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TW 247/83 NOVEMBER

J.V. LANKELMA

STOCHASTIC DYNAMICAL SYSTEMS WITH A CYCLIC STRUCTURE

Preprint

kruislaan 413 1098 SJ amsterdam

Printed at the Mathematical Centre, Kruislaan 413, Amsterdam, The Netherlands.

The Mathematical Centre, founded 11 February 1946, is a non-profit institution for the promotion of pure and applied mathematics and computer science. It is sponsored by the Netherlands Government through the Netherlands Organization for the Advancement of Pure Research (Z.W.O.).

1980 Mathematical subject classification: 35A40, 35B40, 35R60

Stochastic dynamical systems with a cyclic structure *)

by

J.V. Lankelma

ABSTRACT

This paper deals with a stochastic version of the "hypercycle", introduced by Eigen and Schuster. The "cycle" is a dynamical system with a simple cyclic structure. After conversion to a set of stochastic differential equations, Kolmogorov's exit problem is asymptotically solved with the WKB-method.

KEY WORDS & PHRASES: *random perturbations, Fokker Planck equation, exit problems, WKB approximation, hypercycle*

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*) This report will be submitted for publication elsewhere.

1. INTRODUCTION

In this report the hypercycle, a particular kind of dynamical system is considered. The hypercycle of Eigen and Schuster [3,13] is introduced in theoretical molecular evolution theory as a fundamental process, explaining the phenomenon of selforganization as it occurs in prebiotic evolution. The most important feature is the cyclic structure of the equations. In n dimensions we have the following situation:

$$\frac{dx_i}{dt} = b_i(x) \qquad i = 1,n. \tag{1.1}$$

with $b_i(x)$ principally dependent on x_i and x_{i-1}, counting indices modulo n. For each n there is a ω limit set in the positive octant of $\mathbb{R}^n$. For $n \leq 4$ there is an (asymptotically) stable fixed point, for $n \geq 5$ there is (probably) a limit cycle. The last fact has not been proven, but seems almost certain from the large amount of numerical evidence.

Many processes in nature are intrinsically stochastic rather than deterministic, so it seems natural to consider the equations with an extra stochastic component of arbitrarily small covariance ($O(\varepsilon^2)$). For the stochastic equations no stability concept exists and instead we must solve the exit problems as stated by Kolmogorov, in order to determine the persistence of the system under small random perturbations.

An elegant method to solve these problems is due to Matkowsky and Schuss [12]. Formal adjoint equations are solved asymptotically and combined with the original equations. This work is a generalization of earlier results of Grasman and Matkowsky [7] on self adjoint operators. In this report the method in [12] is worked out numerically in a three dimensional problem, which brings about considerable complications compared with two dimensional systems, e.g. Bobrovsky and Schuss [1]. Asymptotic expressions for the adjoint equations are obtained with the WKB-method. This method has its limitations in this problem, since there are points at the boundary where the deterministic vector field (1.1) vanishes. A small neighbourhood of these points has to be excluded in the WKB-approximation. Moreover, as a numerical process the method is rather time consuming, even for the three components.

In section 2 we deal with the model equations. For the dynamical system with a small stochastic perturbation the corresponding Fokker-Planck and backward Kolmogorov equation are formulated. The dynamics of the deterministic hypercycle are described in more detail.

In section 3 the asymptotic approximation of the expected exit time for the attraction domain of a stable point is given. The WKB-Ansatz for the adjoint equation requires a detailed analysis of the eikonal equation at the stable point. This is done in 3.2b. The solution of this equation with the ray method is treated in 3.2c and 3.2d. In 3.3 the method is applied to the cycle with three components. Since the boundary contains singular points, the solution of the adjoint equation will have its largest values on the boundary near these points. However, the WKB-approximation breaks down at such (turning) points. Consequently, the asymptotic method does not hold for $\varepsilon \downarrow 0$, since this limit shifts the maximal boundary value of the solution of the adjoint equation into a singular point.

In section 4 randomly perturbed hypercycles are analyzed by solving stochastic difference equations. Exit times from simulations are compared with the asymptotic expressions of section 3. In first order approximation they agree quite well.

Acknowledgement. The author is indebted to J. Grasman for many stimulating discussions during the preparation of this report.

2. FORMULATION OF THE EQUATIONS

2.1. Model equations for the exitproblem

Let D be an open bounded domain in the positive octant of Euclidean space $\mathbb{R}^n$ with a smooth boundary ∂D. The dynamical system (2.1), with $b(x)$ a smooth vector field in $\mathbb{R}^n$ has by assumption a unique stable fixed point Z in D,

$$\frac{dx}{dt} = b(x). \tag{2.1}$$

On the smooth boundary ∂D the vectorfield is tangential or pointing inside. Writing the outward normal as $\nu(x)$ we have on the boundary

$$(2.2) \qquad b(x).\nu(x) \leq 0.$$

In the deterministic system (2.1) all trajectories not contained in the boundary will approach Z for increasing time t. When the deterministic system (2.1) is replaced by a set of stochastic differential equations with a given arbitrarily small covariance the stability property is lost. The system will leave any bounded domain containing Z in finite time with probability one. Adding a vector $W(t) = (W_1(t),\ldots,W_n(t))^T$ where $W_i(t)$ are n independent Brownian motions, formally gives the Ito equation

$$(2.3) \qquad dX_i(t) = b_i(X)dt + \varepsilon\Sigma_j\sigma_{ij}(X)dW_j(t), \quad i = 1,n, \quad \varepsilon > 0.$$

The symmetric diffusion tensor σ_{ij} joins the j^{th} component of stochastic process W(t) with the i^{th} component of stochastic process X(t). For each component of W(t) the following holds,

$$(2.4) \qquad EW_i(t) = 0, \quad EW_i(t)W_i(s) = \min(t,s).$$

Brownian motion W(t) corresponds to the standard Gaussian white noise $\xi(t)$ denoted as distributional derivative

$$(2.5) \qquad \xi(t) = \dot{W}(t), \quad E\xi(t) = 0 \quad E\xi(t)\xi(s) = \delta(t-s).$$

This results in the infinitesimal displacement dX in (2.3) being normally distributed with expectation b(X)dt and covariance $\varepsilon^2 A(X)dt$, where $A = (a_{ij}) = (\sigma\sigma^T)_{ij}$ is non negative matrix. In the sequel A is assumed to be positive and independent of X. The elements of A and b(X) can be used to define a differential operator L_ε,

$$(2.6) \qquad L_\varepsilon = \tfrac{1}{2}\varepsilon^2 \sum_{ij} a_{ij} \frac{\partial^2}{\partial x_i \partial x_i} + \Sigma_i b_i \frac{b}{\partial x_i} .$$

The Fokker-Planck and backward Kolmogorov equation associated with the

stochastic differential equation (2.3) are

$$\frac{\partial v}{\partial t} + L_\varepsilon^* v = 0 \tag{2.7}$$

$$\frac{\partial u}{\partial t} - L_\varepsilon u = 0 \tag{2.8}$$

where L_ε^* is the formal adjoint of L_ε. The exit problem as formulated by Kolmogorov is split in two parts. In the first place the (asymptotic) expression for the exit time, which is defined as the minimal time $\tau_\varepsilon(x)$ needed to reach the boundary from a given point x in D in stochastic process X(t);

$$\tau_\varepsilon(x) = \inf(t \mid X(t) \in \partial D,\ X(0) = x). \tag{2.9}$$

It is well known that the expected exit time may be obtained by the solution of a Dirichlet boundary value problem (Schuss [12]). The boundary value problem with natural boundary conditions is

$$\begin{aligned} L_\varepsilon u(x) &= -1 \quad x \in D \\ u(x) &= 0 \quad x \in \partial D. \end{aligned} \tag{2.10}$$

For each positive ε the solution $u_\varepsilon(x) = E\tau_\varepsilon(x)$ is bounded so exit will occur from domain D with probability one.

The second part of Kolmogorov's problem is the (asymptotic) distribution of exit points on the boundary. Let f(x) be the characteristic function of a measurable set in the boundary. The probability that exit will occur through the section of ∂D given by f(x) is calculated by solving the boundary value problem

$$\begin{aligned} L_\varepsilon v(x) &= 0 \quad x \in D \\ v(x) &= f(x) \quad x \in \partial D. \end{aligned} \tag{2.11}$$

The solution of this problem is related to the transition probability density function $p_\varepsilon(x,y,t)$ of process X(t), which is defined as the

fundamental solution of (2.12)-(2.14)

$$(2.12) \qquad L_\varepsilon p_\varepsilon = \frac{\partial p_\varepsilon}{\partial t} \qquad x \in D, \quad t > 0$$

$$(2.13) \qquad p_\varepsilon \to \delta(x-y) \qquad x \in D, \quad t \downarrow 0$$

$$(2.14) \qquad p_\varepsilon = 0 \qquad x \in \partial D.$$

The transition probability p_ε defines a density function $q_\varepsilon(x,y)$ on the boundary as follows

$$(2.15) \qquad q_\varepsilon(x,y)dS(y) = \Pr(X(\tau_\varepsilon) \in dS(y) \mid X(0) = x)$$

with $dS(y)$ a surface element of the boundary. Using the density $q_\varepsilon(x,y)$ the solution of (2.11) is given by the expectation of $f(x)$

$$(2.16) \qquad v(x) = E_x f(X(\tau_\varepsilon)) = \int_{\partial D} f(y) q_\varepsilon(x,y) dS(y).$$

It is well known that the exit time is asymptotically given by the reciprocal value of the smallest positive eigenvalue λ_1^ε of the system (2.12)-(2.14). (Friedman [5], Ventsel-Freidlin [14]). This eigenvalue is exponentially small in ε,

$$(2.17) \qquad E\tau_\varepsilon(Z) \sim 1/\lambda_1^\varepsilon \sim W_\varepsilon e^{Q/\varepsilon^2}$$

for certain positive constants W_ε and Q.

2.2. An example: the hypercycle

The molecular evolution theory of Eigen and Schuster is based on the dynamics of systems of coupled nonlinear differential equations. In references [3,13] some interesting sets of equations have been introduced. One of these systems, the so called hypercycle has been chosen as a model for analysis of the influence of stochastic variations. The deterministic equations of the hypercycle in n dimensions are

$$(2.18)\qquad \frac{dx_i}{dt} = b_i(x) = x_i(k_i x_{i-1} - \sum_{j=1}^{n} k_j x_j x_{j-1}) \qquad i = 1,n.$$

The reaction sequence is closed through the counting of indices modulo n. The constants k_i, i = 1,n represent positive reaction rates. When small stochastic perturbations are added to this dynamical system the long term behaviour is completely altered. This will be investigated in the coming sections. Domain D is an open bounded set with smooth boundary ∂D in the positive octant of Euclidean space $\mathbb{R}^n$, which contains all possible ω-limit points in this octant. There is only one fixed point (Z) inside D, with coordinates

$$(2.19)\qquad Z = (z_i) = (1/k_{i+1}/\textstyle\sum_j 1/k_j).$$

Using the variable $c = \Sigma_i x_i$ and adding equations (2.18) gives

$$(2.20)\qquad \frac{dc}{dt} = (1-c) \sum_j k_j x_j x_{j-1}.$$

This shows that the hyperplane c = 1 is attracting. The vector field b(x) vanishes at each coordinate axis. The intersection of the j-th coordinate axis with the hyperplane c = 1 is indicated by X_j. As an example the case n = 3 is illustrated in figure 1.

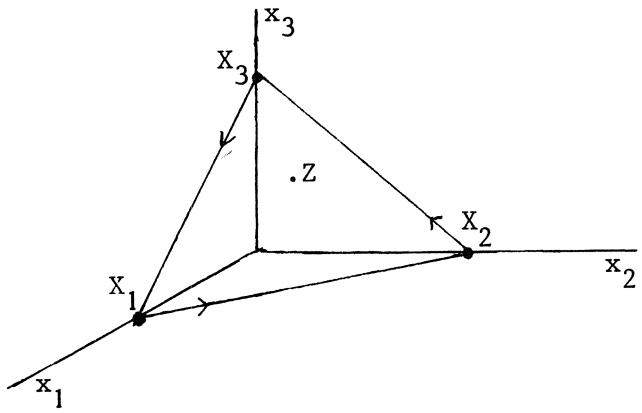


Figure 1. Fixed points in the three dimensional case

The eigenvalues of the Jacobian of b(x) in Z are $\{-1,-\frac{1}{2}\pm\frac{1}{2}i\sqrt{3}\}$, each multiplied by $(\Sigma_j 1/k_j)^{-1}$, so Z is attracting. The eigenvalues in X_i are $\{0,0,k_{i+1}\}$ again counting indices modulo n. The eigenvector associated with the non zero eigenvalue is contained in the hyperplane c = 1 and the plane $x_{i-1} = 0$ (see figure 1). When the flow is restricted to the boundary (planes $x_i = 0$, i = 1,2,3) the points X_1, X_2, X_3 appear to be "saddle" points. For example, in the coordinate plane $x_2 = 0$ consider the function

$$U(x_1,x_3) = (1-x_1)^2 + x_3^2. \tag{2.21}$$

Then

$$\frac{dU}{dt} = -2k_1x_1x_3U(x_1,x_3) \leq 0. \tag{2.22}$$

Consequently U is a Lyapunov function for the flow in the plane $x_2 = 0$, $x_1,x_3 > 0$ and X_1 is in this sense a stable equilibrium. The system (2.18) is structurally unstable since there are many zero eigenvalues.

In our study of the asymptotics of exit problems we deal with one specific example, the cycle with three components, k = (1,3,5) and $\sigma_{ij} = \delta_{ij}$. In the simulations the cycles with two and five components are also treated. In the first case there is a unique attracting fixed point in D, in the second case the fixed point Z with coordinates given by (2.19) is unstable since for all values of $n \geq 5$ the central fixed point Z is a saddle. Schuster et al. [3,13] give numerical evidence for the existence of a limit cycle when $n \geq 5$, for any choice of reaction constants in (2.18). This limit cycle comes near the boundary when the reaction constants are of different order of magnitude.

3. ASYMPTOTIC SOLUTION OF THE EXIT PROBLEM

3.1. Solution with the adjoint equation

In this section we describe some general results obtained by Matkowsky and Schuss [12] for exit problems. The Kolmogorov equation with boundary values

$$
\begin{aligned}
&L_\varepsilon \phi = 0 \qquad x \text{ in } D \\
&\phi(x) = f(x) \quad x \in \partial D
\end{aligned}
\tag{3.1}
$$

is solved in combination with a solution ψ of the homogeneous adjoint Fokker Planck equation, suitably normalized in equilibrium Z.

$$
\begin{aligned}
&L_\varepsilon^* \psi = 0 \quad \text{in } D \\
&\psi(Z) = 1.
\end{aligned}
\tag{3.2}
$$

Accordingly the integral (3.3) vanishes over domain D

$$
\int_D \psi L_\varepsilon \phi - \phi L_\varepsilon^* \psi \, d\sigma = 0. \tag{3.3}
$$

With Gauss' divergence theorem this integral can be written as

$$
\int_{\partial D} \tfrac{1}{2}\varepsilon^2 \left(\psi \frac{\partial \phi}{\partial n} - \phi \frac{\partial \psi}{\partial n}\right) + \psi \phi b.\nu - \varepsilon^2 \psi \phi \frac{\partial a_{ij}}{\partial \nu_i} \, d\sigma = 0 \tag{3.4}
$$

where $\nu(x)$ is the outward normal on the smooth boundary and $\frac{\partial}{\partial n}$ is the conormal derivative $\Sigma_{ij}\, a_{ij} \nu_i \frac{\partial}{\partial x_j}$. For $\varepsilon \downarrow 0$ the solution $\phi(x)$ of the backward equation (3.1) must have a constant value in D outside a small neighbourhood of the boundary; $\phi(x)$ is constant on the characteristics of the lower order operator, which intersect in Z;

$$
\frac{d\phi}{dt} = \Sigma_i b_i \frac{\partial \phi}{\partial x_i} = 0. \tag{3.5}
$$

The constant value of $\phi(x)$ inside domain D is called C_0. At the boundary ∂D there exist two kinds of boundary layers

a. At ∂D_p where $b.\nu(x) = 0$ a parabolic layer,

b. At ∂D_0 where $b.\nu(x) < 0$ an ordinary layer.

To start with the parabolic case, $\phi(x)$ is in the layer approximated by

$$
\tilde{\phi}(x_r, x_t) = f(x_t) + \frac{c_0 - f(x_t)}{\varepsilon} \cdot \sqrt{\frac{2}{\pi}} \int_0^{s(x_r, x_t)} e^{-s^2/2\varepsilon^2} ds \tag{3.6}
$$

with radial coordinate x_r, x_t indicating the set of two tangential coordinates and $s(x_r,x_t)$ to be determined. Since $s = 0$ on the boundary all tangential derivatives are zero on the boundary. With the form (3.6) substituted in (3.1) and retaining only leading terms we obtain

$$(3.7) \qquad \frac{1}{2}\sum_{ij} a_{ij}\frac{\partial s}{\partial x_i}\frac{\partial s}{\partial x_j}s - \sum_i b_i \frac{\partial s}{\partial x_i} = 0.$$

With the assumption that in the boundary layer all tangential derivatives of s are much smaller than the normal derivative, equation (3.7) reduces to

$$(3.8) \qquad \frac{1}{2}\, a_{rr}\left(\frac{\partial s}{\partial x_r}\right)^2 s = b_r(x_r,x_t)\frac{\partial s}{\partial x_r}.$$

The non trivial solution of this equation is

$$(3.9) \qquad s(x_r,x_t) = \frac{2}{\sqrt{a_{rr}}}\left(\int_0^{x_r} b_r(y,x_t)dy\right)^{\frac{1}{2}}.$$

The expression (3.9) used as argument in the error function (3.6) satisfies all conditions. The only property that is needed from $\tilde{\phi}(x)$ is its normal derivative on the boundary. Consequently $b_r(x_r,x_t)$ is written as a linear expression in x_r; $b_r(x_r,x_t) = x_r c_r(x_t)$. The required normal derivative is

$$(3.10) \qquad \left(\frac{\partial\tilde{\phi}}{\partial x_r}\right)(x_t) = \frac{c_0 - f(x)}{\varepsilon}\,\frac{2}{\sqrt{\pi}}\sqrt{\frac{c_r(x_t)}{a_{rr}}}.$$

On the boundary ∂D_0, with $b(x)$ pointing inside domain D there is an ordinary boundary layer. With well known methods the radial derivative on this boundary is computed;

$$(3.11) \qquad \left(\frac{\partial\phi}{\partial x_r}\right)(x_t) = \frac{c_0 - f(x_t)}{\varepsilon^2}\,(b.\nu)(x_t).$$

Together with the asymptotic expansions for $\psi(x)$, to be derived in section 3.2, the radial derivatives of $\phi(x)$ determine the constant $c_0(\varepsilon)$ and implicitly the asymptotic expansion for the distribution of exit points on the boundary, since $c_0(\varepsilon)$ is the only unknown in formula (3.4).

The problem of exit time (2.10) can be treated in the same way.

$$(3.12)\qquad \begin{aligned} L_\varepsilon u &= -1 \quad \text{in } D \\ u &= 0 \quad \text{on } \partial D \end{aligned} .$$

According to the maximum principle the solution u grows very fast, so u is scaled as follows

$$(3.13)\qquad u(x) = e^{K/\varepsilon^2} c_1(\varepsilon) v(x)$$

with unknown constants K and $c_1(\varepsilon)$. The function v(x) is 0(1) in ε and satisfies the boundary condition v = 0. It appears that the same approximation with boundary layers can be applied. As in the previous case tangential derivatives of v are neglected in the normal derivative;

$$\frac{\partial v}{\partial n} = \sum_{ij} a_{ij} \nu_i \frac{\partial v}{\partial x_j} \simeq \frac{a_{rr}}{\varepsilon\sqrt{\pi}} \sqrt{\frac{c_r(x_t)}{a_{rr}}} = \frac{1}{\varepsilon\sqrt{\pi}} \sqrt{c_r(x_t) a_{rr}}.$$

After some calculations the constant $c_1(\varepsilon)$ is evaluated

$$(3.14)\qquad c_1(\varepsilon) = \frac{\int_D \psi \, d\sigma}{\frac{c}{\sqrt{\pi}} \int_{\partial D_p} \psi e^{K/\varepsilon^2} \sqrt{c_r a_{rr}} \, d\sigma - \frac{1}{2} \int_{\partial D_0} \psi e^{K/\varepsilon^2} \sqrt{a_{rr}} b \cdot \nu d\sigma} .$$

When the asymptotic expansion for the forward solution $\psi_\varepsilon(x)$ has been obtained, the constants $c_1(\varepsilon)$ and K can be evaluated.

3.2. WKB-Ansatz for the adjoint equation

3.2a The eikonal and transport equations in three dimensions

In this section a stationary asymptotic solution will be constructed for the Fokker Planck equation. In the WKB-method the solution is assumed to be in the form (Cohen and Lewis [2], Maslow [10])

$$(3.15)\qquad \psi_\varepsilon(x) \sim \exp\left(\frac{1}{\varepsilon^2} \sum_{m=0}^{\infty} \varepsilon^{2m} S_m(x)\right).$$

The expansion truncated after two terms is also known as physical optics approximation. This approximation will be used, it is denoted by

$$(3.16) \qquad \psi_\varepsilon(x) = w(x)e^{-Q(x)/\varepsilon^2}.$$

The physical optics approximation cannot be used when the fixed point is not attracting. For example the case of a saddle is treated by Mangel and Ludwig [9]. They approximate the solution with error functions in analogy with diffraction theory. In our application such points occur at the boundary of the domain of attraction and are, together with a small neighbourhood deleted from domain D. Substitution of (3.16) in the forward equation and sorting terms in powers of ε gives

$$(3.17) \qquad \frac{1}{2}\sum_{ij} a_{ij}\frac{\partial Q}{\partial x_i}\frac{\partial Q}{\partial x_j} + \Sigma_i\, b_i\frac{\partial Q}{\partial x_i} = 0$$

an eikonal or Hamilton-Jacobi equation. The second term gives a transport equation for the function w(x), which contains first and second derivatives of Q(x)

$$(3.18) \qquad \sum_{ij}(a_{ij}\frac{\partial Q}{\partial x_j} + b_i)\frac{\partial w}{\partial x_i} + (\frac{1}{2}\sum_{ij} a_{ij}\frac{\partial^2 Q}{\partial x_i \partial x_j} + \operatorname{div} b(x))w = 0.$$

Since the equations contain only derivatives of Q(x) and the vector field is smooth in D, Q(x) is fixed by prescribing the value at x = Z, where the characteristics intersect.

3.2b Local analysis near the equilibrium

For numerical integration of equations with the ray method, sufficiently accurate local approximations near Z of Q(x) and w(x) are needed. From the eikonal equation we conclude

$$(3.19) \qquad \nabla Q(z) = 0$$

since A is assumed to be positive definite. Then Q(x) is a quadratic function in a neighbourhood of fixed point Z,

$$(3.20) \qquad Q(x) = \frac{1}{2}\sum_{ij} P_{ij}(x_i - z_i)(x_j - z_j) + O(\|x\|^2), \quad P_{ij} = P_{ji}.$$

By differentiating (3.20) the gradient is also known

$$(3.21) \qquad p_i = (\nabla Q)_i = \Sigma_j P_{ij} (x_j - z_j) \quad i = 1,3.$$

The deterministic vector field can be approximated near Z as

$$(3.22) \qquad b_i = \Sigma_j \frac{\partial b_i}{\partial x_j} (x_j - z_j) \quad i = 1,3.$$

Substituting these two approximations in the eikonal equation and sorting powers of x gives with the symmetry of A and P a Riccati equation

$$(3.23) \qquad PAP + BP + PB^T = 0, \quad B = (b_{ij}) = (\frac{\partial b_j}{\partial x_i}).$$

Assuming that P is regular, (3.23) is multiplied from left and right with $S = P^{-1}$. This reduces (3.23) to the simpler Lyapunov equation

$$(3.24) \qquad SB + B^T S = -A.$$

All eigenvalues of B (evaluated at Z) have negative real parts, so matrix S has an integral representation

$$(3.25) \qquad S = \int_0^\infty e^{B^T t} A e^{Bt} \, dt.$$

The quadratic form S is positive definite, since (for $x \neq 0$)

$$(3.26) \qquad x^T S x = \int_0^\infty \| A^{\frac{1}{2}} e^{Bt} x \|_2^2 \, dt > 0.$$

This implies that matrix P is also positive definite. For simplicity A is assumed to be the Kronecker delta δ_{ij}(I). Matrix P in (3.20) is now computed with the Lyapunov equation (3.24). This equation can be written as a linear system of nine equations in the entries of $S(S=P^{-1})$. The coefficient matrix is the sum of two tensor products

$$(3.27) \qquad (B^T \oplus I + I \oplus B^T)\vec{S} = -\vec{I}.$$

The arrows indicate that matrices S and I are written columnwise as vectors. Since eigenvalues of the matrix in (3.27) have the form $\lambda_i + \lambda_j$, with λ in the spectrum of B there are no zero eigenvalues and there exists a unique solution $\bar{S}$. Inverting matrix S gives the required matrix P in the quadratic approximation.

In the computations it is not a priori clear how precise the approximation must be to provide accurate initial values. As a precaution third order terms are introduced

$$(3.28) \qquad Q(x) = \frac{1}{2}\sum_{ij} P_{ij}(x_i-z_i)(x_j-z_j) + \frac{1}{6}\sum_{ijk} R_{ijk}(x_i-z_i)(x_j-z_j)(x_k-z_k)$$

with P_{ij} and R_{ijk} invariant under permutation of indices. The gradient is also better approximated with this relation

$$(3.29) \qquad (\nabla Q)_i \equiv p_i = \Sigma_j P_{ij}(x_j-z_j) + \frac{1}{2}\sum_{jk} R_{ijk}(x_j-z_j)(x_k-z_k).$$

Evaluation of the coefficients R_{ijk} requires knowledge of second order terms in the expansion of b(x) near Z. Substituting the expansion of b(x) and (3.29) in the eikonal equation gives the already known Riccati equation (3.23) and relations which determine the coefficients $R_{k\ell m}$;

$$(3.30) \qquad \Sigma_i T_{ki} R_{i\ell m} = U_{k\ell m} \qquad 1 \le k,\ell,m \le 3,$$

where the symbols are defined as

* $\qquad T_{ij} = P_{ij} + B_{ij}$

* $\qquad U_{k\ell m} = -\Sigma_i B_{i\ell m} P_{ik} = -\Sigma_i \dfrac{\partial^2 b_i}{\partial x_\ell \partial x_m} P_{ik}$ plus terms obtained by permutation of k,ℓ,m.

System (3.30) can be written as a set of 27 linear equations in the unknown variables $R_{i\ell m}$. Reduction to a system of only 10 equations is possible, since the $R_{i\ell m}$ are considered to be invariant under permutation of indices. The Riccati equation implies that

$$T = P + B = (-I)(PB^{T}P^{-1}).$$

Eigenvalues of T are necessarily eigenvalues of B (multiplied by -1). Consequently the coefficient matrix of the original set of 27 linear equations is nonsingular and there is a unique solution R. Approximation of w(x) in a neighbourhood of Z is analogous. According to the normalization $\psi(Z) = 1$ also $w(Z) = 1$. Near Z a quadratic expansion is used for w(x) and the divergence of b(x).

$$\begin{aligned} w(x) &= 1 + \Sigma_i w_i (x_i - z_i) + \frac{1}{2} \sum_{ij} w_{ij} (x_i - z_i)(x_j - z_j) \\ \text{divb}(x) &= \text{divb}(Z) + \Sigma_i F_i (x_i - z_i) + \frac{1}{2} \sum_{ij} F_{ij} (x_i - z_i)(x_j - z_j). \end{aligned} \tag{3.31}$$

Substitution of these expansions in (3.18) gives the coefficients w_i and w_{ij} (i,j=1,3) as the solution of a linear system resp. a matrix equation;

$$\begin{aligned} \Sigma_i T_{ji} W_i &= -(\tfrac{1}{2} \Sigma_i R_{iij} + F_j) \quad j = 1,3 \\ \Sigma_i T_{ji} W_{ik} &= -\tfrac{1}{2}[(\Sigma_i R_{ijk} + B_{ijk}) W_i + (\Sigma_i R_{iij} + F_j) W_k + F_{jk}] \quad j,k = 1,3. \end{aligned} \tag{3.32}$$

The matrix in the right hand side of the last equation can be calculated when the coefficients R_{ijk} and W_i have been determined.

3.2c The ray method

The left hand side of the eikonal equation can be interpreted as Hamiltonian H(x,p), with $p_i = (\nabla Q)_i$. The associated system of bicharacteristics is

$$\frac{dx_i}{ds} = P_i + b_i \qquad i = 1,3 \tag{3.33}$$

$$\frac{dP_i}{ds} = -\Sigma_j B_{ij} p_j \qquad i = 1,3 \tag{3.34}$$

with parameter s defined along the bicharacteristics. The principle of minimal action defines the change in Q(x) along the bicharacteristics to be equal to the Lagrangian,

$$(3.35) \qquad \frac{dQ}{ds} = \Sigma_i p_i \frac{dx_i}{ds} - H(x,p) = \frac{1}{2} \Sigma_i p_i^2 \geq 0.$$

Equation (3.20) implies that Q(x) is positive on a small neighbourhood of Z. Together with (3.35) it is clear that Q(x) is positive on the rays (projection of bicharacteristics on the x-space) emanating from a neighbourhood of Z. The solution w(x) of (3.18) can be obtained after the solution of the Hamilton Jacobi equation. With (3.33) the w equation simplifies to

$$(3.36) \qquad \frac{dw}{ds} + (\tfrac{1}{2}\Delta Q + \mathrm{divb}(x))w = 0.$$

Now there is one more difficulty in the second derivatives of Q(x) being unknown outside a small neighbourhood of Z. As remarked by Ludwig [8] transformation to ray coordinates permits a better statement of the problem. Apart from the s-variable another two variables θ, ϕ are needed. With these two variables the starting point of a ray on a small sphere around Z can be specified. The Jacobian Z of the transformation $(x_1,x_2,x_3) \to (s,\theta,\phi)$ transforms along the rays as

$$(3.37) \qquad \frac{1}{J} \cdot \frac{dJ}{ds} = \Delta Q + \mathrm{divb}(x)$$

the expression in the right hand side is the divergence of the rayfield. When this identity is substituted in the w-equation the result is

$$(3.38) \qquad \frac{d}{ds} \log(w^2 J) = -\mathrm{divb}(x).$$

3.2d Numerical integration of the Hamiltonian equations

Equations (3.17) and (3.33) give the velocity of the rays in x-space $(r=(x_1,x_2,x_3)^T)$

$$(3.39) \qquad \left\| \frac{dr}{ds} \right\|_2 = (\Sigma_i (p_i+b_i)^2)^{\frac{1}{2}} = \|b(x)\|_2.$$

Consequently the velocity of the ray equals the velocity of the deterministic vector field. Equations (3.33)-(3.34) and (3.36)-(3.38) are integrated to obtain w(x) and Q(x).

The initial values needed for numerical integration of the ray equations are given on a small sphere around Z. The two variables describing the sphere are θ and ϕ. When these variables have been initialized also Q(x), $\nabla Q(x)$ and w(x) can be computed on the sphere with the approximations derived before. The system to be integrated is larger than the ten equations of (3.33)-(3.38), since the integration of Jacobian J is only possible with the use of additional variables. Indicating x-coordinates with vector r, J equals

$$(3.40) \qquad J = \frac{\partial r}{\partial \theta} \times \frac{\partial r}{\partial \phi} \cdot \frac{\partial r}{\partial s}.$$

Consequently the 6 variables $\frac{\partial x_i}{\partial \theta}$, $\frac{\partial x_i}{\partial \phi}$, i = 1,2,3 have to be integrated and initialized. Differentiating the Hamiltonian system (3.33)-(3.34) with respect to θ and ϕ results in the necessary equations for these 6 new variables. Also 6 additional variables $\frac{\partial p_i}{\partial \theta}$, $\frac{\partial p_i}{\partial \phi}$ (i=1,2,3) follow from this operation. Details of the computations are omitted. The total number of equations to be integrated is now 20; 7 from the system (3.33)-(3.35), equation (3.38) for $w^2 J$ and 12 equations for $\frac{\partial r}{\partial \theta}$, $\frac{\partial r}{\partial \phi}$, $\frac{\partial p}{\partial \theta}$, $\frac{\partial p}{\partial \phi}$.

In all trajectories integration of the system ends in a caustic surface (Jacobian=0) or an exit in the plane $x_2 = 0$. On regular trajectories the precision is sufficient for 4 significant digits in the answers $(x_1, x_2, x_3, Q(x), w(x))$.

The third order derivative terms seem to have little influence. For each trajectory the traversed path is only slightly different from the path with identical initial values, but only second order approximation for Q(x). Also no significant change in Q values on the boundary is found when the third order terms are neglected.

3.2e Another method for the computation of Q(x)

With the Taylor series of Q(x) around Z on a small sphere another approximation can be obtained on a larger sphere, concentric with the first. From a certain number of initial points, distributed homogeneously over the

first sphere, the ray equations are integrated until the larger sphere is reached. With the collection Q-values an approximation of Q(x) on the larger sphere can be made. For example a polynomial approximation has been made with spherical harmonics.

The integration is carried out with an appropriate NAG-routine [11]. The final sphere is the largest sphere around Z that fits in the positive octant of $\mathbb{R}^3$. This sphere touches the coordinate plane $x_2 = 0$ in the point Z_1, the orthogonal projection of Z onto this plane.

Data gathered from many rays exiting in the plane $x_2 = 0$ indicate that the value $Q(Z_1) = 0.0052 \pm 0.0001$. It appears that the $Q(Z_1)$ value obtained with the method of successive spheres gives the right order of magnitude but nothing more than that. The reason for this phenomenon is the concentration of rays in each step; the rays bend in the direction of caustic surfaces and are contracted into the areas with low divergence of the vector field b(x).

Since the most important ray is the one transporting minimal Q-values (see other sections) a shooting method was constructed in order to find this ray. Two extra variables are introduced:

$$\frac{\partial Q}{\partial \theta} = \nabla Q . \frac{\partial r}{\partial \theta} \tag{3.41}$$

$$\frac{\partial Q}{\partial \phi} = \nabla Q . \frac{\partial r}{\partial \phi} \; . \tag{3.42}$$

Consequently, each of these two is composed of 6 variables which are already computed in the system of 20 equations. With a NAG-routine the integration is repeated over a certain range: parameter s is zero on a small sphere around Z. For a fixed value $s = s_{max}$ the minimum of Q(x) is searched on the surface of end points of rays with $s = s_{max}$, such that $\frac{\partial Q}{\partial \theta} = \frac{\partial Q}{\partial \phi} = 0$. The normal vector on this surface is the product $\frac{\partial r}{\partial \theta} \times \frac{\partial r}{\partial \phi}$. In an extremal point the gradient of Q will be along this normal, giving

$$(\frac{\partial r}{\partial \theta} \times \frac{\partial r}{\partial \phi})(s) = \frac{2J}{\| \nabla Q \|_2^2} \nabla Q(s) \tag{3.43}$$

along the minimal Q ray. In the special case of the hypercycle with three components (see (3.3)) this ray approaches X_1 on the x_1-axis for increasing

values of S_{max}.

3.3 Application to the hypercycle

Again we restrict ourselves to the three dimensional case in (2.18) and diffusion tensor $a_{ij} = \delta_{ij}$. The WKB-solution is supposed to be valid at least in a small neighbourhood of the ray transporting the lowest Q-values. This is supported by the strongly diverging character of the rays near the minimal ray. (see also Ludwig [8]). However, domain D has not been specified up to this moment.

The complete positive octant would be the simplest choice for D. Consider the part of the (non-smooth) boundary ($x_1=0, x_2=0$ or $x_3=0$) where a regular solution ψ_ε is possible. This part will be a non empty set in the boundary since exit will occur with probability one for each $\varepsilon > 0$. As remarked in section 3.2 Q(x) is a Lyapunov function for the deterministic system. In 2.2 it has been shown that the hypercycle with three components has three attracting fixed points in the boundary (X_j, j=1,2,3 in fig. 1). Consequently the only possible minima of Q(x) on the boundary are these three points. In computations carried out in section 3.2 it appears that the minimum of Q is attained in X_1 and that Q is approximately equal to this value in a large neighbourhood of X_1 in the plane $x_2 = 0$. Compare this with results of Bobrovsky and Schuss [1], where in a two dimensional system the same phenomenon occurs. Since Q(x) is approximately constant on a relatively large area in the boundary, the value of w(x) is also important when the maximum of ψ_ε on the boundary is to be determined. This is certainly the case for the ε-values used in the simulations ($\varepsilon \approx 2^{-5}$) in section 4.2. For these ε values the maximum of ψ_ε is approximately on the line X_1Z_1, with Z_1 the orthogonal projection of Z on the boundary plane $x_2 = 0$. When ε decreases the maximum approaches X_1 (table 1). Returning to the question of how to define domain D we conclude that D may be considered to be unbounded. Values of ψ_ε on a hyperplane $\Sigma_i x_i = c \gg 0$ would be vanishingly small compared with ψ_ε near X_1.

Substitution of (3.6) (3.10) and (3.16) in (3.4) gives the following identity

$$(3.44)\qquad \int_{\partial D_p} \frac{1}{2}\varepsilon^2 e^{-Q/\varepsilon^2}\left(w\,\frac{c_0-f(x_t)}{\varepsilon}\cdot\frac{2}{\sqrt{\pi}}\sqrt{c_r(x_t)} - f(x_t)\left(\frac{\partial w}{\partial x_r} - \frac{w}{\varepsilon^2}\frac{\partial Q}{\partial x_r}\right)\right)d\sigma = 0$$

after neglecting terms of smallest order (ε^2) remains

$$(3.45)\qquad \int_{\partial D_p} \frac{1}{2}\varepsilon^2 we^{-Q/\varepsilon^2}\left(\frac{c_0-f(x_t)}{\varepsilon}\cdot\frac{2}{\sqrt{\pi}}\sqrt{c_r(x_t)} + f(x_t)\,\frac{1}{\varepsilon^2}\frac{\partial Q}{\partial x_r}\right)d\sigma(x_t) = 0.$$

It is clear that asymptotically all integrals are determined by the extrema of $Q(x)$. According to section 3.2 the absolute minimum is in Z ($Q(Z) = 0$, $Q(x) > 0$ for $x \neq Z$). For a regular WKB-solution there can be no other extrema inside D, since $\nabla Q = 0$ implies $J = 0$. In equations (3.33) $\frac{dr}{ds}$ would be reduced to $b(x)$ and the ray bends back to Z, resulting in a multi valued function $Q(x)$. In an extremal point X' on the boundary $\nabla Q(X')$ is orthogonal to the boundary, so $(\nabla Q.b)(X') = 0$. The eikonal equation gives $\nabla Q(X') = 0$ which means that also the radial derivative $\frac{\partial Q}{\partial x_r}(X')$ has to be zero.

This eliminates the last term in (3.45) and gives the asymptotic expression for $c_0(\varepsilon)$;

$$(3.46)\qquad c_0(\varepsilon) \sim \frac{\int_{\partial D_p} we^{-Q/\varepsilon^2}\sqrt{c_r(x_t)}\,f(x_t)\,d\sigma(x_t)}{\int_{\partial D_p} we^{-Q/\varepsilon^2}\sqrt{c_r(x_t)}\,d\sigma(x_t)}\ .$$

Each characteristic function $f(x_t)$ with support contained in the boundary, which is identically one on a neighbourhood of the minimum of Q gives $c_0 \sim 1$.

The numerator of the expression for $C_1(\varepsilon)$ (3.14) is evaluated as

$$(3.47)\qquad \frac{(2\pi\varepsilon^2)^{3/2}\,\psi(Z)}{H(Z)^{\frac{1}{2}}} \approx 28.2\,\varepsilon^3$$

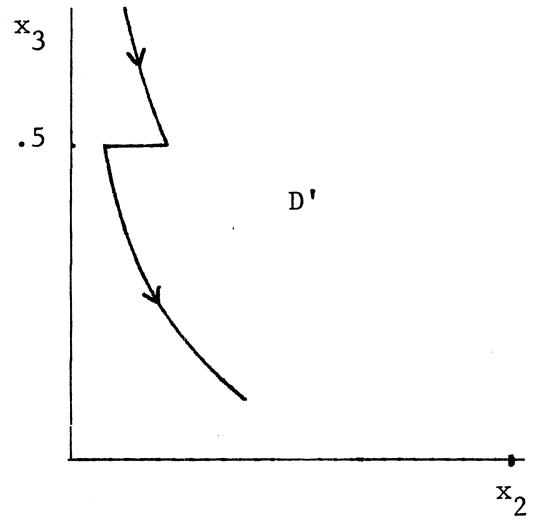
where $H(Z)$ is the Hessian of $Q(x)$ in Z.

The minimum of $Q(x)$ on the boundary (K in (3.13)) is estimated as 0.0038 ± 0.0001. Substituting this in (3.13) we have for the exit time

$$(3.48)\qquad \tau_\varepsilon(Z) \sim C_1(\varepsilon)e^{0.0038/\varepsilon^2}.$$

Only $C_1(\varepsilon)$ remains to determined. The numerical evaluation of the denominator in (3.14) is difficult since information about $\psi_\varepsilon(x)$ near X_1 is incomplete. In this region $Q(x) \approx K$ but unfortunately $w(x)$ is not known. In simulations

and the shooting method it appears that a considerable bundle of rays with low Q-values is close to the boundary plane $x_2 = 0$, but upon approaching X_1 the rays are repelled and either exit in the plane $x_2 = 0$ or enter caustic surfaces. We therefore consider the exit problem for a slightly smaller domain $D' \subset D$, shown in cross section in figure 2.



The main contribution to the first integral in the denominator of (3.14) comes from the boundary $x_3 > 0.5$ and x_2 small. In the approximation we take $x_2 = 0$.

Figure 2. Domain D' in cross section at $x_1 = 0.5$. The boundary consists of deterministic trajectories and the plane $x_3 = 0.5$.

A numerical estimate of the second integral in the denominator of (3.14) over the boundary at $x_3 = 0.5$ equals $6\varepsilon^3$, with a relatively large error (about 25%). As already mentioned the maximum of ψ_ε is located approximately on the line X_1Z_1. By a Gaussian approximation the first surface integral is reduced to a line integral over X_1Z_1. This is accomplished by assuming a quadratic growth of Q(x) in the normal direction (n) on X_1Z_1. The proportionality factor is approximately constant ($\frac{\Delta Q}{(\Delta n)^2} \approx \frac{1}{4}$) in the region of the largest contributions to the integral. After translating and rotating the coordinate system this constant is used to reduce the surface integral to the line integral. $C_1(\varepsilon)$ can then be given as the quotient

$$C_1(\varepsilon) \approx \frac{28.2\varepsilon^3}{2.6\varepsilon^3 I(\varepsilon)+6\varepsilon^3} \tag{3.49}$$

where

$$I(\varepsilon) = \frac{1}{6\varepsilon} \int_{x_1 z_1} we^{(K-Q)/\varepsilon^2} \sqrt{6(1-x)(18-5x)}\, dx \quad \text{is of order 1.}$$

Evaluation of $C_1(\varepsilon)$ for several ε's in the range used for simulations gives the following table

ε	$I(\varepsilon)$	$C_1(\varepsilon)$	$\bar{x}_1$
2^{-4}	0.78	3.4	.30
2^{-5}	1.06	3.1	.38
2^{-6}	.96	3.2	.46

Table 1. The last column gives the x_1-coordinate of the point on the line X_1Z_1 where ψ_ε is maximal.

4. MONTE CARLO SIMULATION

4.1 The stochastic difference equations.

Dynamical systems with small random perturbations can be simulated with the Monte Carlo method. To perform the simulation, the Wiener process W(t) has to be replaced by a pseudo random generator G(t). A NAG routine [11] is used to supply normally distributed random numbers with zero mean and unit variance. Euler's method can be applied to the stochastic difference equations (4.1) with time step h (Franklin [4]).

$$x_i(t+h) = x_i(t) + hb_i(x) + \varepsilon\sqrt{h}\, G_i(t) \qquad i = 1,n. \tag{4.1}$$

The time step h (h=0.03) gives an error in x of order O(h). Define the new stochastic variable $\Delta x_i(t)$, i = 1,n;

$$\Delta x_i(t) = x_i(t+h) - x_i(t). \tag{4.2}$$

This variable has for the first and second moment

$$E\Delta x_i(t) = hb_i(x) + \varepsilon\sqrt{h}\, EG_i(t) = hb_i(x) \tag{4.3}$$

$$\text{Var } \Delta x_i = \varepsilon^2 hEG_i^2(t) = \varepsilon^2 h. \tag{4.4}$$

Consequently in unit time the expectation of Δx_i equals the local vector field $b(x)$ while variance in unit time equals ε^2.

4.2 Results for the hypercycle.

Computations were carried out for the deterministic system (2.18) in the cases n = 2 (A), n = 3 (B) and n = 5 (C). According to equation (4.1) the following stochastic difference equations are obtained:

$$(4.5) \qquad x_i(t+h) = x_i(t) + hx_i(t)(k_i x_{i-1}(t) - \Sigma_j k_j x_j x_{j-1}(t)) + \varepsilon\sqrt{h}\, G_i(t).$$

Each simulation starts in the stable equilibrium and comes to an end when one of the coordinates changes sign.

A. Two components.

In case of two components the reaction constants have been chosen as $k_1 = 1$, $k_2 = 3$. Consequently there is a unique stable equilibrium Z with coordinates (1/4,3/4). Simulation of the exit process gives for $\varepsilon \downarrow 0$ concentration of the exit point distribution on the point in ∂D with minimal distance to Z (this point is (0,3/4)). Averaged over several hundred simulations the mean x_2-coordinate at the moment of exit is 0.742. A least squares approximation of the exit time τ_ε in the form $\tau_\varepsilon \approx ae^{b/\varepsilon^2}$ gives the result

$$(4.6) \qquad \tau_\varepsilon \approx 1.6\, e^{0.033/\varepsilon^2}.$$

B. Three components.

The reaction constants have been chosen as in 2.2 $k_1 = 1$, $k_2 = 3$, $k_3 = 5$. The stable equilibrium Z is consequently at the point

$$(4.7) \qquad (Z_j) = \frac{15}{23}\,(1/3,1/5,1)^T.$$

As in case A there is an exponential growth of the exit time for descending values of ε Table 2 gives for several hundred simulations in each ε the number of exits in each coordinate plane ($x_1=0$, $x_2=0$ or $x_3=0$) and the

averaged exit time τ_ε for that ε-value. Also at each ε the averaged x_1- and x_3-coordinate are given for exits in the plane $x_2 = 0$. The reason for this choice is the concentration of exit points in the plane $x_2 = 0$ for descending ε. In this plane the exits are concentrated on a small area near Z_1, the orthogonal projection of Z on the plane. An approximation of the exit time in exponential form gives the following result

$$\tau_\varepsilon \approx 3.1\, e^{0.0040/\varepsilon^2}. \tag{4.8}$$

		Exits on boundary $x_i = 0$				
ε	τ_ε	$X_1=0$	$X_2=0$	$X_3=0$	$\bar{X}_1$	$\bar{X}_3$
1	.10	81	102	17	.321	.659
1/2	.29	72	118	10	.289	.642
1/4	.79	76	124	0	.268	.636
1/8	2.5	62	138	0	.235	.646
1/16	10	46	154	0	.238	.644
1/32	186	0	10	0	.24	.64

Table 2. For each ε 200 simulations are given on each line, except for $\varepsilon = 1/32$ with only 10. The last two columns give the averaged x_1- and x_3-coordinates for exits in the plane $x_2 = 0$. Coordinates of Z_1, the orthogonal projection of Z on the plane are (0.21, 0.65).

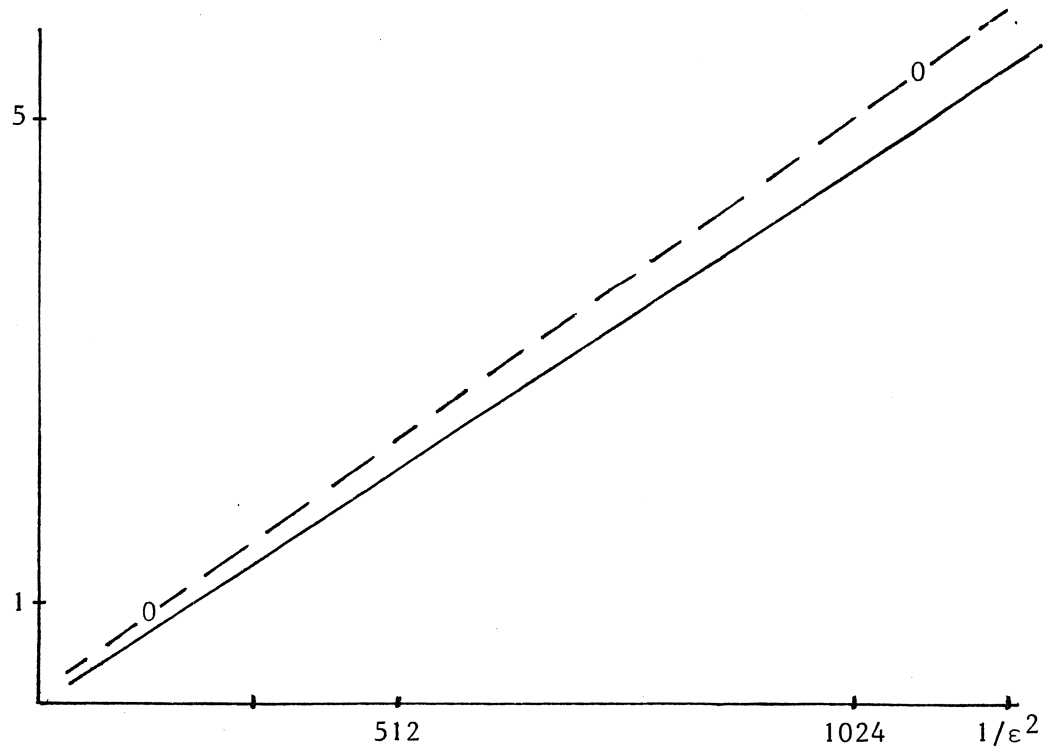


Figure 3. Experimental exit times (4.8) (dashed line) vs. theoretical values (3.48). The vertical axis shows $\log(\tau(Z)/3)$.

C. Five components.

As in preceding cases the starting point of each trajectory is chosen in the ω-limit set of the deterministic system. The fixed point Z however, is a saddle point and the ω-limit set is now (probably) a limit cycle in the plane $\Sigma_{i=1}^{5} x_i = 1$, surrounding Z (Schuster [13]). The five reaction constants come from an example in this reference;

(4.9) $\qquad (k) = (25/13,\ 1/13,\ 19/13,\ 1,\ 7/13).$

For this choice of constants the "limit cycle" is easily found. Starting somewhere in the positive octant in $\mathbb{R}^5$ the deterministic trajectory is followed until the cyclic change in x-coordinates is less than a certain preset tolerance.

The "limit cycle" is numerically represented by 200 step points, distributed

homogeneously in time. The simulation procedure is almost the same as with A and B, the only difference being the starting x-values which are obtained by interpolation on the steppoints. The total collection of starting points is homogeneously distributed over the cycle.
Since the cycle comes very close to the boundary at some points exit times are much lower than in case B or A. The values $\log \tau_\varepsilon$ and $\log \varepsilon$ show an almost linear relation (figure 4), so an approximation of τ_ε was made in the form $a\varepsilon^b$, resulting in

$$\tau_\varepsilon \approx 0.009(\varepsilon^2)^{-0.35}. \tag{4.10}$$

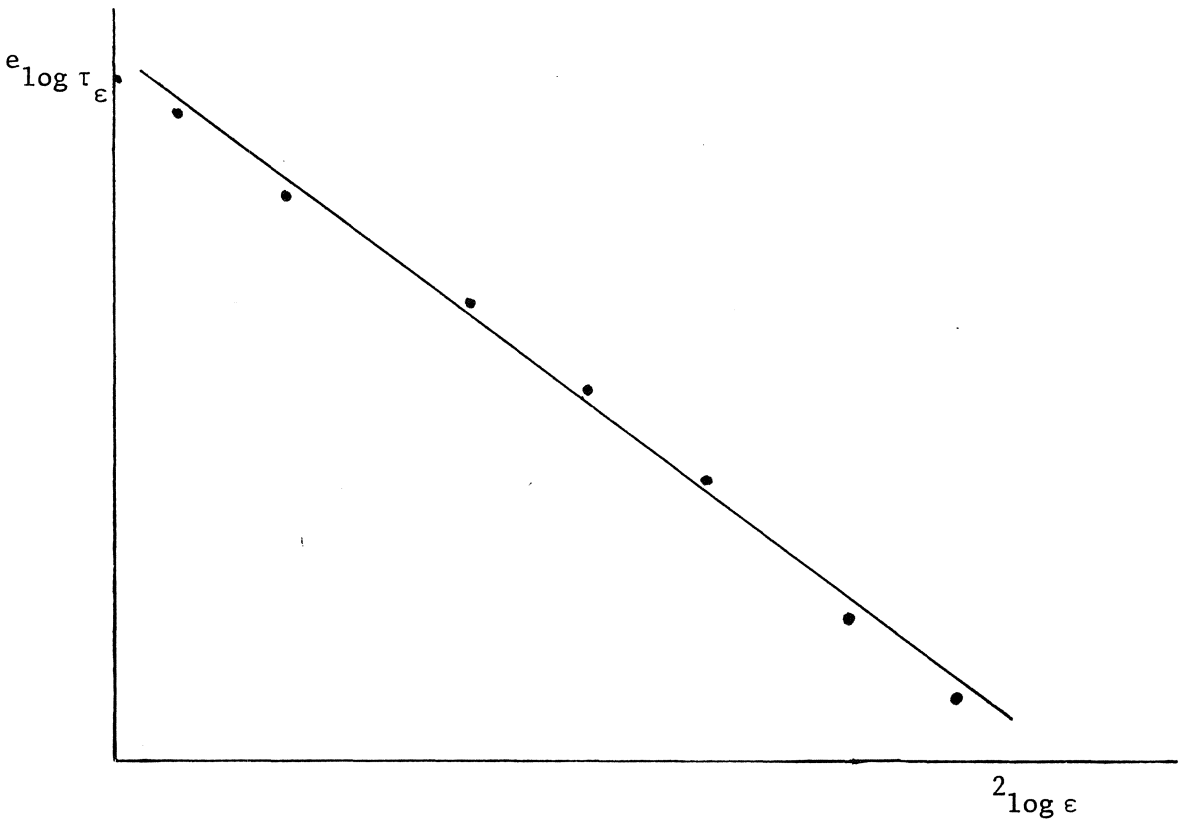


Figure 4. Exit time for the limit cycle with five components. $\log \tau_\varepsilon$ as a function of $^2\log \varepsilon$.

5. CONCLUSIONS

The smaller cycles with 2 or 3 components have an exponential growth of the exit time $\tau_\varepsilon(Z)$ as a function of ε^2. However as indicated in figure 4 for 5 components, the larger cycles will have an algebraic growth of exit time. Only in the special case with all k_i (approximately) equal, Z will be near the center of the hyperplane $\Sigma_i x_i = 1$ and then the stability will be better.

Numerical results from the shooting method appear to be in good agreement with the simulation experiments. The exponential factor 0.0040 in formula (4.8) agrees well with the minimal Q-value on the boundary (0.0038) found in section 3.3. The present approach is related with the following results. In a two dimensional problem with rotational symmetry Williams [15] found an exponential behaviour of exit time from a limit cycle around an unstable fixed point in the origin, where the boundary is taken concentric with the cycle. Bobrovsky and Schuss [1] find algebraic behaviour of the exit time for the case of a center Z in a domain D bounded by a closed trajectory of the vector field b(x).

Graham and Haaken [6] show that the function Q(x) can be interpreted in a very wide sense as a generalized thermodynamic potential for Markov systems that satisfy conditions concerning time reversibility. The shooting method is a very cumbersome way to obtain a single Q-value on the boundary. Due to the strongly diverging character of the rays in the most interesting direction (the minimum on the boundary), convergence in the shooting is hard to obtain. Moreover, the critical points on the boundary have to be excluded. The neighbourhood of a turning point needs a different approach. Since in the precent problem, as well as in the problem of Bobrovsky and Schuss, the minimal Q-value is approximately maintained outside a neighbourhood of the turning point, the asymptotic method will still produce meaningful results. Finally, the ray method does not give values all over the boundary, since the rays may end in a caustic surface, before reaching the boundary.

The structural difficulties mentioned above make it worthwhile to look for a different approach. In a subsequent report we study the same class of problems for a different function ψ. Instead of the WKB-Ansatz ψ will be replaced by a function that allows numerical integration over the volume and boundaries in the divergence theorem.

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