X,t). \tag{8}$$

The time evolution equation for entropy can then be written as

$$\frac{dS}{dt} = \int dX \nabla_X \cdot j \ln \rho, \tag{9}$$

where Eq. (6) is used.

Integrating Eq. (9) by parts, one obtains

$$\frac{dS}{dt} = -\int dX \frac{1}{\rho} j \cdot \nabla_X \rho, \tag{10}$$

where we have used following boundary conditions [6]:

$$j|_{boundary} = 0 \tag{11}$$

and

$$j \ln \rho|_{boundary} = 0. \tag{12}$$

In the next step an application of the Schwartz inequality $|\int dX g h|^2 \leqslant \int dX |g|^2 \int dX |h|^2$ to the integral (10) where g and h can be appropriately identified yields an upper bound for the rate of entropy change

$$\frac{dS}{dt} \leqslant U_B(t),$$

$$U_B(t) = \left(\int dX \frac{j^2}{\rho} \right)^{1/2} \left(\int dX \frac{(\nabla_X \rho)^2}{\rho} \right)^{1/2}. \tag{13}$$

It is important to note that the second integral is same as the trace of Fisher information matrix [8] and this inequality is valid if and only if $j/\sqrt{\rho}$ is not a constant multiple of $(\nabla_X \rho)/\sqrt{\rho}$. To find the explicit time dependence of the upper bound we work out simple examples for each of the noise processes in the following section.

III. APPLICATIONS

A. The upper bound for a dynamical system driven by an external color noise

As a simple illustration, we consider a Langevin equation of motion for a dissipative dynamical system driven by an external, Gaussian Ornstein-Uhlenbeck noise η_1,

$$\dot{X}_1 = -\gamma X_1 + f_c + \eta_1. \tag{14}$$

The noise correlation of η_1 is given by

$$\langle \eta_1(t) \eta_1(t') \rangle = \frac{D^0}{\tau} \exp\left(-\frac{|t-t'|}{\tau} \right), \tag{15}$$

where γ in Eq. (14) is the dissipative parameter and f_c is a constant external applied force term that is used to identify specific interplay between γ and τ.

For the Langevin Eq. (14) the Fokker-Planck Eq. (2) becomes (see Ref. [11])

$$\frac{\partial \rho}{\partial t} = \gamma \frac{\partial X_1 \rho}{\partial X_1} - f_c \frac{\partial \rho}{\partial X_1} - X_2 \frac{\partial \rho}{\partial X_1} + \frac{1}{\tau} \frac{\partial X_2 \rho}{\partial X_2} + \frac{D^0}{\tau^2} \frac{\partial^2 \rho}{\partial X_2^2}, \tag{16}$$

where $X_2 = \eta_1$.

We now use the following transformation in the Eq. (16):

$$U = aX_1 + X_2, \tag{17}$$

where a is a constant to be determined.

Then Eq. (16) reduces into the following one-dimensional form:

$$\frac{\partial \rho(U,t)}{\partial t} = \frac{\partial}{\partial U}(\Gamma U)\rho - F_u \frac{\partial \rho}{\partial U} + D_s \frac{\partial^2 \rho}{\partial U^2}, \tag{18}$$

where

$$\Gamma U = \gamma a X_1 - a X_2 + \frac{X_2}{\tau}, \quad F_u = a f_c \quad \text{and} \quad D_s = \frac{D^0}{\tau^2}. \tag{19}$$

Here Γ is again a constant to be determined. Using Eq. (17) in Eq. (19) and comparing the coefficients of X_1 and X_2 we find

$$\Gamma = \gamma \quad \text{and} \quad a = \frac{1-\gamma\tau}{\tau}. \tag{20}$$

We then search for the Green's function or conditional probability solution for the system at U at time t for the initial condition given by

$$\rho(U,t=0)=\lim_{\epsilon\to\infty}\frac{\epsilon}{\pi}\exp[-\epsilon(U-U')^2]. \tag{21}$$

We now look for a solution of the Eq. (18) of the form

$$\rho(U,t|U',0)=\exp[G(t)], \tag{22}$$

where

$$G(t)=-\frac{1}{\sigma(t)}[U-\beta(t)]^2+\ln\nu(t). \tag{23}$$

We will see that by suitable choice of $\beta(t)$, $\sigma(t)$, $\nu(t)$ we can solve Eq. (18) subject to the initial condition,

$$\rho(U,0|U',0)=\lim_{\epsilon\to\infty}\frac{\epsilon}{\pi}\exp[-\epsilon(U-U')^2]. \tag{24}$$

Comparison of this with Eq. (22) and $G(0)$ shows that

$$\sigma(0)=\frac{1}{\epsilon},\quad \beta(0)=U',\quad \nu(0)=\frac{\epsilon}{\pi}. \tag{25}$$

If we put Eq. (22) in Eq. (18) and equate the coefficients of equal powers of U we obtain after some algebra the following set of equations:

$$\dot{\sigma}(t)=-2\Gamma\sigma(t)+4D_s, \tag{26}$$

$$\dot{\beta}(t)=-\beta(t)+F_u, \tag{27}$$

$$\frac{1}{\nu(t)}\dot{\nu}(t)=-\frac{1}{2\sigma(t)}\dot{\sigma}(t). \tag{28}$$

The relevant solutions of $\sigma(t)$ and $\beta(t)$ for the present problem that satisfy the initial conditions as stated earlier are given by

$$\sigma(t)=\frac{2D_s}{\Gamma}[1-\exp(-2\Gamma t)]+\sigma(0)\exp(-2\Gamma t) \tag{29}$$

and

$$\beta(t)=\frac{F_u}{\Gamma}[1-\exp(-\Gamma t)]+\beta(0)\exp(-\Gamma t). \tag{30}$$

Now making use of Eqs. (22), (29), and (30) in Eq. (13) we finally obtain explicit time dependence of the upper bound $U_B(t)$ for the rate of entropy change as

$$\frac{dS}{dt}\leqslant U_B(t),$$

where

$$U_B(t)=\frac{(2\beta^2\Gamma^2\sigma-4\beta\Gamma F_u\sigma+2F_u^2\sigma+\Gamma^2\sigma^2+4D_s^2-4D_s\Gamma\sigma)^{1//2}}{\sigma}. \tag{31}$$

We now examine specifically the long time limit, i.e., $t\to\infty$ of the above result (31). As $t\to\infty$ Eqs. (29) and (30) reduce to

$$\sigma(\infty)=\frac{2D_s}{\Gamma}\quad\text{and}\quad\beta(\infty)=\frac{F_u}{\Gamma}. \tag{32}$$

It is easy to check that as $t\to\infty$ the numerator of the right hand side of Eq. (31) vanishes both in presence or absence of F_u. Therefore we obtain the equation

$$\frac{dS}{dt}=0. \tag{33}$$

This equality holds since in the long time limit $j=0$ [see Eq. (18)]. At any other time the time dependence of the upper bound U_B for the rate of entropy change is explicitly shown in Fig. 1. We choose the initial conditions $\sigma(0)=0$, $\beta(0)=1.0$ and parameter values $D^0=1.0$, $f_c=1.0$, $\gamma=1.0$, and $\tau=1.0$. Figure 1 shows that except for an initial short period $U_B(t)$ decreases almost exponentially with time. In absence of f_c the time dependence of U_B follows a similar pattern. In Fig. 2(a) and 2(b) we plot U_B at $t=5$ vs correlation time τ in absence and presence of the external forcing f_c. As expected U_B increases monotonically with τ [in Fig. 2(a)], which is a clear signature of the persistence of the nonequilibrium situation in contrast to the case in Fig. 2(b) where the interplay of τ with external forcing f_c results in a minimum in U_B. The result of Fig. 2(b) is qualitatively same to that of the Fig. 1 of Ref. [11] where only entropy produc-

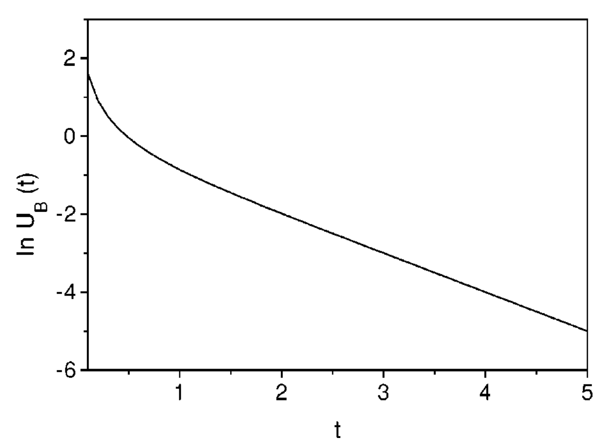

FIG. 1. Plot of upper bound for the time derivative of entropy $\ln U_B(t)$ vs time t for the Eq. (31) using $\gamma=1.0$, $f_c=1.0$, $D^0=1$, $\tau=1.0$, $\beta(0)=1.0$, and $\sigma(0)=0.0$ (units are arbitrary).

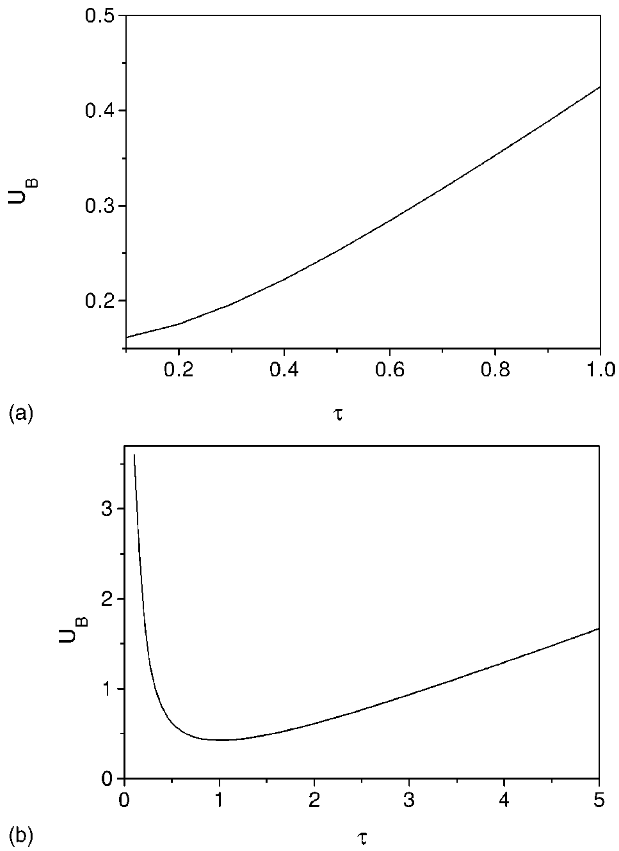

FIG. 2. (a) Plot of U_B vs correlation time τ at $t=5.0$ for the Eq. (31) using $f_c=0.0$ and values of other parameters same as in Fig. 1 (units are arbitrary). (b) Same as in Fig. 2(a) but for $f_c=1.0$ (units are arbitrary).

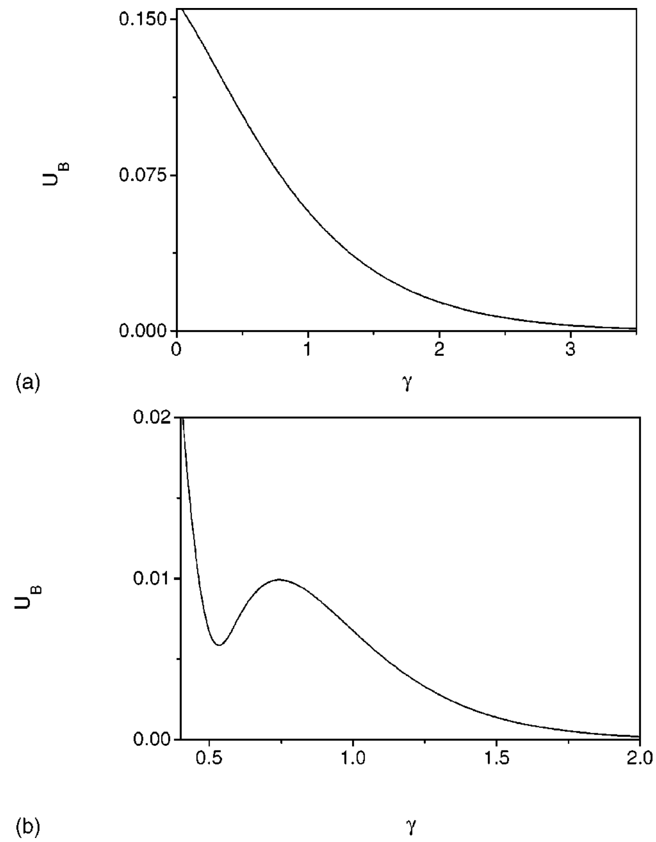

FIG. 3. Plot of U_B vs dissipative constant γ at $t=5.0$ for the Eq. (31) using $\tau=1.0$ and values of other parameters same as in Fig. 2(a) (units are arbitrary). (b) Same as in (a) but for $f_c=1.0$ (units are arbitrary).

tion in the stationary state is considered. In the present context, however, the upper bound of the sum of entropy production and entropy flux [11] at any arbitrary time is considered. The relation between entropy flux (E_F) and entropy production (E_P) in the long time limit for the present model [11] is

$$E_P=-E_F=\frac{(1-\gamma\tau)^2 f_c^2}{D^0}. \tag{34}$$

Using above equation in Eq. (31) at time $t\to\infty$ we have

$$U_B=[2\gamma E_P+2\gamma E_F]^{1/2}=0. \tag{35}$$

Since near equilibrium E_P approaches $-E_F$ the upper bound of time derivative of entropy as shown in Fig. 2(b) mimics the result of Fig. 1 of Ref. [11].

In Figs. 3(a) and 3(b) we plot the variation of U_B (at $t=5.0$) vs dissipative constant γ in absence [Fig. 3(a)] and presence [Fig. 3(b)] of the external force f_c. While an increase in γ facilitates the approach to stationarity as evident from the monotonic decrease of the bound in Fig. 3(a), its effect becomes more interesting when the external f_c is switched on [Fig. 3(b)]. One observes that the bound passes first through minimum followed by a maximum to settle down at the vanishing level for the large values of dissipation. It is thus apparent that in presence of the external constraint the properties of the noise processes and the dynamical characteristics of the system play an important part for the upper bound for the rate of entropy change.

B. The upper bound in a cross-correlated noise-driven system

We now turn to the second case where a simple dissipative system is driven by both additive and multiplicative noises,

$$\dot{X}_1=-\gamma X_1-\zeta_1 X_1+\eta_1. \tag{36}$$

Equation (5) for this system reduces to (for details, see Ref. [11])

$$\frac{\partial\rho(X_1,t)}{\partial t}=-\frac{\partial(F_1\rho)}{\partial X_1}+D_1\frac{\partial^2\rho}{\partial X_1^2}, \tag{37}$$

where the drift term is

$$F_1=-(\gamma+2D'_{11}-\nu)X_1+l \tag{38}$$

with

$$l=(2-\nu)\lambda_{11}\sqrt{D'_{11}\alpha_{11}}, \tag{39}$$

and

$$D_1 = \frac{[\alpha_{11}\gamma^2 + (2-\nu)D'_{11}\alpha_{11}\{(2-\nu)D'_{11} + 2\gamma - 2\gamma\lambda_{11}^2 - \lambda_{11}^2(2-\nu)D'_{11}\}]}{\Gamma'^2}, \quad (40)$$

where

$$\Gamma' = \gamma + 2D'_{11} - \nu. \quad (41)$$

Here D'_{11} and α_{11} are the multiplicative and additive noise strength, respectively. λ_{11} is the cross correlation between the noise processes. $\nu = \mathbf{1}$ stands for the Startonovich and $\nu = 0$ for the Ito convention, respectively.

The Eq. (37) is very much similar to Eq. (18). Hence, the upper bound for the rate of entropy change can be calculated as in the previous case and the final expression for the upper bound U_B is given by

$$\frac{dS}{dt} \leqslant U_B(t),$$

where

$$U_B(t) = \frac{(2\beta_1^2\Gamma'^2\sigma_1 - 4\beta_1\Gamma' l\sigma_1 + 2l^2\sigma_1 + \Gamma'^2\sigma_1^2 + 4D_1^2 - 4D_1\Gamma'\sigma_1)^{1/2}}{\sigma_1}. \quad (42)$$

Here the time evolution of $\sigma_1(t)$ and $\beta_1(t)$ can be written as

$$\sigma_1(t) = \frac{2D_1}{\Gamma'}[1 - \exp(-2\Gamma' t)] + \sigma_1(0)\exp(-2\Gamma' t) \quad (43)$$

and

$$\beta_1(t) = \frac{l}{\Gamma'}[1 - \exp(-\Gamma' t)] + \beta_1(0)\exp(-\Gamma' t). \quad (44)$$

The initial conditions for $\sigma_1(0)$ and $\beta_1(0)$ can be chosen as in Eq. (25). l, D_1, and Γ' are determined by Eqs. (39), (40), and (41). Again it is easy to check that for the correlated noise process under stationary condition we obtain the usual equality

$$\frac{dS}{dt} = 0. \quad (45)$$

The time dependence of U_B for a correlated noise process [we fix the parameter values as $\gamma = 1.0, D_{11} = 1.0$, $\lambda_{11} = 0.5$, $\alpha_{11} = 1.0$ and the initial conditions $\sigma_1(0) = 0$, $\beta_1(0) = 0$] is more or less same as that of Fig. 1. In Fig. 4 we exhibit the variation of U_B (at $t = 5.0$) with the strength of correlation λ_{11}. It is interesting to note that although both multiplicative and additive noises are independently and instantaneously correlated their mutual strength of correlation λ_{11} drives the system away from stationarity more strongly [as compared to the case corresponding to the variation of correlation time τ in Fig. 2(b)]. No minimum, however, is obtained. We men tion, in passing, that since the models considered here are linear and are exactly solvable by Green's function of Gaussian form the computed upper bound is an exact one.

IV. CONCLUSIONS

Based on Fokker-Planck description of color and cross-correlated noise-driven dynamical systems we have shown how the intrinsic properties of a noise process can set an upper bound for the rate of entropy change in a nonequilibrium system. Since the dissipative forces tend to equilibrate the system while an increase in the noise correlation time in a color noise process or an increase in the strength of correlation in cross-correlated noise processes acts in the opposite direction, an interplay of them makes the dynamical system exhibit interesting extremum properties of this upper bound. This is manifested in the maxima and minima of the bound for the time derivative of Shanon entropy as a function of the strength of dissipation, correlation time, or strength of correlation in presence or absence of the external forces acting on

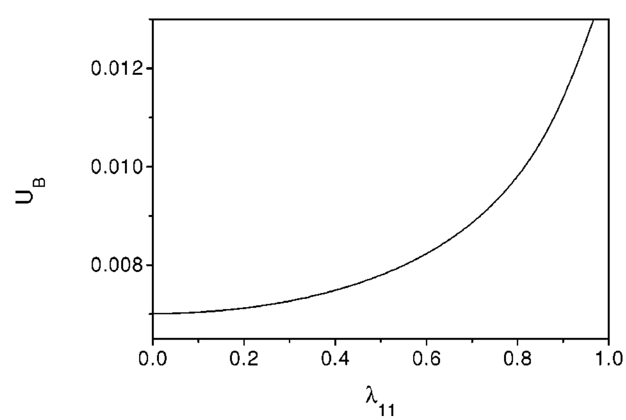

FIG. 4. Plot of U_B vs noise correlation strength λ_{11} at $t = 5.0$ for the Eq. (42) using $\gamma = 1.0$, $D_{11} = 1$, $\alpha_{11} = 1.0$, $\beta_1(0) = 1.0$, and $\sigma_1(0) = 0.0$ (units are arbitrary).

the dynamics. Since the color and cross-correlated noise processes occur in many situations in physics and chemistry, the observation made in this paper, we hope, will be useful for understanding the close connection between irreversible thermodynamics and dynamical systems in many related issues.

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