Journal of Statistical Physics, Vol. 15, No. 6, 1976

An Observation on the Effect of Fluctuations Far from Equilibrium: The Lotka–Volterra Model

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Received February 5, 1976; revised March 22, 1976

Spontaneous fluctuations in the Lotka–Volterra model of chemical reactions are known to grow in an unbounded way when species held in excess are neglected. This result is obtained in a simple way using generalized fluctuation-dissipation principles but appears to be an artifact of ignoring fluctuations in the variables that are held fixed. When fluctuations in the other concentrations are included in the model, the spontaneous fluctuations become bounded.

KEY WORDS: Stochastic process; chemical fluctuations; Lotka–Volterra model; stability.

1. INTRODUCTION

Spontaneous fluctuations in systems far from equilibrium may be qualitatively quite different from those near equilibrium. An example of this is provided by the Lotka–Volterra equations, which have been used as a model of both coupled chemical reactions and ecological competition.(1) When fluctuations in this model are treated by the birth and death (master equation) formalism,(2,3) it is found that near the steady state deviations from the average grow in an unbounded way. In this sense the model is unstable to spontaneous fluctuations. This is somewhat perplexing since the averages from the mass action rate law are stable in the Liapunov sense that concentrations which are originally close to the steady state remain close to the steady state.

The purpose of this note is to understand the instability with respect to spontaneous fluctuations. The work is based on generalized fluctuation-

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This work was supported by the National Science Foundation through Research Grant No. MPS 74-00483 A01.

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dissipation principles(4) which are known to agree with the macroscopic limit of the master equation formalism.(5) When fluctuations are neglected for species which are held fixed in the Lotka–Volterra model, an unbounded growth of the fluctuations is obtained. To examine the reason for this divergence, an extension of the Lotka–Volterra model is introduced. In the extended model an external source term is explicitly added to the kinetic equations in order to fix the concentration of species held in excess. In this extended model, the equations satisfied by the conditionally averaged concentrations are *identical* to those in the Lotka–Volterra model. Thus the average behavior is stable and the temporal oscillations are identical to those found in the Lotka–Volterra model. However, using the generalized fluctuation-dissipation principles, the equations satisfied by the fluctuations are substantially different from those which are found when fluctuations in the externally fixed variables are ignored. Indeed the fluctuations in this extended model are easily shown to be bounded. This demonstrates the importance of considering the effect of fluctuations in all variables and shows that special care should be used in treating fluctuations far from equilibrium.

2. FLUCTUATIONS IN THE LOTKA–VOLTERRA MODEL WITH BATH MOLECULES NEGLECTED

The mechanism for the Lotka–Volterra model involves three irreversible elementary reactions:

$$E + C_1 = 2C_1 \tag{1}$$

$$C_1 + C_2 = 2C_2 \tag{2}$$

$$C_2 = G \tag{3}$$

In this mechanism the concentrations of the bath molecules E and G are supposed to be fixed, the forward rate constants are k_1, k_2, and k_3, and the rate constants of the back reactions are taken to be zero. It is easily verified that these reactions are linearly dependent, but that the concentrations of the molecules C_1 and C_2 are independent variables. Thus the generalized fluctuation-dissipation principles(4,5) for describing concentration fluctuations are easily applied. These principles associate a conditional probability with transport equations, and according to the first principle the conditionally averaged concentrations satisfy the phenomenological rate laws. For this model the rate law is

$$d\bar{n}_1/dt = k_1 E\bar{n}_1 - k_2\bar{n}_1\bar{n}_2, \qquad d\bar{n}_2/dt = k_2\bar{n}_1\bar{n}_2 - k_3\bar{n}_2 \tag{4}$$

where $\bar{n}_1$ and $\bar{n}_2$ are the average concentrations conditioned on the precise values $n_1{}^0$ and $n_2{}^0$ at $t = 0$ and E represents the fixed concentration of the molecule E. In treating fluctuations in this way, the common point of view(2,3) has been adopted that the concentrations of the bath molecules E and G are parameters, not variables, of the system. Thus they do not fluctuate. This is not the only possible point of view, and a more complete treatment is given below. The second fluctuation-dissipation principle describes the deviations from the conditional averages, $\delta\mathbf{n} = \mathbf{n} - \bar{\mathbf{n}}$, which are supposed to satisfy a linearized version of Eq. (4):

$$d\delta\mathbf{n}/dt = H(\mathbf{n}^0, t)\,\delta\mathbf{n} + \tilde{\mathbf{f}}(t) \tag{5}$$

where $H(\mathbf{n}^0, t)$ is the matrix

$$H(\mathbf{n}^0, t) = \begin{pmatrix} k_1E - k_2\bar{n}_2(\mathbf{n}^0, t) & -k_2\bar{n}_1(\mathbf{n}^0, t) \\ k_2\bar{n}_2(\mathbf{n}^0, t) & k_2\bar{n}_1(\mathbf{n}^0, t) - k_3 \end{pmatrix} \tag{6}$$

and $\tilde{f}(t)$ is a nonstationary Gaussian process whose average vanishes and whose covariance matrix is

$$\langle\tilde{\mathbf{f}}(t)\tilde{\mathbf{f}}(s)^T\rangle = \gamma(\mathbf{n}^0, t)\,\delta(t - s) \tag{7}$$

with

$$\gamma(\mathbf{n}^0, t) = V^{-1}\begin{pmatrix} k_1E\bar{n}_1(\mathbf{n}^0, t) + k_2\bar{n}_1(\mathbf{n}^0, t)\bar{n}_2(\mathbf{n}^0, t) & -k_2\bar{n}_1(\mathbf{n}^0, t)\bar{n}_2(\mathbf{n}^0, t) \\ -k_2\bar{n}_1(\mathbf{n}^0, t)\bar{n}_2(\mathbf{n}^0, t) & k_2\bar{n}_1(\mathbf{n}^0, t)\bar{n}_2(\mathbf{n}^0, t) + k_3\bar{n}_2(\mathbf{n}^0, t) \end{pmatrix} \tag{8}$$

In Eq. (8), V is the volume. Equations (4)–(8) produce a Gaussian conditional probability density $P_2(\mathbf{n}^0|\mathbf{n}t)$ and can be used to predict the future probability distribution in an ensemble. For example, if the concentrations n_1 and n_2 are originally distributed with the density $W_1(\mathbf{n}, 0)$, then at a time t later the probability density will be

$$W_1(n, t) = \int W_1(\mathbf{n}^0, 0)P_2(\mathbf{n}^0|\mathbf{n}t)\,d\mathbf{n}^0 \tag{9}$$

The difficulty in treating fluctuations resulting from coupled nonlinear reactions is apparent in the expressions for H and γ since the solutions to the nonlinear average equations, Eq. (4), for arbitrary initial condition $\mathbf{n}^0$ are required. Even for as simple a case as the Lotka–Volterra model, no analytical solutions are known, except close to the steady state. This steady state is at $n_1^{\text{ss}} = k_3/k_2$, $n_2^{\text{ss}} = Ek_1/k_2$ and the solutions to the average equation are closed trajectories around the steady state. For initial values $\mathbf{n}^0$ close to $\mathbf{n}^{\text{ss}}$ the solutions are approximately circular trajectories moving counterclockwise in the (n_1, n_2) plane. Because of the simplicity of these trajectories, attention is restricted to initial ensembles which are *close to the steady state.* According to Eq. (9), the conditional probability density $P_2(\mathbf{n}^0|\mathbf{n}t)$ can be used to predict the future behavior in this ensemble. However, since the steady state is stable and the initial distribution $W(\mathbf{n}^0, 0)$ is sharply peaked around it, one has

$$W_1(\mathbf{n}, t) = \int W_1(\mathbf{n}^0, 0) P_2(\mathbf{n}^0|\mathbf{n}t)\, d\mathbf{n}^0 \approx P_2(\mathbf{n}^{ss}|\mathbf{n}t) \tag{10}$$

Thus the approximate future behavior of the ensemble can be determined by evaluating the conditional probability density solely at the initial steady state. This is done by setting $\mathbf{n}^0 = \mathbf{n}^{ss}$ in Eqs. (4)–(8) and gives

$$\bar{\mathbf{n}}(\mathbf{n}^{ss}, t) = \mathbf{n}^{ss}, \qquad d\delta\mathbf{n}/dt = H(\mathbf{n}^{ss})\,\delta\mathbf{n} + \tilde{\mathbf{f}}(t) \tag{11}$$

with the *time-independent* matrices

$$H(\mathbf{n}^{ss}) = \begin{pmatrix} 0 & -k_3 \\ k_1E & 0 \end{pmatrix} \equiv \Lambda \tag{12}$$

and

$$\gamma(\mathbf{n}^{ss}) = \frac{Ek_1k_3}{Vk_2} \begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix} \tag{13}$$

It is easily verified that $\gamma(\mathbf{n}^{ss})$ is positive definite and that the eigenvalues of Λ are $\lambda_\pm = \pm i\omega$, $\omega = (k_3k_1E)^{1/2}$. The conditional probability is

$$P_2(\mathbf{n}^{ss}|\mathbf{n}t) = [(2\pi)^2 \det \sigma(\mathbf{n}^{ss})]^{-1/2} \exp[-\tfrac{1}{2}(\mathbf{n} - \mathbf{n}^{ss})^T \sigma^{-1}(\mathbf{n}^{ss}, t)(\mathbf{n} - \mathbf{n}^{ss})]$$

with

$$\sigma(\mathbf{n}^{ss}, t) = \int_0^t \exp[\Lambda(t - s)]\, \gamma(\mathbf{n}^{ss}) \exp[\Lambda^T(t - s)]\, ds \tag{14}$$

The covariance matrix $\sigma(\mathbf{n}^{ss}, t)$ is obtained using the representation

$$\exp(\Lambda t) = I \cos \omega t + \Lambda \sin \omega t$$

which leads to

$$\begin{aligned} \sigma(\mathbf{n}^{ss}, t) = {} & \frac{\omega}{2k_2} \begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix} (\cos \omega t \sin \omega t + t) \\ & + \frac{1}{k_2} \begin{pmatrix} k_3 & k_1E - k_3 \\ k_1E - k_3 & -k_1E \end{pmatrix} \sin^2 \omega t \\ & + \frac{\omega}{2k_2} \begin{pmatrix} 2k_3/k_1E & 1 \\ 1 & 2k_1E/k_3 \end{pmatrix} (t - \cos \omega t \sin \omega t) \end{aligned} \tag{15}$$

The oscillatory terms are a consequence of the fact that the eigenvalues of Λ are pure imaginary. It is clear from Eq. (15) that as time proceeds there is a linear divergence of the variance of n_1 and n_2. Thus when only fluctuations in

C_1 and C_2 are considered the present formalism predicts that the Lotka–Volterra model—while stable to macroscopic deviations—is unstable to microscopic fluctuations. That is to say, the noise level soon obscures the average behavior. This is closely connected to the fact that the eigenvalues of Λ are pure imaginary and should not occur for models in which the oscillations are due to a stable limit cycle.

3. INCLUSION OF FLUCTUATIONS FOR BATH MOLECULES

The treatment of fluctuations in the preceding section is based on the assumption that the concentration of the reactant E does not fluctuate. This certainly cannot be correct since E is constantly reacting with C_1. In fact to keep the amount of E fixed, an external source—which just balances the depletion of E by reaction (1)—must be added to the system. Hence the complete average equations should be

$$\begin{aligned} d\bar{E}/dt &= -k_1\bar{E}\bar{n}_1 + K(t) \equiv 0 \\ d\bar{n}_1/dt &= k_1\bar{E}\bar{n}_1 - k_2\bar{n}_1\bar{n}_2 \\ d\bar{n}_2/dt &= k_2\bar{n}_1\bar{n}_2 - k_3\bar{n}_2 \end{aligned} \tag{16}$$

The external source term is $K(t)$ and by varying its strength the constant average concentration $\bar{E}$ can be changed, since $\bar{E} = K(t)/k_1\bar{n}_1(t)$. In this extended Lotka–Volterra model the average concentration of E is fixed and so the time dependence of $\bar{n}_1(\mathbf{n}^0, t)$ and $\bar{n}_2(\mathbf{n}^0, t)$ will be *precisely the same as in the usual model described by Eq. (4)*. However, spontaneous deviations in the concentration of E may now be easily included. Restricting attention again to distributions which are sharply peaked around the steady state $\mathbf{n}^{ss} = (\bar{E}, k_3/k_2, \bar{E}k_1/k_2)$, the deviations from the average concentrations, $\delta\mathbf{n} \equiv (\delta E, \delta n_1, \delta n_2)$, obey

$$d\delta\mathbf{n}/dt = \Lambda' \,\delta\mathbf{n} + \tilde{\mathbf{f}}(t) \tag{17}$$

where the external source term does not appear(4) since only dissipative events contribute to the fluctuations. The matrix Λ' is found from Eq. (16),

$$\Lambda' = \begin{pmatrix} -k_1k_3/k_2 & -k_1\bar{E} & 0 \\ k_1k_3/k_2 & 0 & -k_3 \\ 0 & k_1\bar{E} & 0 \end{pmatrix} \tag{18}$$

and the covariance matrix of the random terms $\tilde{\mathbf{f}}(t)$ is(5)

$$\gamma' = \frac{k_1k_3\bar{E}}{Vk_2}\begin{pmatrix} 1 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{pmatrix} \tag{19}$$

Again γ' is a positive-definite matrix. For initial distributions sharply peaked around the steady state, Eq. (10) can be applied. Such a distribution can be approximated by the Gaussian distribution $P_2(\mathbf{n}^{ss}|\mathbf{n}t)$ with fixed average value $\mathbf{n}^{ss}$ and a covariance matrix whose time dependence is given by

$$\sigma(\mathbf{n}^{ss}, t) = \int_0^t \exp[\Lambda'(t-s)]\,\gamma'\,\exp[\Lambda'^T(t-s)]\,ds$$

An explicit expression for $\sigma(\mathbf{n}^{ss}, t)$ may be found using the same methods which were employed in obtaining Eq. (15). In particular, since the Routh–Hurwitz criterion(6) shows that all the eigenvalues of Λ' have negative real parts, it follows that *covariance matrix converges to a finite limit* as time proceeds. The exact time dependence of the matrix elements has been evaluated for arbitrary k_3 and $\bar{E}$ when $k_1 = k_2 = 1$, and representative results are shown in Fig. 1. For values of the parameter $\bar{E}/k_3$ between 1 and 1000 the imaginary parts of the eigenvalues of Λ' produce oscillations in the covariance matrix, which are damped by the real part of the eigenvalues as time proceeds. Thus fluctuations, which grew in an unbounded way when E was treated as a parameter, become bounded when E is allowed to fluctuate! This points out the importance of including all the physical variables when treating spontaneous fluctuations and shows that far from equilibrium, fluctuations in one variable may drastically effect those in another.

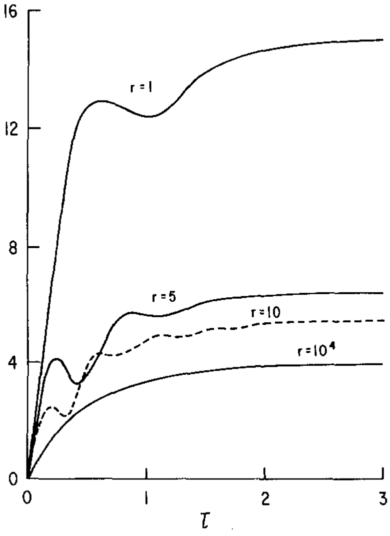

Fig. 1. The time dependence of the variance of n_1 for the extended Lotka–Volterra model for several values of $r = \bar{E}/k_3$ when $k_1 = k_2 = 1$. The ordinate represents $V\langle(\delta n_1)^2\rangle/\bar{E}$ and the abscissa is the scaled time $\tau = k_3 t/3$. The shapes of the curves are representative of the time dependence of all the matrix elements, although the magnitude of the curves for $V\langle(\delta E)^2\rangle/\bar{E}$ and $V\langle\delta E\ \delta n_2\rangle/\bar{E}$, for example, is an increasing function of r.

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