Influence of Gaussian fluctuations on a model kinetic system exhibiting explosive behavior[a)]

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(Received 17 June 1982; accepted 17 September 1982)

We examine the influence of fluctuations on a model kinetic equation which exhibits explosive behavior. The particular model kinetic equation $\dot{x} = kx^2 - \alpha x$ has fixed points at $x = 0$ and $x = x_1 = (\alpha/k)$. For constant coefficients k and α, the trajectory $x(t)$ diverges in a finite time if the initial value $x_0 > x_1$, and $x(t)$ approaches zero if $x_0 < x_1$; fluctuations in the coefficients may change this deterministic behavior. We consider three different models incorporating Gaussian fluctuations. In case A, the rate coefficient $k(t)$ has a fluctuating part; in this case it is possible to determine exactly the entire probability distribution $p(x,t|x_0)$ as well as $N(t)$ the probability that the system has not exploded (for a given x_0) at time t. In case B, the rate coefficients $k(t)$ and $\alpha(t)$ contain identical fluctuating parts; we show that this type of fluctuating behavior has no influence on the transition between stable and unstable behavior. In case C, the rate coefficient $\alpha(t)$ contains a fluctuating part. An approximation solution leads to an effective kinetic equation which is identical to the deterministic equation except that α is replaced by $\alpha_{\text{eff}} = \alpha(1 - \alpha q)$, where q is a measure of the strength of the fluctuation in $\alpha(t)$. This model kinetic equation is helpful for illustrating how fluctuations may influence kinetic systems that contain explosive character, including the problem of passage over a barrier in the overdamped limit.

I. INTRODUCTION

In recent years there has been growing interest in the influence of fluctuations on chemically reacting systems that are controlled by nonlinear mechanisms which support multiple steady states.[1–4] Several investigations have studied the role of fluctuations in the dynamics of such systems, focusing on the stability of the steady state and transitions among the states.[5–10] These studies have considered states of local or marginal stability and described the influence of fluctuations included as a appropriate random terms, usually assumed to be Gaussian.

Our purpose in this paper is to describe the influence of fluctuations on a simple reaction mechanism which exhibits *explosive behavior*. Specifically we wish to examine how fluctuations may drive the system from a region of stability into a region of explosive instability. We introduce fluctuations in the reaction mechanism in several ways and discover that each way influences the transition quite differently.

The reaction mechanism that we examine is one of the simplest that exhibits explosive behavior[11]:

$$\begin{aligned} &x \xrightarrow{\alpha} B\,, \\ &A + 2x \xrightarrow{k} 3x\,. \end{aligned} \tag{1.1}$$

For simplicity we assume that the reactant A is supplied in a manner that maintains its concentration constant; we choose this concentration to be unity. We also neglect diffusion and other transport processes that are pertinent in the description of chemically reactive fluids.

Evidently the reaction mechanisms Eq. (1.1) is highly artificial although it mimics some features of models of combustion.[12] The major deficiency of the model is the nonconservation of species x. The model's advantage, however, is that it is one of the simplest examples of a nonlinear dynamical equation that exhibits both regions of stable and unstable behavior.

The deterministic kinetic equation for the reaction mechanism (1.1) is

$$\frac{dx}{dt} = kx^2 - \alpha x\,, \quad k\,, \alpha > 0\,. \tag{1.2}$$

Note that this equation has two stationary points, $x = 0$ and $x_1 = (\alpha/k)$. The former point is stable and the latter, unstable; thus for any initial condition in the interval $0 \le x_0 < x_1$ all trajectories will approach $x = 0$ as $t \to \infty$, while for any initial condition $x_0 > x_1$ all trajectories lead to *explosive behavior* $x(t) \to \infty$.

The explicit solution to Eq. (1.1) is

$$x(t) = [\exp(\alpha t)(x_0^{-1} - x_1^{-1}) + x_1^{-1}]^{-1}\,. \tag{1.3}$$

For $x_0 > x_1$, $x(t)$ diverges in a *finite time* t_∞, dependent upon initial conditions, given by

$$\alpha t_\infty = -\ln\left[1 - \frac{x_1}{x_0}\right]\,. \tag{1.4}$$

The time t_∞ increases as the initial concentration approaches x_1 from above.

An interesting limiting case of Eq. (1.2) is $\alpha = 0$. For this case, all initial trajectories lead to explosive behavior, according to

$$x(t) = [x_0/(1 - kx_0 t)]\,, \tag{1.5}$$

with $t_\infty = (kx_0)^{-1}$. The more usual case of a *stable* sta-

a)Supported in part by the Defense Advanced Research Projects Agency.

tionary state x_1 is realized by changing the sign of both k and α.

Our purpose is to examine how fluctuations influence the transition from stable to explosive behavior. In particular, we seek an answer to the question: "In the presence of fluctuations, what is the chance that the system in an initial state $x_0 < x_1$ will make a transition to explosive behavior?" In the next section we demonstrate that the answer to this question depends on how fluctuations are introduced into the mechanism. We consider three different models and solve two of these exactly and the third approximately.

II. INFLUENCE OF FLUCTUATIONS ON EXPLOSIVE BEHAVIOR

We modify the deterministic kinetic equation (1.2) to permit time-dependent rate coefficients that include the influence of fluctuations

$$\frac{dx(t)}{dt} = k(t)x^2(t) - \alpha(t)x(t) . \qquad (2.1)$$

Here the influence of fluctuations is introduced through a a multiplicative time dependence of the rate coefficients in contrast to an additive external random flux.

The key to our attack consists of recognizing that Eq. (2.1) is a Bernoulli equation and making the standard substitution[12] $u(t) = x(t)^{-1}$ transforms Eq. (2.1) into a linear equation,

$$\frac{du}{dt} = \alpha(t)u(t) - k(t) . \qquad (2.2)$$

If $\alpha(t)$ and/or $k(t)$ are considered Gaussian random variables then Eq. (2.1) or (2.2) can be transformed into a Fokker–Planck equation. This approach has been pursued with some success for the Verhults type population growth differential equation considered here by Keizer[9] and by Fox.[2] We proceed to consider three different models for the fluctuations.

III. MODEL A—QUADRATIC FLUCTUATIONS ONLY

For this model we assume that the rate coefficient of the first order term does not contain fluctuations $\alpha(t) = \alpha$ and that the rate coefficient of the second order term includes a fluctuating part $f(t)$ which is Gaussian; thus $k(t) = k + f(t)$ with

$$\overline{f(t)}^{x_0} = 0 \quad \text{and} \quad \overline{f(t_1)f(t_2)}^{x_0} = q\delta(t_1 - t_2) . \qquad (3.1)$$

A note of caution is required in the use of the white noise condition (3.1) in Eq. (2.1). The delta function makes the value of x jump in such a singular way that the appropriate value for x on the right-hand side of Eq. (2.1) at the moment of action of $f(t)$ is unclear.[13] This question does not arise if the Gaussian fluctuation has a finite correlation time τ_c and we follow, in principle, the approach of Stratonovich,[14] of taking the limit $\tau_c \to 0$ at the end of the calculation.

For this model Eq. (2.2) becomes

$$\frac{du}{dt} = \alpha u(t) - k - f(t) . \qquad (3.2)$$

If we make the substitution

$$y = u - \frac{k}{\alpha} = \frac{1}{x} - \frac{1}{x_1} \quad , \qquad (3.3)$$

Eq. (3.3) becomes

$$\dot{y} = \alpha y - f(t) \qquad (3.4)$$

which, except for sign changes, is the form of the Langevin equation. A lemma due to Chandrasekhar[15] immediately leads to an exact expression for $\hat{p}(y, t|y_0)$, the probability that the variable is in the neighborhood of y at time t, given that it was in the neighborhood of y_0 at $t = 0$,

$$\hat{p}(y, t|y_0) = \left[\frac{2\pi q}{\alpha}(e^{2\alpha t} - 1)\right]^{-1/2} \exp\left\{-\frac{(y - y_0 e^{\alpha t})^2}{\left(\frac{2q}{\alpha}\right)(e^{2\alpha t} - 1)}\right\} . \qquad (3.5)$$

In terms of the variable of interest x the probability distribution is

$$p(x, t|x_0) = \left[\frac{2\pi q}{\alpha}(e^{2\alpha t} - 1)\right]^{-1/2} \frac{1}{x^2} \times \exp\left\{-\frac{\left[\left(\frac{1}{x} - \frac{1}{x_0}e^{\alpha t}\right) + \frac{k}{\alpha}(e^{\alpha t} - 1)\right]^2}{\left(\frac{2q}{\alpha}\right)(e^{2\alpha t} - 1)}\right\} . \qquad (3.6)$$

Note that as $t \to 0$,

$$p(x, t|x_0)_{t \to 0}\ \delta(x - x_0) , \qquad (3.7)$$

and that in the limit of vanishing fluctuations $q \to 0$,

$$p(x, t|x_0) \underset{q \to 0}{\to} \delta\left[\left(\frac{1}{x} - \frac{1}{x_0}e^{\alpha t}\right) + \frac{k}{\alpha}(e^{\alpha t} - 1)\right]\frac{1}{x^2} . \qquad (3.8)$$

The expression (3.6) is one of the main results of our inquiry. It provides an exact expression for the probability distribution function, not just a few moments of the distribution, for the model of Gaussian quadratic fluctuations. Various moments may be found according to the prescription

$$\overline{X(t)^n}^{x_0} = \int_0^\infty x^n p(x, t|x_0)\, dx . \qquad (3.9)$$

The limit $q \to 0$ leads to an expression for $\overline{x(t)}^{x_0}$ from Eq. (3.8) which, as expected, is identical to the deterministic expression (1.3).

The numerator of the argument of the exponential in the probability distribution (3.6) vanishes when

$$\frac{1}{x} = \left(\frac{1}{x_0} - \frac{1}{x_1}\right)e^{\alpha t} + \frac{1}{x_1} \quad , \qquad (3.10)$$

where $x_1 = (\alpha/k)$. If $x_0 < x_1$, then $x \to 0$ as $t \to \infty$. However, if $x_0 > x_1$ then the right-hand side of Eq. (3.10) vanishes and x diverges in the finite time t_∞ given by Eq. (1.4). Thus for $x_0 < x_1$, the peak of the probability distribution moves gradually toward the origin. But for $x_0 > x_1$, the probability distribution peak only remains on the interval $0 < x < \infty$ during the time interval $0 < t < t_\infty$. We may conclude that there is an abrupt change in behavior of the probability distribution depending upon the initial condition just as in the deterministic case.

The critical quantity of interest is the probability at time t that the system is within the range $0 \le x \le \infty$. This probability $N(t)$ is given by

$$N(t)=\int_0^\infty dx\,p(x,t\,|\,x_0)=\int_0^\infty du\,w(u,t\,|\,u_0)\ , \qquad (3.11)$$

where $p(x,t\,|\,x_0)$ is given by Eq. (3.6); and $w(u,t\,|\,u_0)$, with $u=x^{-1}$, is found from Eq. (3.6) to be

$$w(u,t\,|\,u_0)=\left[\frac{2\pi q}{\alpha}\,(e^{2\alpha t}-1)\right]^{-1/2}\exp\left\{-\frac{[u-u_0(t)]^2}{\left(\frac{2q}{\alpha}\right)(e^{2\alpha t}-1)}\right\}\ ,$$

where

$$u_0=\frac{1}{x_1}+\left(\frac{1}{x_0}-\frac{1}{x_1}\right)e^{\alpha t}\ .$$

Examination of the explicit expressions for $p(x,t\,|\,x_0)$, $0<x<\infty$ and $w(u,t\,|\,u_0)$, $0<u<\infty$, indicate the behavior to be expected from the quantity $N(t)$. In terms of the variable u, the probability distribution w and the flux $(\partial w/\partial u)$ is nonzero at $u=0$, but these quantities vanish at $u=\infty$. This means that the dynamics carries the system into the region $u<0$ but never into the neighborhood of $u=\infty$. It follows that in terms of the variable x, the flux vanishes at $x=0$ but is finite at $x=\infty$. Thus the dynamics carries the system beyond $x=\infty$, at which point we may refer to the system as having exploded. Similar conclusions about the behavior of the probabilities w and p and their associated fluxes at the extreme points zero and infinity can be reached by examining the Fokker–Planck equation which the probability distributions must satisfy.[2,15]

It should be noted that the behavior at $x=0$ can be anticipated from the model stochastic dynamical equation (3.1). Regardless of the sign or magnitude of the fluctuations, the system cannot reach the point $x=0$ because the random rate coefficients are multiplied by terms involving x which vanish as $x\to 0$. In contrast, stochastic differential equations of the Langevin form that involves the stochastic term as a linear forcing function, e.g., Eq. (3.2), can arrive at the origin.

This reasoning leads one to conclude that $N(t)$ gives the probability that the system has not exploded by time t, i.e., the fraction of the probability distribution $w[p]$ that initially was a delta function centered at $u_0[x_0]$ which has not yet vanished past the point $0[\infty]$.

An explicit expression for $N(t)$ may be obtained by substitution of Eq. (3.6) into Eq. (3.11). The result is

$$N(t)=\frac{1}{\sqrt{\pi}}\int_{-h(t)}^{\infty}dy\,e^{-y^2/2}\ , \qquad (3.12)$$

where

$$h(t)=\frac{1}{x_1}+\left(\frac{1}{x_0}-\frac{1}{x_1}\right)e^{\alpha t}\Big/\left[\frac{2q}{\alpha}\,(e^{2\alpha t}-1)\right]^{1/2}\ . \qquad (3.13)$$

All limits of interest may be extracted from this expression. For example, as $t\to\infty$,

$$h(t)\to h_\infty=\left[\left(\frac{1}{x_0}-\frac{1}{x_1}\right)\Big/\sqrt{2q/\alpha}\right] \qquad (3.14)$$

and $N(t)\to N_\infty$ with

$$N_\infty=\frac{1}{\sqrt{\pi}}\int_{-h_\infty}^{\infty}dy\,e^{-y^2/2}\ . \qquad (3.15)$$

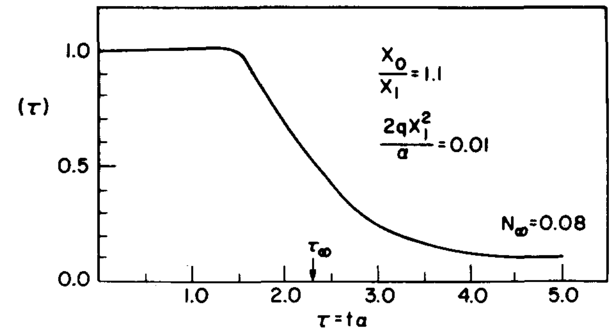

FIG. 1. Probability $N(\tau)$ that system has not exploded vs reduced time $\tau=\alpha t$ for initial condition $x_0=x_1/(0.9)$. Reduced fluctuation strength $2q\,x_1^2/\alpha=0.01$. See Eqs. (3.12) and (3.13).

If $x_0<x_1$, then $h_\infty>0$ and N_∞ lies between the limits $1\le N_\infty\le 1/2$. As $q\to 0$, the influence of fluctuations is negligible and $N_\infty\to 1$; the system does not explode, in agreement with the prediction of the deterministic equation. As $q\to\infty$, the fluctuations dominate and $N_\infty\to 1/2$ indicating that, at most, one-half the systems will explode from the stable region.

If $x_0>x_1$, then $h_\infty<0$ and N_∞ lies between the limits $1/2<N_\infty<0$. As $q\to 0$ the results of deterministic equations with explosive behavior are found; $N_\infty\to 0$. As $q\to\infty$, $N_\infty\to 1/2$ indicating that large fluctuations have, at most, a probability of 1/2 of preventing the system from exploding.

The specific value $N_\infty=1/2$ that is realized for large fluctuations is best understood from Eq. (3.5). For $q\to\infty$ the p.d.f. $w(u,t\,|\,u_0)$ is spread progressively more uniformly over the entire u axis. The fraction of the probability density which lies on the negative u axis is counted by us as "exploded." This fraction approaches (1/2) as $q\to\infty$. Evidently it is sensitive to our treatment of the boundary condition at $u=0$ $(x=\infty)$.

Figure 1 presents a plot of $N(t)$ vs time to illustrate the difference in the behavior of the deterministic explosive behavior $[q=0$, Eq. (1.2)] and the results of this model of fluctuations in rate coefficients. We have selected a case where the initial point x_0 lies in the unstable region, i.e., $x_0>x_1$. If fluctuations were not present $(q\to 0)$, we would find $N=1$ for $t<t_\infty$, and then an abrupt jump to $N=0$ for $t>t_\infty$. The curve exhibits the influence of fluctuations and the nonvanishing limit N_∞. For this model it is always true that $N(t_\infty)=1/2$.

IV. MODEL B–EQUAL FLUCTUATIONS

The second model we consider has equal fluctuations for both the first and second order terms. Thus we assume

$$\alpha(t)=\alpha[1+f(t)] \quad\text{and}\quad k(t)=k[1+f(t)] \qquad (4.1)$$

with $f(t)$ a Gaussian random variable as defined by Eq. (3.1). The rate equation (2.1) becomes

$$\frac{dx}{dt}=[1+f(t)][kx^2(t)-\alpha x(t)]\ . \qquad (4.2)$$

In this model, the effect of the fluctuation is simply to rescale the time. Thus if we let

$$\tau(t) = t + \int_0^t f(s)\, ds \tag{4.3}$$

and define $x[\tau] = x(t)$, one finds

$$\frac{dx[\tau]}{d\tau} = kx^2[\tau] - \alpha x[\tau] \tag{4.4}$$

which is precisely the deterministic equation except that τ varies over the entire range $-\infty < \tau < +\infty$. Thus one finds

$$\left[\frac{1}{x[\tau]} - \frac{1}{x_1}\right] = \left[\frac{1}{x_0} - \frac{1}{x_1}\right] \exp(\alpha\tau) \tag{4.5}$$

or, in terms of the real time t,

$$\left[\frac{1}{x(t)} - \frac{1}{x_1}\right] = \left[\frac{1}{x_0} - \frac{1}{x_1}\right] \exp\left\{\alpha\left[t + \int_0^t f(s)\, ds\right]\right\} . \tag{4.6}$$

Regardless of the behavior of the fluctuations, the region where x decays $0 < x(t) < x_1$, and the region where x explodes $x(t) > x_1$ will not be connected. This follows immediately by noting that the exponential factor is nonnegative and does not change sign regardless of events in its argument. Thus if x_0 is greater (less) than x_1, it follows that $x(t)$ will be greater (less) than x_1 for all time.

An exact expression can be found for the probability density, provided $f(t)$ is Gaussian. The substitution (3.3) leads to

$$\frac{dy(t)}{dt} = \alpha[1 + f(t)]y(t) \tag{4.7}$$

and

$$y(t) = y_0 \exp\left\{\alpha\left[t + \int_0^t f(s)\, ds\right]\right\} . \tag{4.8}$$

If $y_0 > 0$ then $y(t)$ will be nonnegative so we can make the substitution $z(t) = \ln y(t)$ with

$$\frac{d}{dt}[z(t) - \alpha t] = \alpha f(t) . \tag{4.9}$$

Application of Chandrasekhar's lemma[15] leads to the result

$$p(z, t \mid z_0) = [4\pi q\alpha^2 t]^{-1/2} \exp\left\{-\frac{[z - z_0 - \alpha t]^2}{4q\alpha^2 t}\right\} , \tag{4.10}$$

or in terms of the variable of interest x,

$$p(x, t \mid x_0) = [4\pi q\alpha^2 t]^{-1/2} \exp\left\{-\frac{\left[\ln\left[\left(\frac{x_1 - x}{x_1 - x_0}\right)\frac{x_0}{x_1}\right] - \alpha t\right]^2}{4q\alpha^2 t}\right\} \times \frac{x_1}{x(x_1 - x)} \qquad 0 < x < x_1 . \tag{4.11}$$

On the other hand, if $y_0 < 0$, we set $z(t) = \ln[-y(t)]$ and obtain by a precisely similar argument

$$p(x, t \mid x_0) = [4\pi q\alpha^2 t]^{-1/2} \exp -\frac{\left[\ln\left[\left(\frac{x - x_1}{x_0 - x_1}\right)\left(\frac{x_0}{x_1}\right)\right] - \alpha t\right]^2}{4q\alpha^2 t} \times \frac{x_1}{x(x - x_1)} . \tag{4.12}$$

Thus we have been able to obtain an exact expression for the probability distribution for model B when there are Gaussian fluctuations. For model B, in contrast to model A, we find that fluctuations do not influence the transition. If the system has an initial value in the interval $0 < x_0 < x_1$, it will remain in that interval and never exhibit explosive behavior. The parameter x_1 remains a discrete boundary between decaying and explosive behavior. However, the fluctuations do influence the time to probable explosion when the system is initially in the explosive region $x_0 > x_1$.

V. MODEL C—LINEAR FLUCTUATIONS

The third model we consider contains fluctuations in the linear term $\alpha(t) = \alpha[1 + f(t)]$ in Eq. (2.1), with $f(t)$ a Gaussian random variable, and a constant second order term. The resulting rate equation is

$$\frac{dx}{dt} = kx^2 - \alpha[1 + f(t)]x . \tag{5.1}$$

We define the propagator $Q(t)$ as a solution to the stochastic equation

$$\frac{dQ(t)}{dt} = -\alpha[1 + f(t)]Q(t) , \qquad Q(0) = Q_0 = 1 \tag{5.2}$$

a special case of model B, Eqs. (4.7) and (4.8). This equation has the solution

$$Q(t) = \exp\left[-\alpha t - \alpha \int_0^t f(s)\, ds\right] . \tag{5.3}$$

In terms of this propagator the solution for $x(t)$ becomes

$$x(t) = Q(t)\left[\frac{1}{x_0} - k\int_0^t Q(\tau)\, d\tau\right]^{-1}$$

$$= \left[\frac{Q^{-1}(t)}{x_0} - k\int_0^t Q^{-1}(\tau)\, d\tau\right]^{-1} . \tag{5.4}$$

In contrast to the treatment of models A and B, we are unable to find an exact solution for the probability distribution of $x(t)$. The reason for this difficulty is that the random propagator in the expression for $x(t)$ enters in a nonlinear manner and involves values of Q at different times. Accordingly we must resort to an approximation.

The approximation we introduce[16] consists of replacing $Q(\tau)$ in the denominator of $x(t)$ [Eq. (5.4)], by its average value $\overline{Q(\tau)}^{Q_0}$. Thus

$$x(t) \simeq Q(t)\left[\frac{1}{x_0} - k\int_0^t \overline{Q(\tau)}^{Q_0}\, d\tau\right]^{-1} . \tag{5.5}$$

For a Gaussian random variable the average value of Q may be easily determined:

$$\overline{Q(t)}^{Q_0} = e^{-\alpha t} \exp\left[\frac{\alpha^2}{2}\int_0^t \int_0^t d\tau_1\, d\tau_2 \overline{f(\tau_1)f(\tau_2)}^{Q_0}\right] . \tag{5.6}$$

In the simple case of a delta-function correlation in the random fluxes [Eq. (3.1)] one finds

$$\overline{Q(t)}^{Q_0} = \exp[-(\alpha - \alpha^2 q)t] . \tag{5.7}$$

The possibility of more complex correlation functions may also be explored, e.g., an exponential form in place of the delta function in Eq. (3.1).

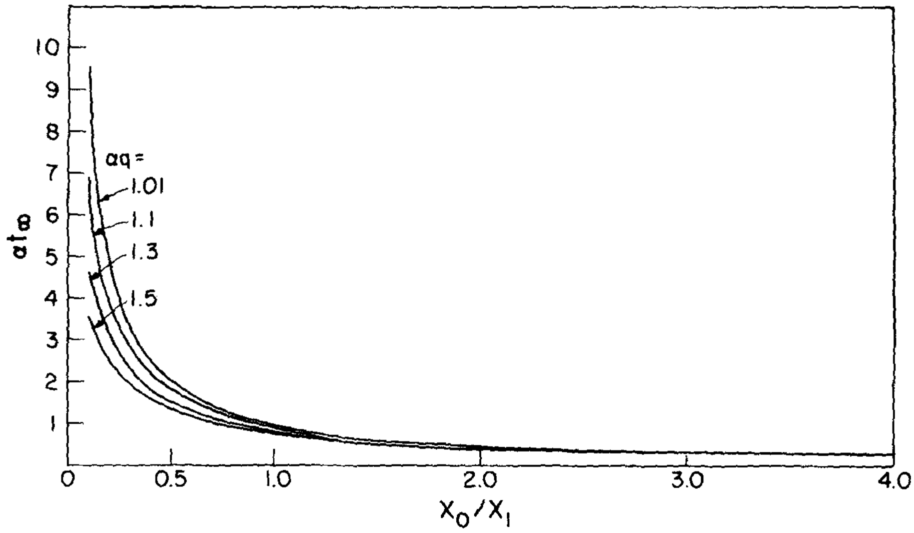

FIG. 2. Reduced explosion time (αt_∞) vs initial position for various values of the strength of large fluctuations (αq) < 1 according to Eq. (5.9).

With this approximation and the result [Eq. (5.7)] one obtains the following result for $\overline{x(t)}^{x_0}$:

$$\overline{x(t)}^{x_0}=\frac{x_0\exp[-(\alpha-\alpha^2 q)t]}{\left\{1-\frac{x_0}{x_1}\frac{1}{(1-\alpha q)}\{1-\exp[-(\alpha-\alpha^2 q)t]\}\right\}} . \tag{5.8}$$

For *large* amplitude fluctuations $(q\alpha>1)$, $\overline{x(t)}^{x_0}\to\infty$ for long times for all values of the initial value x_0 excluding the case $x_0=0$. The finite explosion time t_∞ is found from Eq. (5.8) to be

$$t_\infty=\frac{1}{\alpha(\alpha q-1)}\ln\left[1+\frac{x_1}{x_0}(\alpha q-1)\right] . \tag{5.9}$$

For these large fluctuations the system is always driven to explode regardless of whether the initial condition was in the stable $(x_0<x_1)$ or unstable $(x_0>x_1)$ region. This behavior is shown in Fig. 2.

For *small* amplitude fluctuations $(q\alpha)<1$, the long time behavior of $\overline{x(t)}^{x_0}$ depends upon the magnitude of the initial condition. For $(x_0/x_1)<(1-\alpha q)<1$, the system begins in the stable region and the strength of the fluctuations is insufficient to cause an explosion. For $(x_0/x_1)>(1-\alpha q)$ the system will explode in a finite time given by

$$t_\infty=\frac{1}{\alpha(\alpha q-1)}\ln\left[1-\frac{x_1}{x_0}(1-\alpha q)\right] \quad (\alpha q<1) . \tag{5.10}$$

Thus the strength of the fluctuations, measured by αq, has effectively lowered the unstable fixed point of the system from x_1 to $x_1(1-\alpha q)$. Furthermore, comparison of this expression with Eq. (1.4) demonstrates that an additional effect of the fluctuations, if the system is initially in the unstable regime $(x_0>x_1)$, is to decrease the time to divergence as illustrated in Fig. 3.

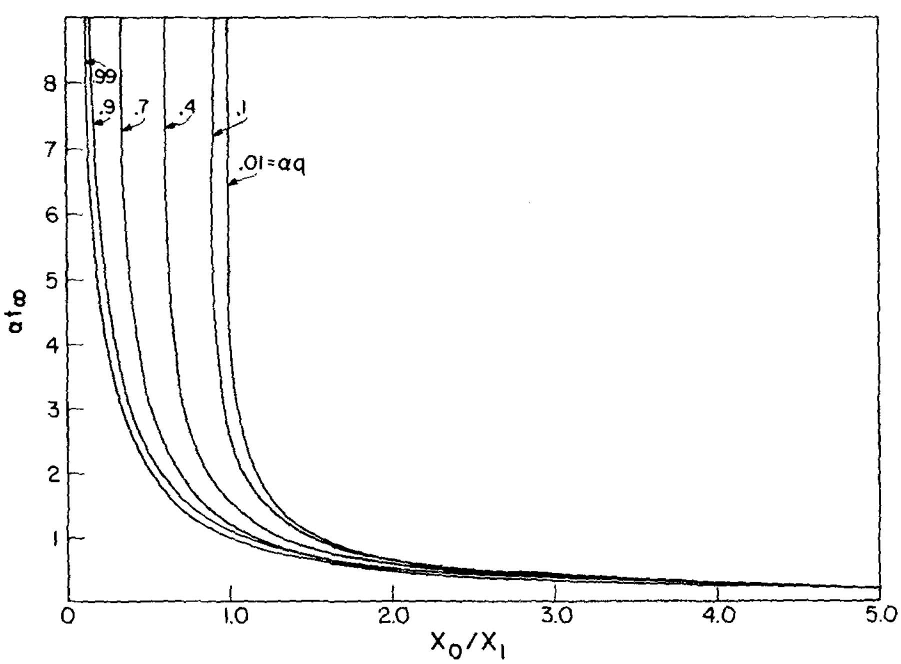

FIG. 3. Reduced explosion time (αt_∞) vs initial position for various value of the strength of small fluctuations (αq) < 1 according to Eq. (5.10).

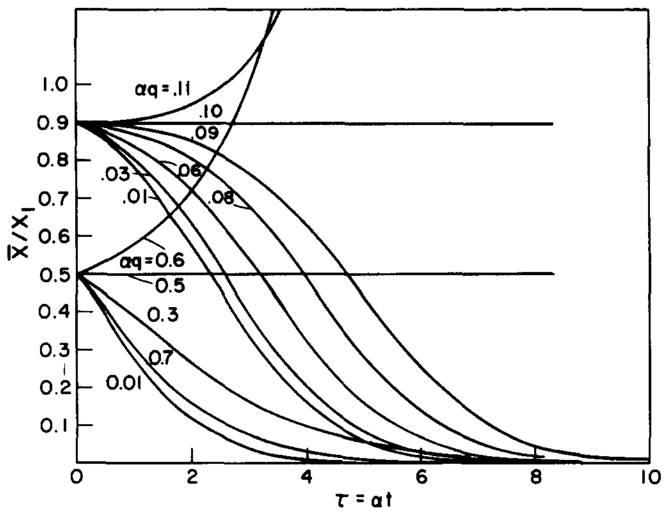

FIG. 4. Average concentration $\overline{x(t)}^{x_0}$ vs reduced time αt for initial conditions $x_0 = 0.9$ and 0.5 for various values of the reduced strength of fluctuations $\alpha q < 1$. See Eq. (5.8).

Finally we note that a consequence of this new fixed point is that if the system begins exactly at the special point $x_0 = x_1(1-\alpha q)$ then $\overline{x(t)}^{x_0} = x_0$ for all succeeding time.

Figure 4 illustrates the behavior in model C for two initial conditions $x_0 = 0.5x_1$ and $x_0 = 0.9x_1$ for various values of $\alpha q < 1$. For example, note the behavior for $x_0 = 0.5x_1$: For values of $\alpha q < 0.5$, $x(t)$ decays, while for values of $\alpha q > 0.5$, the system explodes; it remains constant if $\alpha q = \frac{1}{2}$.

In summary, for this model system with the approximation introduced in Eq. (5.5) we find that the behavior of the first moment with fluctuations Eq. (5.8) is identical to the behavior of the deterministic system (1.3) with the identification of a new linear rate α_{eff},

$$\alpha_{\text{eff}} = \alpha(1-\alpha q) . \qquad (5.11)$$

The behavior of the first moment is described by an effective nonlinear kinetic equation

$$\frac{dx}{dt} = kx^2 - \alpha_{\text{eff}} x \qquad (5.12)$$

which exhibits a shifted fixed point if $(\alpha q) < 1$ given by

$$x_{1\,\text{eff}} = (\alpha_{\text{eff}}/k) = (\alpha/k)(1-\alpha q) . \qquad (5.13)$$

VI. BERNOULLI EQUATIONS OF HIGHER DEGREE

We point out that the method we have introduced may be applied to the general Bernoulli equation

$$\dot{x} = -\alpha x + kx^n , \quad n > 1 . \qquad (6.1)$$

The substitution

$$u = x^{-(n-1)} \qquad (6.2)$$

leads to the equation

$$(n-1)^{-1}\dot{u} = \alpha u - k \qquad (6.3)$$

which should be compared to Eq. (2.2). For models A and B one immediately obtains results identical to Eqs. (3.5) and (5.10) with the rescaling

$$t \to (n-1)t \quad \text{and} \quad q \to (n-1)q . \qquad (6.4)$$

For model C an additional modification of the approximation introduced in Sec. V is required if one wishes to determine $\overline{X(t)}^{x_0}$ for the case $n > 2$.

VII. CONCLUDING REMARKS

In this paper we have explored how fluctuations can modify the deterministic dynamics of a system that can exhibit explosive behavior. The simple model we have examined illustrates several distinct effects of fluctuations. Indeed, according to the mechanisms of the fluctuations one finds either no effect on the stability (model B), a broadening of the deterministic result (model A), or a shift in the transition point between stable and unstable behavior (model C). In two cases, models A and B, we have found it possible to determine exact expressions for the probability distribution of the system trajectory.

The main limitation of this work is the unphysical nature of the reaction mechanism and the resulting kinetic equation. Future work will focus on more realistic reaction mechanisms that may exhibit explosive behavior locally, e.g., the "Brusselator,"[17] and on the coupling of chemical reactions with heat evolution.[18]

Finally, it should be noted that the central dynamical equation under study may also be employed as a model for barrier crossing. From this viewpoint the equation of motion for a particle of mass m, moving in an effective one-dimensional potential $v[x(t)]$ subject to linear dissipation is

$$m\ddot{x} = -\gamma\dot{x} - \frac{\partial V}{\partial x} . \qquad (7.1)$$

The overdamped limit $(m \to 0)$ with choice of potential

$$V(x) = \gamma^{-1}\left[\frac{\alpha}{2}x^2 - \frac{k}{3}x^3\right] \qquad (7.2)$$

corresponds precisely to Eq. (1.2) with the restriction that the particle remains on the positive x axis. Thus our considerations apply with appropriate modification to the influence of fluctuations on barrier crossing; in this case the potential barrier has a maximum at $x = \alpha/k$ and crosses the x axis at $x = (\frac{3}{2}\alpha/k)$ proceeding toward $(-\infty)$. The situation we have examined differs from the usual case of fluctuations arising from a linear inhomogeneous random force added to the right-hand side of Eq. (1.2). Here we have been concerned with fluctuations in the parameters that characterize the effective potential.

The method of recursive functions introduced by Feigenbaum[19] to describe nonlinear dynamic system perhaps may be usefully applied to the problem of explosive behavior. However we note that the description of the dynamical flows[20] in these nonlinear, usually dissipative systems, normally involve transitions between locally stable steady states.

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[16]An alternative and easily calculable approximation $\overline{x(t)}^{x_0} \sim [\overline{x(t)^{-1}}^{X_0}]^{-1}$ has been rejected. This approximation is a lower limit on $\overline{x(t)}^{x_0}$ and leads to an elevated effective unstable fixed point and an unphysical increase in the stability of the system. This unpleasant result is a consequence of the Gaussian approximation which does not preserve the unitarity of $Q(t)$, i.e., $Q(t)Q^{-1}(t)=1$, but $\overline{Q(t)}^{Q_0} \cdot \overline{Q(t)^{-1}}^{Q_0} \neq 1$.

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