KINETICS OF NONLINEAR SYSTEMS WITH WEAK INTERNAL AND PARAMETRIC FLUCTUATIONS*

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(Received May 6, 1993)

For nonlinear systems which can be described using simple generic forms of kinetic equations, with a priori unspecified but still present internal and parametric fluctuation terms, it is possible to extract noise characteristics from simple experimental data. Several examples are provided to illustrate this point.

PACS numbers: 05.45. +b, 05.70. Ln, 82.20. Mj

1. Introduction

The influence of noise on kinetics of nonlinear systems has been studied in numerous papers [1–6]. It is known that behavior of a system can be drastically changed by the influence of noise and the modes of the change are sensitive to the specific properties of the noise [1–9].

One can notice that most of the authors employ kinetic equations with ad hoc noise terms. Naturally one can never be sure if the noise was modelled properly and which noise terms are important and which are not.

The simplest is the Gaussian white noise. There are excellent methods for its description such as Fokker–Planck equation [1, 2]. On the other hand for more realistic colored noise easy to apply and general methods of description are virtually nonexistent. This is unfortunate as for many models white noise assumption is inadequate.

The coloured noise can enter into the kinetic equations in either way: additively and/or multiplicatively. To distinguish between different situations can be a very challenging experimental problem. (Various aspects of this problem were already addressed in several papers [3, 5, 7] and the theoretical considerations were applied, with success, to dye-laser [7].

* This work was supported by the KBN Grant No 02 0387 91 01.

This problem is also considered in the present paper. We will show that for a number of simple, generic forms of kinetic equations with ápriori unknown stochastic parts it is possible to determine directly which type of the noise is the dominant one. Our approach is limited to models which can be analytically treated. Thus it is not universal. Moreover it is applicable to the case of a weak noise, only. Still for a number of important models it gives plenty of very useful information (which is lacking or difficult to obtain in different approaches). In particular one can distinguish if the noise is white or coloured and if it is coupled additively or multiplicatively. This knowledge about the noise can be obtained through experimental determination of a few observables and comparison with the analytical formula. In below we provide several examples.

2. The Verhulst type kinetic equations

The general equation of Verhulst type

$$\frac{dx(t)}{dt} = a(t)x - b(t)x^{1+\mu} + c(t)\,, \tag{2.1}$$

was discussed frequently and is applicable to many different systems [3]. The solution for the deterministic (no noise) system with $c(t) = 0$ is

$$x(t) = x_0 \exp\left\{\int_0^t a(r)dr\right\}\left\{1 + \mu x_0{}^{\mu}\int_0^t dsb(s)\exp\left[\mu\int_0^s a(p)dp\right]\right\}^{-1/\mu} \tag{2.2}$$

The parameter μ is usually taken to be 1 or 2. To fix attention in the following we will consider only the models for which $x \geq 0$. These are for example: chemical models with x being some concentration or ecological models with x being the population density.

In real systems the internal (additive) noise $c(t)$ is present in the equation (2.1). It can crudely model all internal or so called "thermal" fluctuations coming from cooperative action of the neglected irrelevant degrees of freedom of the system.

The additive noise can be accompanied by so called external, or multiplicative, or parametric noise. The multiplicative, parametric noise corresponds to errors in control parameters. Namely the fixed values of control parameters a = const, b = const correspond to ideal situation. In reality $a = a_0[1 + \xi_a(t)]$ and $b = b_0[1 + \xi_b(t)]$ where a_0, b_0 are constants and ξ_a, ξ_b are the noise terms coming from imperfect control. The multiplicative parametric noise can contain contribution from internal stochastic processes as well.

Given the general form of the kinetic equation of the Verhulst type with $a = a_0[1 + \xi_a(t)]$, $b = b_0[1 + \xi_b(t)]$, $c = \xi_c(t)$ (where $x \geq 0$), not much can be said about relative importance of different noise terms for specific systems. (One of the attempts to obtain the information on interference effects of the different types of white noise in the system (2.1) was given in Ref. [9].)

There are many situations when white noise assumption is not adequate. Clearly, much more natural is the coloured noise. The simplest type is Ornstein and Uhlenbeck coloured noise with properties [1, 2]:

$$\langle \xi(t) \rangle = 0\,, \quad \langle \xi(t)\xi(t') \rangle = \sigma^2 \tau^{-1} \exp\left(-\frac{|t - t'|}{\tau} \right), \tag{2.3}$$

where ξ stands for the noise (sometimes a subscript to distinguish between different noises will be added to ξ) and σ, τ are amplitude and correlation time of the noise, respectively. For zero correlation time we recover the white noise. In the following we will always assume the Ornstein–Uhlenbeck noise.

After this introduction let us assume that we want to study the general situation. Our aim will be to apply analytical treatment and to get all the relevant data about the noises. First we consider the problem of parametric noise, only. We assume that the noise is weak; the terms of the order σ^3 and higher are neglected. Taylor expanding the formula (2.2) and performing statistical averages after simple but tedious calculations we obtain the moments $\langle x(t)^m \rangle$, $m = 1, 2, 3, \ldots$ for the case of parametric noise:

$$\begin{aligned} \lim_{t\to\infty} \langle x^m(t) \rangle &= \langle x(\infty)^m \rangle \\ &= \left(\frac{a_0}{b_0} \right)^{m/\mu} \left\{ 1 + \tfrac{1}{2}\sigma^2 m(m \mp \mu) \left[\frac{a_0}{\mu} - a_0^2 \tau \frac{\beta}{\beta + \mu a_0} \right] \right\}, \end{aligned} \tag{2.4}$$

where $\beta = 1/\tau$ (for white noise β is infinity), $a_0 > 0$, $b_0 > 0$. The signs $-, +$ correspond respectively to the assumptions $a = a_0[1 + \xi_a(t)]$, $b = b_0$, $c = 0$ and $a = a_0$, $b = b_0[1 + \xi_b(t)]$, $c = 0$. For $a < 0$, $b > 0$ all $\langle x^m(\infty) \rangle$ are zero. In the following we will always assume $a > 0$.

To check the correctness of formula (2.4) we can assume white noise with Stratonowich interpretation ($\tau = 0$ limit) and use Fokker–Planck equation to obtain $\langle x \rangle$ and $\langle x^2 \rangle$ in the independent way. Indeed the results (2.4) in the limit $\tau = 0$ agree with the Fokker–Planck results. Note that the most important conclusion coming from these exercises is the possibility to distinguish the white from coloured noise and to treat both of them within one formalism.

One more remark which is proper is that to check the formulas (2.4) for $\tau \neq 0$ one could, in principle, employ the new steepest-descent technique due to Gang and Haken [10]. However the lowest order approximation which is still analytically feasible [10] does not reproduce the exact results.

It is also proper at this place to repeat once more that there exist many other approaches which deal with small noise assumption in coloured noise problems [3–6]. In particular there exists the so called best Fokker–Planck approximation [4] which range of validity was shown to be rather small [5, 6]. This follows from truncation or in other cases from approximation to infinite Kramers–Moyal expansion [3, 5, 6]. In our approach, however, thanks to analytical solvability of the model this problem does not arise. Neither the small correlation time assumption is necessary [5].

After obtaining the formulas for the case of parametric noise let us return to the problem of internal fluctuations (additive noise) modeled by the equation $dx(t)/dt = a_0 x - b_0 x^{1+\mu} + \xi_c(t)$. As before we assume $x \geq 0$. For this equation the analytical solution is not available. Luckily for a weak noise a certain simpleminded approximation is possible. Namely we will make a substitution:

$$\underset{(x\geq 0)}{\frac{dx(t)}{dt} = a_0 x - b_0 x^{1+\mu} + \xi_c} \rightarrow \underset{\text{(no condition on x)}}{\frac{dx(t)}{dt} = a_0 x - b_0 x^{1+\mu} + a_0 x \tilde{\xi}_c} \tag{2.5}$$

where

$$\langle \tilde{\xi}_c(t) \tilde{\xi}_c(t') \rangle = \tilde{\sigma}^2 \tau^{-1} \exp\left(-\frac{|t-t'|}{\tau}\right),$$

$$\tilde{\sigma} = \frac{1}{a_0}\left(\frac{b_0}{a_0}\right)^{1/\mu} \sigma . \tag{2.6}$$

(For properties of ξ_c — see Eq. (2.3)). This approximation can be explained in the following way. For a weak noise, when probability distribution is centered more or less around deterministic $\bar{x}_{\text{det}} = (a_0/b_0)^{1/\mu}$ and is very narrow — for many physical characteristics of the system it does not matter whether we are dealing with $\sigma\xi_c$ or with $a_0 x \tilde{\xi}_c \approx a_0 \bar{x}_{\text{det}} \tilde{\xi}_c$. As bonus for our crude approximation (2.5) the condition $x \geq 0$ disappears. On the other hand the price one has to pay is distortion of probability distribution (the higher moments of probability distribution will be incorrect). Using approximation (2.5) by simple substitution directly into formula (2.4) we obtain

$$\langle x(\infty)^m \rangle \approx \left(\frac{a_0}{b_0}\right)^{m/\mu} \left\{ 1 + \tfrac{1}{2} m(m-\mu) \frac{\sigma^2}{a_0{}^2} \left(\frac{b_0}{a_0}\right)^{2/\mu} \left[\frac{a_0}{\mu} - a_0^2 \tau \frac{\beta}{\beta + \mu a_0}\right] \right\},$$

$$\text{(intrinsic noise; } m = 1,2). \tag{2.7}$$

We would like to stress that the equation (2.7) is valid upon assumption of weak noise provided a_0 is not too close to zero.

Let us now make short summary. For the Verhulst model with $x \geq 0$ constraint and with different types of noise the equations (2.4) and (2.7) are our main result. Provided one knows nothing about the type of the noise in the real system it is only necessary to perform some precise measurements on $\langle x \rangle$ and $\langle x^2 \rangle$ for several values of deterministic (kinetic) parameters a_0, b_0 and then to compare results with formulas (2.4) and (2.5). If the parameter and internal additive noise are present at the same time one simply has to be more careful. More experimental data and generalization of (2.4) and (2.7) into one "synthetic" formula will be needed.

3. One-dimensional overdamped rotator with friction and forcing

This model was studied by means of numerical simulation in [11]. The equation for the deterministic case reads

$$\gamma \frac{d\theta}{dt} = \epsilon \sin(\omega t) \sin(\theta) \, , \tag{3.1}$$

where θ is the angle of the rotation, t is the time, γ is friction coefficient and ϵ is the amplitude of forcing. The deterministic solution is

$$\tan\left(\frac{\theta_{\text{det}}}{2}\right) = \tan\left(\frac{\theta_0}{2}\right) \exp\left\{\frac{\epsilon}{\gamma\omega}[1 - \cos(\omega t)]\right\} . \tag{3.2}$$

It is known [11] that the additive noise gives rise to erratic motion with $\langle \theta \rangle = 0$. The frequency of jumps of θ from the interval $[0, \pi]$ into $[-\pi, 0]$ is dependent on the noise amplitude and on $\epsilon/(\gamma\omega)$. For small σ, small $\epsilon/(\gamma\omega)$ and for $\tan(\theta_0/2) \sim 1$ the waiting time for a single jump can be very large.

In contrast to additive noise the parametric noise does not give rise to jumps. The equation (3.1) in the presence of parametric noise becomes

$$\gamma \frac{d\theta}{dt} = \epsilon[1 + \xi(t)] \sin(\omega t) \sin(\theta) . \tag{3.3}$$

The solution of (3.3) is simple:

$$\frac{\tan\left(\frac{\theta}{2}\right)}{\tan\left(\frac{\theta_{\text{det}}}{2}\right)} = \exp\left\{\frac{\epsilon}{\gamma} \int\limits_0^t \sin(\omega r)\xi(r) dr\right\} . \tag{3.4}$$

Using (3.3), performing Taylor expansion and averaging over noise we obtain

$$\lim_{t\to\infty}\left\langle \ln\left\{\frac{\tan\left(\frac{\theta}{2}\right)}{\tan\left(\frac{\theta_{\rm det}}{2}\right)}\right\}\right\rangle = 0\,, \tag{3.5}$$

$$\lim_{t\to\infty}\left\langle \ln^2\left\{\frac{\tan\left(\frac{\theta}{2}\right)}{\tan\left(\frac{\theta_{\rm det}}{2}\right)}\right\}\right\rangle = \left(\frac{\epsilon}{\gamma}\sigma\right)^2\left\{1-\frac{\omega^2}{\omega^2+\beta^2}\right\}t\,. \tag{3.6}$$

The time "going to infinity" from the computational point of view has the meaning: $t\omega \gg 1$, $t\beta \gg 1$, and $^1/_2 t\beta(\beta^2+\omega^2) \gg \beta\omega\exp(-\beta t)$. The formulas (3.5) and (3.6) together with the results of Ref. [11] clearly demonstrate a possibility of experimental discrimination between the different types of noise.

Let us note that the other types of parametric noise are also possible. Consider for example forcing with imperfect periodicity — $\sin[\omega t+\xi(t)]$. For this type of the noise the result is:

$$\lim_{t\to\infty}\left\langle \ln\left\{\frac{\tan\left(\frac{\theta}{2}\right)}{\tan\left(\frac{\theta_{\rm det}}{2}\right)}\right\}\right\rangle = -\frac{\epsilon\sigma^2}{2\tau\gamma\omega}[1-\cos(\omega t)]\,. \tag{3.7}$$

The equation for $\langle\ln^2[\tan(\theta/2)/\tan(\theta_{\rm det}/2)]\rangle$ is identical to (3.6). The formula (3.7) together with experimental data can answer the question if the forcing is ideal periodic one or not.

4. Simple chemical reaction. Fluctuating temperature and concentrations

One of the simplest chemical reactions is

$$A_1 + X \underset{k_2}{\overset{k_1}{\rightleftharpoons}} A_2 + Y\,. \tag{4.1}$$

This corresponds for enzymatic (catalytic) conversion of A_1 into A_2 with X, Y being two different states (conformations) of the enzyme.

The concentrations of molecules A_1, A_2, X, Y are denoted by a_1, a_2, x, y. We consider the situation when a_1, a_2 are kept constant and when $x+y=1$. (This experimental setup requires that appropriate control system and external reservoirs has to be used).

The kinetic equation for x is of the well known form [12, 13]:

$$\frac{dx}{dt} = k_2a_2 - (k_1a_1+k_2a_2)x\,. \tag{4.2}$$

Suppose that one is dealing with temperature fluctuations in the reaction rates (parameters) k_i controlling the speed and the direction in which the reaction is going. Assume the Arrhenius dependence $k_i = k_i^0 \exp\{-E_i/k_B T(t)\}$ where $i = 1,2$, a_i k_i^0 are constants, E_i are activation energies, k_B is the Boltzmann constant, and where the temperature $T(t)$ is fluctuating around T_0, *i.e.*, $T(t) = T_0[1+\xi_T(t)]$. The analytic solution for the present problem is:

$$x(t) = \exp\big(-G(t)\big)\left\{x_0 + \int_0^t dr a_2 k_2(r)\exp[G(r)]\right\},$$

$$G(t) = \int_0^t ds\big(a_1k_1(s) + a_2k_2(s)\big). \tag{4.3}$$

Taylor expanding up to σ^2 and subsequently averaging over the noise we obtain

$$\frac{1}{\sigma}\left\{\frac{\langle x(\infty)\rangle}{x_{\rm det}(\infty)} - 1\right\} = \beta\left\{\epsilon_2(\epsilon_2-2) - \frac{g_2}{g_0} - \frac{g_1\epsilon_2}{g_0+\beta} + \frac{g_1^2}{g_0(g_0+\beta)}\right\}, \tag{4.4}$$

where $\epsilon_i = E_i/(k_B T_0)$, $g_0 = \sum_{i=1}^2 a_i k_i$, $g_1 = \sum_{i=1}^2 a_i k_i \epsilon_i$ and where $\beta < g_0$. For β equal and greater than g_0 the higher moments $(\langle x^m(\infty)\rangle\ m = 2,3,\ldots)$ are divergent.

Much simpler is the model of parametric fluctuations in concentration $a_1(t) = a_1^0[1+\xi(t)]$, with a_2 constant $(a_2 = a_2^0)$. In this case we obtain

$$\frac{2}{\sigma}\left\{\frac{\langle x^m(\infty)\rangle}{{x_{\rm det}}^m(\infty)} - 1\right\} \approx m(m+1)\frac{g^2}{g_0}\frac{\beta}{g_0+\beta}, \tag{4.5}$$

where $g_0 = k_1a_1^0 + k_2a_2^0$, $g = k_1a_1^0$.

5. Conclusions

We have shown that for a number of simple generic forms of kinetic equations such for which analytic treatment is available, it is possible to extract from the experimental data and analytic formula the information about the properties of noise present in real experimental systems. It is possible to discriminate if this is Gaussian white noise or coloured noise. Furthermore it is possible to distinguish between additive and parametric noises. The method presented in the paper seems to be the only one which works for the problem of temperature fluctuations in chemical kinetic equations. For other systems (where many other methods to extract the information about the noise are available) it provides the additional, very simple to use, tools for the experimentalist.

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