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Coloured thermal noise-driven dynamical system: upper bound of time derivative of information entropy

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Abstract

In this paper we have studied the upper bound of the time derivative of information entropy for non-Markovian and thermodynamically closed system(s) using *reduced model theory* (RMT). The upper bound is calculated on the basis of the Fokker–Planck equation and the Schwartz inequality principle. Our calculation shows that the upper bound exhibits extremal nature in the variation of system parameters such as noise correlation time, dissipation strength. The present calculation also considers how the upper bound does change if we increase the number of auxiliary variables involved in the RMT.

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In the present paper we consider relaxation of a non-Markovian and thermodynamically closed system, from a given non-equilibrium state to an equilibrium state. Non-Markovian stochastic processes play an important role in noise-driven dynamical systems [1, 2]. In traditional classical thermodynamics the specific nature of the stochastic process is irrelevant, but it may play an important role in the process of equilibration for a given non-equilibrium state of the noise-driven dynamical system. Thus an understanding of the interplay among frictional force, random force, noise strength and external force, if any, has become a subject in the recent past [1–5]. In this context, Shannon's information measure [6]

$$S = -\int W(U,t)\ln W(U,t)\,\mathrm{d}U \tag{1}$$

is a very important tool for the study of non-equilibrium and stationary states of a Brownian particle. Here S is called information entropy, and $W(U,t)$ is the continuous probability distribution function in phase space. If one considers Boltzmann's constant as the information unit and identifies Shannon's measure with the thermodynamic entropy, then the whole of statistical mechanics can be elegantly reformulated by the extremization of S, subject to the

constraints imposed by the *a priori* information one may possess about the system of interest [6]. Very recent studies show that the information entropy and Fisher information, which are proportional to the upper bound of the time derivative of S [3], are vital to the detailed study of the noise-driven dynamical system [3–5]. Since the time evolution of the phase space of the stochastic process is very sensitive to the characteristics of the frictional and random forces, the specific nature of the random process has a strong role to play in deciding the upper bound of the rate of change of information entropy. In an earlier paper [5] we have discussed the time dependence of this upper bound, with the frictional force being proportional to the momentum, and the Ornstein–Uhlenbeck noise process corresponding to the random force. Thus it considers a thermodynamically open system, the random force and the dissipative force having different origins. In view of the importance of the role that dissipation plays while the system approaches a stationary state, it is worthwhile to consider a dissipation with finite memory, in a thermodynamically *closed* system (dissipative memory kernel is related to fluctuating force through fluctuation–dissipation relation), which can influence the upper bound of the time derivative of S in non-equilibrium states. The objective of the present paper is to address this specific issue.

For the calculation of the upper bound we consider a simple thermodynamically closed system where the stochastic process is non-Markovian in nature. The generalized Langevin equation of motion for this process can be written as

$$\dot{x} = p \qquad \text{and} \qquad \dot{p} = -\omega^2 x - \int_0^t \beta(t-t')\,p(t')\,\mathrm{d}t' + f(t), \tag{2}$$

where x and p correspond to the position and momentum of a harmonic oscillator with frequency ω. Here $\beta(t-t')$ is the dissipative memory kernel, and $f(t)$ represents Gaussian fluctuations that satisfy the fluctuation–dissipation relation

$$\langle f(t)\,f(t')\rangle = k_B T \beta(t-t'). \tag{3}$$

k_B is the Boltzmann constant and T is the temperature of the thermal bath. The system described by equations (2) and (3) is sometimes termed the *thermodynamically closed system*, and the stochastic process lacking relation (3) is accordingly called the *thermodynamically open system*. Thus the present model differs from that of [5] in three aspects, namely, fluctuation–dissipation relation, external force and nature of dissipation.

We are now in a position to introduce an interesting method which is known as *reduced model theory* (RMT) developed by Grigoloni and co-workers [7] to study non-Markovian stochastic processes in an extended phase space. Following [7] one can write the above equations of motion in an equivalent form using n-number auxiliary variables $(\zeta_1, \zeta_2, \ldots, \zeta_n)$ as

$$\frac{\mathrm{d}A}{\mathrm{d}t} = HA(t) + R(t), \tag{4}$$

where

$$A = \begin{pmatrix} x \\ p \\ \zeta_1 \\ \zeta_2 \\ \vdots \\ \zeta_n \end{pmatrix}, \qquad H = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & \cdots & 0 \\ -\omega^2 & 0 & 1 & 0 & 0 & \cdots & 0 \\ 0 & -\Delta_1^2 & 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & -\Delta_2^2 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & 0 & -\Delta_n^2 & -\gamma_n \end{pmatrix} \tag{5}$$

and

$$R(t) = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ f_n(t) \end{pmatrix}, \tag{6}$$

f_n appearing in equation (6) is Gaussian white noise with $\langle \zeta(t) \rangle = 0$ and $\langle f_n(t) f_n(t') \rangle = 2D_n \delta(t - t')$, $D_n = \gamma_n k_B T \left(\Delta_1^2 \cdot \Delta_2^2 \cdots \Delta_n^2 \right)$. The form of Δ_i^2 and γ_n are described in detail in [7–9].

The Fokker–Planck equation corresponding to the above Langevin equation of motion can be written as [1, 7]

$$\frac{\partial W(A_1, A_2, \ldots, A_{n+2}, t)}{\partial t} = \left[-\sum_{i=1}^{n+2} \frac{\partial F_i}{\partial A_i} + D_n \frac{\partial^2}{\partial A_{n+2}^2} \right] W(A_1, A_2, \ldots, A_{n+2}, t), \tag{7}$$

where

$$F_i = \sum_{j=1}^{n+2} H_{ij} A_j \qquad \text{and} \qquad F = HA.$$

It is now important to note that one can use the linear transformation (with $\alpha_{n+2} = 1$)

$$U = \sum_{i=1}^{n+2} \alpha_i A_i, \tag{8}$$

on the Fokker–Planck equation (7), since the differential equation for each component of A (4) is linear in terms of the phase-space variables. U being a linear combination of the extended phase-space variables $\{A_j\}$, takes care of their stochastic behaviour in entirety. The transformation (8) is generally used [4, 5, 10] with the purpose of reducing the dimension of the Fokker–Planck equation for a linear stochastic process. The parameters $\alpha_1, \alpha_2, \ldots, \alpha_{n+1}$ in the above equation are constants to be determined.

By virtue of the above transformation, the Fokker–Planck equation (7) becomes

$$\frac{\partial W(U, t)}{\partial t} = \frac{\partial \Gamma_n W}{\partial U} + D_n \frac{\partial^2 W}{\partial U^2}, \tag{9}$$

where

$$\Gamma_n U = -\sum_{i=1}^{n+2} \alpha_i F_i. \tag{10}$$

Putting equation (8) into equation (10) and comparing the coefficients of A_i on both sides we obtain $n+2$ algebric equation (for $\alpha_i, \ldots, \alpha_{n+1}$ and Γ_n). The set $\{\alpha_i\}$ and Γ_n are therefore known [4, 5, 10]. Here we would like to point out that the linear transformation (8) can also be applied directly to the Langevin dynamics described by equation (4) to derive the Fokker–Planck equation (9). Multiplying α_i on both sides of the time evolution equation of A_i (equation (4)) and then adding for all i we have

$$\frac{\mathrm{d}U}{\mathrm{d}t} = -\Gamma_n U + f_n(t). \tag{11}$$

This is the Langevin equation of motion corresponding to the Fokker–Planck equation (9). The above equation implies that the time evolution equations corresponding to all A_i indeed

can become again a Markovian process for the projection of U. In the weak noise limit equation (11) becomes

$$\frac{\mathrm{d}U}{\mathrm{d}t} = -\Gamma_n U. \tag{12}$$

The solution of this equation is

$$U(t) = U(0)\exp(-\Gamma_n t). \tag{13}$$

The effective damping constant Γ_n in the above equation is finite for finite values of the parameters in the set $\{\Delta_i^2\}$, ω and γ_n and it does not correspond to a particular eigenvalue of the matrix H. The above equation implies that $U(t)$ is finite at a finite time t, and it is not the slow variable of the original dynamics since it satisfies the initial condition taking the contribution of all the modes and Γ_n is not smallest eigenvalue of the matrix H. Thus U in equation (13) considers the contribution from all the variables at arbitrary time. Hence the linear transformation (8) being used to reduce the Fokker–Planck equation (7) into (9) works at any time.

The Fokker–Planck equation (9) can be rearranged into the general form of the continuity equation

$$\frac{\partial W(U,t)}{\partial t} = -\frac{\partial j_c}{\partial U}, \tag{14}$$

where the current, $j_c = -\Gamma_n U W - D_n \frac{\partial W}{\partial U}$. We shall now define the upper bound for the time derivative of information entropy using equations (1) and (14). The time evolution equation for S can be written as

$$\frac{\mathrm{d}S}{\mathrm{d}t} = \int \mathrm{d}U \frac{\partial j_c}{\partial U} \ln W. \tag{15}$$

Performing partial integration on the right-hand side of the above equation and then putting the natural boundary conditions, $j_c|_{\text{boundary}} = 0$ and $j_c \ln W|_{\text{boundary}} = 0$, one obtains

$$\frac{\mathrm{d}S}{\mathrm{d}t} = -\int \mathrm{d}U \frac{1}{W} j_c \frac{\partial W}{\partial U}. \tag{16}$$

Identifying g as $j_c/\sqrt{W}$ and h as $\frac{\partial W}{\partial U}\Big/\sqrt{W}$ we can apply the Schwartz inequality $|\int \mathrm{d}U gh|^2 \leqslant \int \mathrm{d}U|g^2| \int |h^2|\,\mathrm{d}U$ to the integral (16). This yields an upper bound for the rate of information entropy change

$$\frac{\mathrm{d}S}{\mathrm{d}t} \leqslant U_B(t)^{(n)} \tag{17}$$

where

$$U_B(t)^n = \left(\int \mathrm{d}U \frac{j_c^2}{W}\right)^{1/2} \left(\int \mathrm{d}U \left(\frac{\partial W}{\partial U}\right)^2 \frac{1}{W}\right)^{1/2}. \tag{18}$$

The strict equality is valid if and only if g is not a constant multiple of h. The second factor of the right-hand side in the above equation is the square root of the Fisher information (I) [3].

To find the explicit time dependence of the upper bound, we use the following standard solution [1, 11] of the Fokker–Planck equation (21):

$$W(U,t) = N \exp\left[-\frac{U^2}{\sigma_n(t)}\right] \tag{19}$$

where $\sigma_n(t) = \frac{2D_n}{\Gamma_n}(1-\exp(-2\Gamma_n t)) + \sigma_n(0)\exp(-2\Gamma_n t)$, and N is the normalization constant. Here we have chosen the initial value of U as $U_0 = 0.0$. Now by making use of equation (20)

in equation (19) we finally obtain an explicit time dependence of the upper bound $U_B^{(n)}(t)$ for the rate of entropy change (given by equation (19)) as,

$$U_B^{(n)} = \left[\frac{\Gamma_n^2\sigma_n^2 - 4\Gamma_n\sigma_n D_n + 4D_n^2}{2.0\sigma_n}\right]^{1/2}\left[\frac{2}{\sigma_n}\right]^{1/2}. \tag{20}$$

It can be rearranged into another form of the bound [3] as

$$U_B^{(n)} = \frac{1}{2} I \frac{\mathrm{d}\langle U\rangle}{\mathrm{d}t}, \tag{21}$$

since $I = 2/\sigma_n$ and $\frac{\mathrm{d}\langle U^2\rangle}{\mathrm{d}t} = 2D_n - \Gamma_n\sigma_n$.

The above form of upper bound describes how it depends on noise correlation time, strength of dissipation, system frequency and number of auxiliary variables introduced in RMT for the non-Markovian system. For example, we choose the model memory function for the $\beta(t)$ appearing in equation (2) as an exponentially decaying form [12]. It can be represented as

$$\beta(t) = \frac{\gamma}{\tau}\,\mathrm{e}^{-\frac{|t|}{\tau}} \tag{22}$$

where γ is the dissipation parameter and τ corresponds to the correlation time of the coloured noise process. Then the two-time correlation of f for the thermodynamically closed system in equation (3) becomes

$$\langle f(t)f(0)\rangle = \frac{\gamma k_B T}{\tau}\,\mathrm{e}^{-\frac{|t|}{\tau}}. \tag{23}$$

The above equation implies that for the present example $f(t)$ in equation (2) corresponds to the Ornstein–Uhlenbeck noise process [1]. Thus, effectively, we study the thermodynamically closed system given by equation (2), along with equations (22) and (23), by increasing the auxiliary variables one by one. First of all we consider the simplest form of RMT with only one auxiliary variable ζ_1. Then equation (4) yields

$$\dot{A}_1 = A_2, \tag{24}$$

$$\dot{A}_2 = -\omega^2 A_1 + A_3, \tag{25}$$

$$\dot{A}_3 = -\frac{\gamma}{\tau}A_2 - \frac{1}{\tau}A_3 + f_3. \tag{26}$$

For the above Langevin equation of motion the Fokker–Planck equation (7) becomes

$$\frac{\partial W(U,t)}{\partial t} = \frac{\partial \Gamma_1 W}{\partial U} + D_1\frac{\partial^2 W}{\partial U^2}, \tag{27}$$

with

$$\Gamma_1 = \left(-\frac{r}{2} + \sqrt{\frac{r^2}{4} + \frac{q^3}{27}}\right)^{1/3} + \left(-\frac{r}{2} - \sqrt{\frac{r^2}{4} + \frac{q^3}{27}}\right)^{1/3},$$

where

$$q = \omega^2 + \frac{\gamma}{\tau} - \frac{1}{3\tau^2} \qquad r = -\frac{2\omega^2}{3\tau} + \frac{\gamma}{3\tau^2} - \frac{2}{27\tau^3} \qquad \text{and} \qquad D_1 = \frac{\gamma k_B T}{\tau^2}.$$

To keep Γ_1 positive we choose $r < 0$ and $\left(\frac{r^2}{4} + \frac{q^3}{27}\right) > 0$ since the distribution function W must vanish at the boundary. Thus the Fokker–Planck equation (27) describes the original non-Markovian system through the appearance of the noise correlation time in both Γ_1 and D_1, the effective dissipation and diffusion coefficient, respectively. The effective dissipation

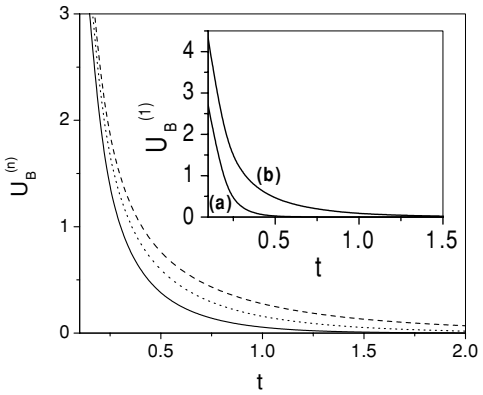

Figure 1. Plot of $U_B^{(n)}(t)$ versus time t using equation (20) for $\sigma(0) = 0.0, k_B T = 0.5, \omega = 2.0, \tau = 0.25$ and $\gamma = 1.0$. n has values 1, 3 and 5 for the solid, dotted and dashed curves respectively. In the inset $U_B^{(1)}$ is plotted versus t for the same parameter set as in the main figure: (a) $\tau = 0.1$ and (b) $\tau = 0.3$ (units are arbitrary).

appearing in [5] is not a function of the noise correlation time τ and ω, but is same as the constant dissipation parameter γ. It makes the present model much more general than the model described in [5].

Thus one can now calculate the upper bound of the time derivative of information entropy using the values of Γ_1 and D_1 in equation (20) for one auxiliary variable ($n = 1$). Repeating this calculation it can be calculated for any n. The time evolution of $U_B^{(n)}$ is shown in figure 1. The upper bound in each case monotonically decreases to the limiting value zero. It so happens because of the fact that with the increase of time the random force becomes more effective in the dynamics and consequently both the rate of change of width of distribution function $\left(\frac{\mathrm{d}\langle U^2\rangle}{\mathrm{d}t^2}\right)$ and Fisher information (I) decrease. At equilibrium I reaches a minimum value and $\frac{\mathrm{d}\langle U^2\rangle}{\mathrm{d}t^2}$ becomes zero and thus $U_B^{(n)}$ is zero in the long time limit. Figure 1 shows that the relaxation time of coloured noise-driven thermodynamically closed systems depends on the number of auxiliary variables used in the RMT. It increases with the increase of the number of auxiliary variables, and the value of the upper bound becomes higher for larger n at a given time since effective damping decreases with the increase of n. In the inset of figure 1 we plot $U_B^{(1)}$ versus t for different noise correlation times to examine how τ affects the equilibration time. It shows that the smaller the noise correlation time, the faster is the relaxation to equilibrium from a non-equilibrium condition. As the effective damping constant decreases with the increase of the noise correlation time, the relaxation time increases with the increase of τ. But the equilibration time is not affected by the noise correlation time in our earlier paper [5]. However, the upper bound is calculated using equation (20) at time $t = 2.5$ for different values of noise correlation time and is plotted in figure 2. Here, with increasing τ, we find the upper bound to increase first till it attains a maximum and then decrease. But in the previous model [5], U_B passes through a minimum in the presence of a constant force, and without the constant force the bound monotonically increases. Thus in the present model, τ has a different role in the persistence of the non-equilibrium situation.

We now examine the influence of the constant dissipation parameter γ on the upper bound. In figure 3 we plot the variation of $U_B^{(1)}$ versus γ. The upper bound first decreases followed by an increase after passing through a minimum. But it decreases monotonically in the previous model [5] since the decrease of the rate of change of the width of distribution function $\left(\frac{\mathrm{d}\langle U^2\rangle}{\mathrm{d}t}\right)$

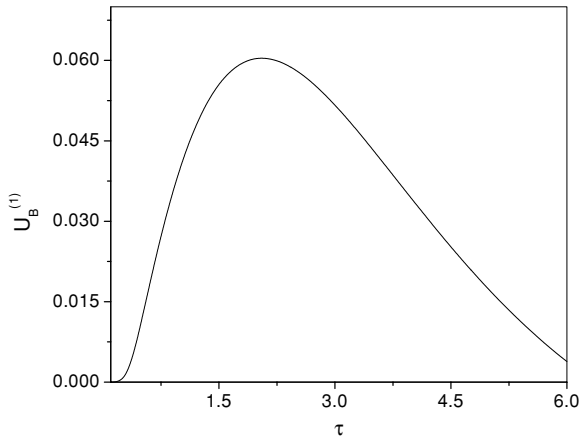

Figure 2. Plot of $U_B^{(1)}(t)$ versus τ using equation (20) for the same parameter set as in figure 1 at time $t = 2.5$ (units are arbitrary).

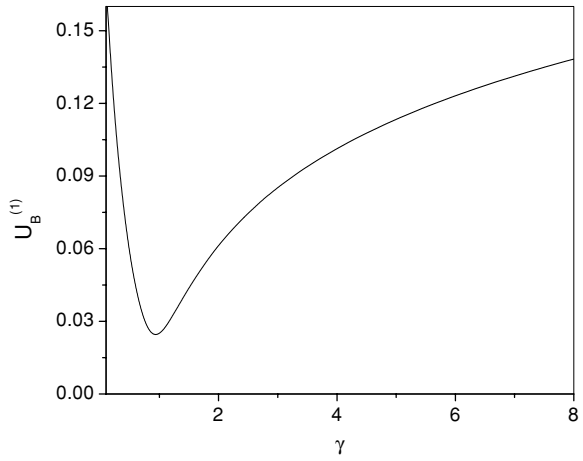

Figure 3. Plot of $U_B^{(1)}$ versus γ using equation (20) at time $t = 2.5$ for the same parameter set as in figure 2 and $\tau = 3.0$ (units are arbitrary).

very strongly dominates over the increase in Fisher information with the increase of dissipation parameter γ. However, in the present model the upper bound increases because of the decrease in effective damping with the increase of γ.

In conclusion, it may be said that we have considered the passage to equilibrium, from a given non-equilibrium state, of a coloured thermal noise-driven harmonic oscillator system. It is a thermodynamically closed system since in the present model the random force and frictional force have a common origin, and they follow the standard fluctuation–dissipation relation. Here we have studied the upper bound of the rate of change of information entropy in the non-equilibrium state based on the RMT, the Fokker–Planck description of the noise processes and the Schwartz inequality principle. In this paper we have derived a general formula by which one can calculate the bounds for a large number of auxiliary variables introduced in the RMT. The upper bound of the time derivative of the information entropy shows extremal behaviour of the variation of system parameters such as the noise correlation

time (τ) and the time-independent dissipation parameter (γ). The noise correlation time affects the equilibration time in addition to the value of the upper bound. Since *coloured noise-driven thermodynamically closed systems* are found in many situations in biology, physics and chemistry such as barrier crossing dynamics, stochastic resonance, reaction diffusion processes etc, we hope that our present studies will be useful for the understanding of experimental results in these areas.

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