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## SMALL FLUCTUATIONS IN SYSTEMS WITH MULTIPLE STEADY STATES\*

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**Abstract.** We consider the effect of small random perturbations on deterministic systems with multiple steady states. The deterministic systems of interest may have two stable nodes and a saddle point. As parameters vary, two or three of the steady states coalesce. This work is concerned with the long time behavior of the system, when it starts near the deterministic separatrix. The separatrix is surrounded by a tube that may contain two stable steady states. The quantity of basic interest is the conditional probability of first exit from the tube through a specified boundary, conditioned on initial position. We use the diffusion approximation, so that the conditional probability satisfies the Kolmogorov backward equation. Formal asymptotic solutions of the backward equation are constructed. The solutions are obtained by a generalized "ray method" and are given in terms of various incomplete special functions. In the appendices, we construct asymptotic solutions of the equation satisfied by the mean value of the first exit time.

**1. Introduction.** The evolution of natural systems is often described by a deterministic differential equation:

$$(1.1) \quad \dot{x}^i = b^i(x, \eta, \delta), \quad x^i(0) = x_0^i, \quad i = 1, \dots, n.$$

In equation (1),  $\eta$  and  $\delta$  are parameters. A steady state is characterized by  $b^i(x, \eta, \delta) = 0$ ,  $i = 1, \dots, n$ . If  $b(x, \eta, \delta)$  is nonlinear, the system may possess multiple steady states. As the parameters  $\eta$  and  $\delta$  vary, it is possible that the steady states coalesce and annihilate each other, or exchange stability.

The variable  $x$  in (1.1) is a macrovariable: it describes the average state of a large system and is obtained by averaging over many independent, microscopic subunits. Equation (1.1) provides only an approximate description of the evolution of the system. In particular, it ignores fluctuations that are inherent to all natural systems. If the system has multiple stable steady states ( $P_0, P_2$ ), fluctuations may drive the system against the deterministic flow so that  $P_0(P_2)$  is reached from an initial point which deterministically is attracted to  $P_2(P_0)$ . In this case, the quantity of basic interest is the probability of a specified outcome, conditioned on the initial data. In this work, the behavior of the conditional probability is determined by solving the diffusion equation that it satisfies, for the case of noise of small intensity.

Many physical, chemical and biological systems fit into the framework of fluctuations superposed on a deterministic differential equation. Examples are: 1) Lasers, in which fluctuations are caused by the quantum nature of radiation (Graham (1974)). 2) Tunnel diode circuits may exhibit multiple steady states. Fluctuations are caused by the random motion of electrons (Landauer and Woo (1972)). 3) The mean field ferromagnet exhibits multiple steady states below the critical temperature (Griffiths, Weng and Langer (1966), Goldstein and Scully (1973)). 4) Isomerization, autocatalytic, chain and substrate inhibited reactions in open vessels may exhibit multiple steady states (Perlmutter (1972), Higgins (1967)). Fluctuations are caused by the random motion of the molecules, which may lead to a birth and death description of the reaction process. 5) Membranes may exhibit states of high and low conductivity, separated by a threshold (e.g. Lecar and Nossal (1971a, b)). 6) The equations used in theoretical ecology may exhibit multiple steady states (Bazekin (1975)). Fluctuations are caused by the elementary birth and death processes. The theory developed in this work is applicable to all of

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the above systems. Elsewhere, we discuss autocatalytic reactions and substrate inhibited reactions (Mangel (1977a)).

This work is concerned with the effects of fluctuations on systems initially in the vicinity of an unstable steady state. We assume that the unstable steady state is a saddle point, so that a deterministic separatrix  $\mathcal{S}$  exists. The separatrix divides the phase plane into two domains of attraction of the stable steady states (Fig. 1). The solutions of (1.1) exhibit a discontinuity of the following type. As  $t \rightarrow \infty$ , phase points initially on one side of  $\mathcal{S}$  approach  $P_0$ . Points on the other side of  $\mathcal{S}$  approach  $P_2$ . Points initially on  $\mathcal{S}$  approach the saddle  $P_1$ .

When fluctuations are included in the kinetic equations, the deterministic description must be modified. With probability 1, all phase points leave a vicinity of  $\mathcal{S}$  and approach  $P_0$  or  $P_2$ . More importantly, phase points which are deterministically attracted to  $P_0(P_2)$  might approach  $P_2(P_0)$ . Our goal is to calculate the probability of this event, as a function of initial position.

In § 2, we discuss the stochastic set up for this problem. The deterministic kinetic equation is converted to a Langevin-like stochastic equation. We use the diffusion approximation, so that the desired probability satisfies a backward diffusion equation.

We will construct formal asymptotic solutions of the diffusion equation. Our technique is a generalization of the "ray method" of Luneberg (1948), Keller (1958) and Cohen and Lewis (1967). In § 3, we study the exact solution of a one dimensional equation. We are lead to certain canonical integrals. These integrals are used in § 4–6 in the asymptotic solution of the two dimensional backward equation. In the appendices, we show how to construct the leading term in the asymptotic solution of the equation for the first exit time.

The theory given here has applications to chemical, physical and biological systems. These applications are discussed elsewhere (Mangel and Ludwig (1977), Mangel (1977a)).

**2. Stochastic kinetic equation, backward equation and the exit problem.** The macrovariable  $x(t)$  is the average value of a stochastic variable  $\tilde{x}(t)$  and evolves according to

$$(2.1) \quad \dot{x}^i = b^i(x, \eta, \delta) \equiv b^i(x), \quad x^i(0) = x_0^i.$$

The random variable  $\tilde{x}(t)$  will satisfy a stochastic kinetic equation. Ideally, we would derive this kinetic equation from basic principles. For instance, for physical and chemical systems, we would start with the Liouville equation and reduce it to a stochastic kinetic equation. This reduction has been performed only on the simplest system (Sinai (1970)). Instead, we shall use a Langevin method (Lax (1966)) and add a stochastic term to the right hand side of (2.1). We assume that the random effects occur rapidly, and are characterized by a time scale  $\tau$ , small compared to the macroscopic time scale  $t$ , on which measurements are made.

The increments in  $\tau$  and  $t$  are related by a parameter  $\alpha$ :

$$(2.2) \quad \Delta\tau = \Delta t \cdot \alpha^2,$$

where  $\alpha^2$  will characterize the fast time scale. The random process generated by the microscopic motions is assumed to be a mixing process  $\tilde{Y}$ . In most of the physical literature (e.g. Mori (1965), Ma (1976)), it is assumed that

$$(2.3) \quad E[\tilde{Y}^k(s)\tilde{Y}^l(0)] = \delta^{kl}(s)$$

where  $\delta^{kl}(s) = 0$  unless  $k = l$  and  $s = 0$ . We shall not make this assumption and define

$$(2.4) \quad \gamma^{kl} = \int_0^\infty E[\tilde{Y}^k(s)\tilde{Y}^l(0)] ds.$$

In the case that (2.3) holds,  $\tilde{Y}(\tau)$  is the "white noise" process. We assume that the stochastic variable  $\tilde{x}(t; \alpha)$  satisfies

$$(2.5) \quad \frac{d\tilde{x}^i(t; \alpha)}{dt} = b^i(\tilde{x}) + \sqrt{\varepsilon} \frac{\sigma_i^j(\tilde{x})}{\alpha} \tilde{Y}^j(t/\alpha^2), \quad i = 1, \dots, n.$$

Langevin was the first to use a kinetic equation of the form (2.5) (Lax (1966)). Such equations have been used in the last fifty years by most physical scientists working in this field. The use of (2.5) represents an approximate, somewhat ad hoc, way of treating stochastic effects in macroscopic systems. Equation (2.5) is the stochastic kinetic equation that will be used in the rest of this work. We assume that  $E(\sigma_i^j \tilde{Y}^j) = 0$ .

The parameter  $\varepsilon$  appearing in (2.5) characterizes the intensity of the fluctuations. We assume that  $\varepsilon$  is small. In most chemical systems, for instance,  $\varepsilon = V_c/V$ , where  $V_c$  is the characteristic volume of a subunit and  $V$  is the volume of the whole system (Keizer (1975), Van Kampen (1976)). For the case of stochastic mechanics (Nelson (1967))  $\varepsilon = \hbar^2/2m$ , and is small for macroscopic or meso-macroscopic particles.

There is considerable argument and confusion about the relationship between (2.5) and (2.1) (Van Kampen (1976)). Namely, if we average (2.5), we obtain

$$(2.5a) \quad E\left\{\frac{d\tilde{x}^i}{dt}\right\} = \frac{dx^i}{dt} = E\{b^i(\tilde{x})\}.$$

For nonlinear systems  $E\{b^i(\tilde{x})\} \neq b^i(E\{\tilde{x}\}) = b^i(x)$  in general. A solution to this "paradox" is the following.

First, we rewrite (2.1) as

$$(2.5b) \quad x^i(t+dt) - x^i(t) = b^i(x) dt.$$

In (2.5b), there is an implicit conditioning that  $x(t) = x$ . If we construct a probabilistic model that allows the calculation of

$$(2.5c) \quad \begin{aligned} E\{\tilde{x}^i(t+dt) - \tilde{x}^i(t) | \tilde{x}(t) = x\} \\ = x^i(t+dt) - x^i(t) \\ \equiv b^i(x) dt; \end{aligned}$$

then when (2.5) is averaged, we obtain (2.1).

In particular, suppose that

$$b(x) = b^+(x) - b^-(x)$$

with  $b^+, b^- > 0$ . We assume that

$$(2.5d) \quad \Pr\{\tilde{x}(t+dt) - \tilde{x}(t) = \pm 1 | \tilde{x}(t) = x\} = b^\pm(x) dt + o(dt),$$

$$(2.5e) \quad \Pr\{\text{all other transitions}\} = o(dt).$$

Then

$$(2.5f) \quad \lim_{dt \rightarrow 0} E\left\{\frac{d\tilde{x}}{dt}\right\} = \frac{dx}{dt} = b^+(x) - b^-(x) = b(x)$$

and we obtain the deterministic equations as an appropriate *conditioned* average of

stochastic equations. Keizer (1975) uses an equivalent procedure, without introducing (2.5d, e).

This type of conditioning is a backward approach that we will follow throughout.

The field  $\sigma_i^j(x)$  is assumed to be known. It characterizes the  $x$  dependence of the fluctuations. Since (2.5) is not derived from first principles, we need to provide a prescription for the calculation of  $\sigma(x)$ . Elsewhere, we discuss how  $\sigma(x)$  can be calculated for chemical systems by a birth-and-death approach (Mangel (1977b)).

For the remainder of this paper, we assume that  $\sigma(x)$  is known. We assume that  $\tilde{x}(0; a) = x_0$  remains a deterministic initial condition.

As  $\alpha \rightarrow 0$ ,  $\tilde{x}(t; \alpha)$  converges to a diffusion process  $\tilde{x}(t)$  (Papanicolaou and Kohler (1974)). Let  $E$  denote expectation with respect to the diffusion and set:

$$(2.6) \quad u(t, x) = E\{u_0(\tilde{x}(t)) | \tilde{x}(0) = x\}.$$

Then  $u(t, x)$  satisfies the backward equation

$$(2.7) \quad u_t = \frac{\varepsilon a^{ij}}{2} u_{ij} + b^i u_i + \varepsilon c^i u_i$$

where

$$(2.8) \quad a^{ij}(x) = \sigma_k^i(x) \sigma_l^j(x) (\gamma^{kl} + \gamma^{lk}),$$

$$(2.8a) \quad c^i(x) = \gamma^{kl} \sigma_k^j \frac{\partial}{\partial x^i} (\sigma_l^i).$$

The function  $u_0(x)$  in the definition of  $u(t, x)$  is the initial data for (2.7).

If  $\tilde{Y}(\tau)$  were white noise, the resulting diffusion equation would be

$$(2.9) \quad u_t = \frac{\varepsilon a^{ij}}{2} u_{ij} + b^i u_i.$$

If  $a^{ij}$  is independent of  $x$ , then equations (2.7) and (2.9) are identical. Elsewhere (Mangel (1977a)) we present a numerical comparison of solutions of equations (2.7) and (2.9). Our results indicate that (2.9) is an excellent approximation to (2.7) if the boundaries are nonsingular.

The fundamental equation derived above is (2.7) or its time independent version

$$(2.10) \quad 0 = \frac{\varepsilon a^{ij}}{2} u_{ij} + b^i u_i + \varepsilon c^i u_i.$$

Equation (2.10) must be supplemented by boundary conditions if the problem is to be properly posed. We surround the separatrix by a tube with boundaries I, II. If  $u = 0$  on I,  $u = 1$  on II, then  $u(x)$  is the probability that  $\tilde{x}(t)$  first exits from the tube around the separatrix through boundary II. Alternatively, let  $\tilde{\tau}(x)$  be the first time that  $\tilde{x}(t)$  hits either boundary I or II, given that  $\tilde{x}(0) = x$ . Let  $u(x) = \Pr \{\tilde{x}(\tilde{\tau}(x)) \in \text{II}\}$ ; Matkowsky and Schuss (1977) show that  $u(x)$  satisfies (2.10), with  $u(x) = 0$  for  $x \in \text{I}$  and  $u(x) = 1$  for  $x \in \text{II}$ . In order that the asymptotic solutions satisfy the boundary conditions, the boundaries must have certain regularity properties. These conditions are formulated in § 4.

A first exit problem of this type was studied by Levinson (1950). He noted that the solution relies heavily on the characteristics of the reduced ( $\varepsilon = 0$ ) problem

$$(2.10a) \quad u_t = b^i u_i.$$

These characteristics are determined by:

$$(2.10b) \quad \dot{x}^i = b^i(x),$$

i.e. the deterministic trajectories. Levinson treated the problem in which  $b(x)$  did not vanish in the domain of interest (i.e. characteristics do not intersect). Visik and Lynsternik (1962) treated the problem in which the characteristics intersect at one point and all characteristics point outwards. Matkowsky and Schuss (1977) treated the analogous problem when the characteristics point inwards. Here we treat the problem in which (a)  $b(x)$  may vanish at up to three points in the domain of interest, (b) two characteristics never leave the domain.

We distinguish three cases of increasing complexity.

1) *The normal case* in which the separatrix tube contains only the unstable steady state.

2) *The marginal case* in which the separatrix tube contains the unstable steady state and one stable steady state. As one parameter varies, the two steady states coalesce and annihilate each other (the marginal bifurcation). After the bifurcation, only one stable steady state remains. This steady state is not in the separatrix tube, so that the deterministic flow is always across the tube in the same direction (see Fig. 2). The first exit problem as formulated is of little interest. A more interesting question involves the expected time to reach boundary II, given that  $\tilde{x}(0) = x$ ,  $T(x)$ . Let  $d(x)$  denote the distance from the point  $x$  to II. Let

$$(2.11) \quad T(x) \equiv \int_0^\infty tu_t(x, t) dt$$

where  $u(x, t)$  satisfies (2.7) with boundary conditions  $u(x, t) = 1$  on II,  $u_t \rightarrow 0$  as  $d \rightarrow \infty$ ,  $u(x, 0) = 0$  unless  $x \in \text{II}$ . Then  $u(x, t)$  is the probability that  $\tilde{x}(t)$  has reached II by time  $t$ , given that  $\tilde{x}(0) = x$ .

$T(x)$  satisfies (Gihman and Skorohod (1972))

$$(2.12) \quad \frac{\varepsilon a^{ij}}{2} T_{ij} + b^i T_i + \varepsilon c^i T_i = -u(x)$$

where  $u(x)$  is the probability of eventually reaching II, given that  $\tilde{x}(0) = x$ .  $T(x)$  satisfies the boundary conditions

$$(2.13) \quad T(x) = 0, \quad x \in \text{II}; \quad T < \infty \text{ as } d \rightarrow \infty.$$

3) *The critical case* in which the separatrix tube contains the unstable steady state and both stable steady states. As two parameters vary the three steady states move together and coalesce (the critical bifurcation). The remaining steady state is assumed to be stable.

In § 4–6, we shall give explicit characterizations of normal, marginal and critical type dynamical systems. Our classification scheme generalizes the one of Kubo et al. (1973), who only treated one dimensional problems.

Recently, Matkowsky and Schuss (1977), Schuss (1977) and Williams (1977) have studied stochastic exit problems. They were interested in the exit distribution and mean exit time from a domain containing a simple, stable steady state. Their results are obtained by matched asymptotic solutions of (2.7). There is little overlap between their work and this one.

**3. Three canonical integrals.** Equations (2.10) and (2.12) are singularly perturbed elliptic equations. The equations are further complicated by the fact that  $b(x)$  vanishes

at one or more points in the separatrix tube. We seek approximate solutions of the equations. We will use formal asymptotic methods for the calculation of the first exit probability. Similar methods apply to the first exit time (Appendix A). The form of the asymptotic solutions will be suggested by the analysis of a one-dimensional version of (2.10):

$$(3.1) \quad 0 = \frac{\varepsilon a(x)}{2} u_{xx} + b(x, \eta, \delta) u_x + \varepsilon c u_x.$$

The analysis of (3.1) will lead to three canonical integrals which will be used in the solution of (2.10).

The use of the canonical problems helps to identify the characteristics of the multidimensional problem. This is an essential idea of the ray method of Luneberg (1948) and Keller (1958). Our results are a generalized ray method.

The reduced ( $\varepsilon \equiv 0$ ) deterministic system is

$$(3.2) \quad \dot{x} = b(x, \eta, \delta) = b(x)$$

which may have three steady states,  $x_0$ ,  $x_1$  and  $x_2$  (1st case). As  $\eta$ ,  $\delta$  vary, two steady states coalesce (2nd case) or all three coalesce (3rd case). The 2nd case is the marginal type steady state,  $x_m$ , characterized by (Kubo et al. (1973))

$$(3.3) \quad \begin{aligned} b(x_m) &= 0; & b'(x_m) &= 0; & b''(x_m) &\neq 0, \\ \eta &= \eta_m, & \delta &= \delta_m. \end{aligned}$$

The third case is the critical type steady state,  $x_c$ , characterized by ( $\eta = \eta_c$ ,  $\delta = \delta_c$ )

$$(3.4) \quad b(x_c) = b'(x_c) = b''(x_c) = 0, \quad b'''(x_c) \neq 0.$$

Equation (3.1) must be supplemented by boundary conditions. We choose  $l_1, l_2$  so that  $x_1 \in [l_1, l_2]$ , where  $x_1$  is the unstable steady state. If  $u(l_1) = 0$ ,  $u(l_2) = 1$ , then  $u(x)$  is the probability that the process first exits from  $[l_1, l_2]$  through the right hand boundary. The solution of (3.1) is

$$(3.5) \quad u(x) = \frac{\int_{l_1}^x \exp \left[ -\int_{l_1}^{x'} \frac{2(b(s) + \varepsilon c(s))}{\varepsilon a(s)} ds \right] dx'}{\int_{l_1}^{l_2} \exp \left[ -\int_{l_1}^{x'} \frac{2(b(s) + \varepsilon c(s))}{\varepsilon a(s)} ds \right] dx'}.$$

When  $\varepsilon$  is small, the behavior of (3.5) will be determined by the  $2b/(\varepsilon a)$  term. Thus, we shall consider the simpler integral

$$(3.6) \quad v(x) = \int_{l_1}^x \exp \left[ -\int_{l_1}^{x'} \frac{2b(s)}{\varepsilon a(s)} ds \right] dx'.$$

By using (3.6) rather than (3.5), the algebraic details of the analysis are simplified, but the main points remain unchanged. The two results will differ by terms  $O(\varepsilon)$  or less. Our analysis will be based upon Laplace's method (Olver (1974), Bleistein and Handelsman (1975)). It is assumed that  $a(x) > 0$  for  $x \in [l_1, l_2]$ .

**3.1. Normal case: The error integral.** In the normal case, only one steady state is contained in  $[l_1, l_2]$ . The main contribution to (3.6) will come from the minimum of

$$(3.7) \quad \phi(x') = \int_{l_1}^{x'} \frac{2b(s)}{a(s)} ds.$$

Since  $\phi'(x_1) = 0$  and  $\phi''(x_1) = 2b'(x_1)/a(x_1) > 0$ , the minimum of  $\phi(x')$  is at  $x' = x_1$ .

Using a Taylor expansion of  $\phi$  about  $x_1$  in (3.6) yields

$$(3.8) \quad v(x) = k \int_{x_1}^x \exp \left[ -\frac{b'(x_1)}{\varepsilon a(x_1)} (x' - x_1)^2 \right] dx' + O(\sqrt{\varepsilon}),$$

where  $k$  is constant. Differentiation of (3.8) gives

$$(3.9) \quad v_x(x) \sim k \exp \left[ -\frac{b'}{\varepsilon a} (x - x_1)^2 \right].$$

For small  $\varepsilon$ ,  $v_x$  is very small, except in a region around  $x_1$ . Hence, we obtain an internal boundary layer about  $x_1$  of width  $O((\varepsilon a(x_1)/b'(x_1))^{1/2})$ . A change of variables converts (3.8) to

$$(3.10) \quad v(x) = k \int^{\tilde{x}(x)} \exp(-s^2/2\varepsilon) ds + O(\sqrt{\varepsilon}).$$

The integral in (3.10) is the error integral

$$(3.11) \quad E(z) = \int_{z_0}^z e^{-s^2/2} ds.$$

The function  $E(z)$  satisfies the following equation

$$(3.12) \quad \frac{d^2 E}{dz^2} = -z \frac{dE}{dz}, \quad z_0 \leq z \leq z_1.$$

The error integral is closely related to the normal distribution function (Abramowitz and Stegun (1965)).

**3.2. Marginal case: The Airy integral.** In § 3.1 we assumed that  $b'(x_1)$  does not vanish. This assumption is not valid at a marginal or critical type steady state. Thus, the error integral no longer adequately represents the asymptotic behavior of the probability. The cause of the breakdown is clear: the error integral corresponds to linear dynamics, but the dynamics at the marginal and critical steady states are totally nonlinear.

Apparently, this breakdown of mathematical method has not been appreciated in the physical literature. The use of the error integral at a marginal or critical type steady state leads to an "infinite variance", i.e.  $E(\tilde{x}^2) = \infty$ . This result has nothing to do with the physics of the problem, but is due to the misuse of the mathematics. (This topic is discussed in detail in Mangel (1978).)

In order to obtain an expansion at a marginal type steady state, a more complicated special function is needed. We use a third term in the Taylor expansion of  $\phi$ :

$$(3.13) \quad \phi(x) = \phi(x_1) + \frac{b'(x_1)}{a(x_1)}(x - x_1)^2 + \frac{b''(x_1)}{3a(x_1)}(x - x_1)^3 + O((x - x_1)^4).$$

A change of variable converts (3.13) to

$$(3.14) \quad \phi = \frac{b''(x_1)}{a(x_1)} \left[ \frac{1}{3} y^3 - \tilde{\alpha} y + \beta \right] + O(y^4)$$

where  $y$  is a regular function of  $x$  and  $\tilde{\alpha}, \beta$  are functions of  $b'(x_1)$ ,  $b''(x_1)$  and  $a(x_1)$ ;  $\tilde{\alpha}$  vanishes when  $b'$  vanishes. Another change of variables converts (3.6) to the form

$$(3.15) \quad v(x) = c \int^{\tilde{x}(x)} \exp \left[ -\frac{1}{\varepsilon} \left( \frac{1}{3} r^3 - \alpha r \right) \right] dr + O(\varepsilon^{2/3})$$



where  $c$  is a constant and  $\alpha = (b''/a)^{1/3}\tilde{\alpha}$ . The integral (3.15) can be obtained by applying Levinson's result directly to (3.6) (Levinson (1962)). Differentiation of (3.15) gives

$$(3.16) \quad v_{\tilde{x}} \sim \exp \left[ -\frac{1}{\varepsilon} \left( \frac{1}{3} \tilde{x}^3 - \alpha \tilde{x} \right) \right].$$

Hence, for small  $\varepsilon$ ,  $v_{\tilde{x}}$  will be very small except in a region around the origin where  $\frac{1}{3}\tilde{x}^3 - \alpha\tilde{x}$  is  $O(\varepsilon)$ . Thus we obtain an internal boundary layer of width  $O(\varepsilon^{1/3})$ .

The integral in (3.15) is an incomplete Airy integral

$$(3.17) \quad A(z, \alpha) = \int_{z_0}^z \exp \left( -\frac{1}{3}s^3 + \alpha s \right) ds.$$

The function  $A(z, \alpha)$  satisfies the differential equation

$$(3.18) \quad \frac{d^2 A(z, \alpha)}{dz^2} = -(z^2 - \alpha) \frac{dA(z, \alpha)}{dz}, \quad z_0 \leq z \leq z_1.$$

Equation (3.17) is analogous to the incomplete Airy function, which arises in diffraction problems (Levey and Felsen (1969)). The asymptotic properties of  $A(z, \alpha)$ , for large  $\alpha$ , can be determined by Laplace's method and repeated integration by parts (Olver (1974)). We obtain

$$(3.19) \quad A(z, \alpha) \sim \frac{k(\alpha)}{2\sqrt{\alpha}} E(\tilde{z}) + O(1/\alpha)$$

where  $\tilde{z}$  is a regular function of  $z$  and  $k(\alpha)$  is a function of  $\alpha$ :

$$(3.20) \quad k(\alpha) = \exp \left[ \left( \frac{2}{3} \right) \alpha^{3/2} \right].$$

The result (3.19) ignores endpoint contributions, and is obtained by assuming that  $-\sqrt{3\alpha} < z_0$ . The condition on  $z_0$  can be further weakened, but it will not be necessary to do so in this work.

**3.3. Critical case: The Pearcey integral.** The analysis in § 3.2 is not valid at a critical type steady state, since  $b''(x_c, \eta_c, \delta_c) \equiv 0$ . Thus the Airy integral does not provide an adequate asymptotic representation. In order to obtain the expansion of (3.6), another term must be used in the Taylor expansion of  $\phi(x')$ . If a Taylor expansion of  $\phi$  up to  $(x - x_1)^4$  and two changes of variable are used, then (3.6) can be put into the form

$$(3.21) \quad v(x) = c \int_{\tilde{x}(x)}^{\tilde{x}(x)} \exp \left[ \frac{1}{\varepsilon} \left( \frac{1}{4} y^4 - \frac{\alpha y^2}{2} - \beta y \right) \right] dy + O(\varepsilon^{3/4})$$

where  $c$  is a constant,  $\tilde{x}(x)$  is a regular function of  $x$ . The parameters  $\alpha, \beta$  are functions of  $b'(x_1), b''(x_1), b'''(x_1)$  and  $a(x_1)$ , and vanish at the critical bifurcation. In this case, the boundary layer around  $x_1$  clearly has width  $O(\varepsilon^{1/4})$ .

The integral in (3.21) is the incomplete Pearcey integral

$$(3.22) \quad P(z, \alpha, \beta) = \int_{z_0}^z \exp \left[ \left( \frac{1}{4} s^4 - \frac{\alpha s^2}{2} - \beta s \right) \right] ds$$

and satisfies

$$(3.23) \quad \frac{d^2 P}{dz^2} = (z^3 - \alpha z - \beta) \frac{dP}{dz}, \quad z_0 \leq z \leq z_1.$$

An integral analogous to (3.22) was discovered by Pearcey (1946) during his investigation of the electromagnetic field at a cusped caustic. The asymptotic properties of  $P(z, \alpha, \beta)$ , for large  $\alpha, \beta$  can be determined by Laplace's method. Let  $\tilde{s}$  be the middle root of

$$(3.24) \quad s^3 - \alpha s - \beta = 0$$

and

$$(3.25) \quad \tilde{\gamma} = \frac{\tilde{s}^4}{4} - \alpha \frac{\tilde{s}^2}{2} - \beta \tilde{s}.$$

Then we find that

$$(3.26) \quad P(z, \alpha, \beta) \sim \begin{cases} \frac{e^{\tilde{\gamma}}}{\sqrt{\alpha}} E(\tilde{z}_1), & \alpha \text{ large, } |\beta| \text{ small, i.e., } |\beta^2|/\alpha^3 \ll 1, \\ e^{\tilde{\gamma}} k(\alpha, \beta) A(z'_1, \eta), & \alpha \text{ large, } |\beta| \text{ large, i.e. } \beta^2 = O(\alpha^3). \end{cases}$$

In (3.26),

$$(3.27) \quad k(\alpha, \beta) = \frac{1}{(3|\tilde{s}|)^{1/3}} \exp \left[ -\frac{2}{3} \left( \frac{3\tilde{s}^2 - \alpha}{2} \right)^3 \frac{1}{9\tilde{s}^2} \right].$$

The parameter  $\eta$  is given in terms of  $\alpha$  and  $\beta$ . The functions  $\tilde{z}_1$  and  $z'_1$  are regular functions of  $z$  and  $\alpha$  or  $\alpha$  and  $\beta$ . The results given in (3.26) are obtained by ignoring endpoint contributions to the integrals, so that we assume  $r_0 < z_0$  and  $z_1 < r_4$ , where  $r_0$  is the minimum and  $r_4$  is the maximum root of

$$(3.28) \quad \frac{s^4}{4} - \alpha \frac{s^2}{2} - \beta s = 0.$$

When  $\alpha$  is small and  $|\beta|$  is large (i.e.,  $\alpha^3/\beta^2 \ll 1$ ), the main contribution to (3.22) comes from the endpoints  $z_0$  and  $z_1$ , so that simple exponential estimates are obtained (Olver (1974, p. 80)).

Asymptotic analysis of the exact solution of a one dimensional version of (2.12) leads to special functions that satisfy inhomogeneous versions of (3.12), (3.18) and (3.23). The results given above indicate that it may be possible to solve the two dimensional problems (2.10, 12) by an asymptotic method. The separatrix would be surrounded by a boundary layer. Outside of the boundary layer  $u(x)$  is approximately constant and inside the boundary layer,  $u(x)$  changes rapidly. The width of the boundary layer will depend upon the type of deterministic dynamics. Consequently, we shall construct formal asymptotic solutions of the backward equation in the normal, marginal and critical cases. Although the solutions will be formal, the numerical results indicate that they are satisfactory.

The results obtained in this section could also have been obtained by the use of the method of matched asymptotic expansions (Nayfeh (1973)).

*Remark. Dual problems and their special functions.* There are three dynamical systems which are closely related to the ones discussed above. A study of the canonical problems leads to three "dual" special functions. The three cases are:

1) *The dual normal case* consists of a single, stable steady state in the tube. Instead

of the error integral, we are lead to a special function  $\hat{E}(z)$  that satisfies

$$(3.29) \quad \frac{d^2 \hat{E}}{dz^2} = z \frac{d\hat{E}}{dz}, \quad z_0 \leq z \leq z_1.$$

2) *The dual marginal case* is the same as the marginal case, except that the roles of  $Q_0$  and  $P_2$  are reversed. We are lead to the dual incomplete Airy integral  $\hat{A}(z, \alpha)$ , which satisfies

$$(3.30) \quad \frac{d^2 \hat{A}}{dz^2} = (z^2 - \alpha) \frac{d\hat{A}}{dz}, \quad z_0 \leq z \leq z_1.$$

3) *The dual critical case* is identical to the critical case, except that the critical type steady state is unstable. We are lead to the dual incomplete Pearcey integral  $\hat{P}(z, \alpha, \beta)$ , satisfying

$$(3.31) \quad \frac{d^2 \hat{P}}{dz^2} = -(z^3 - \alpha z - \beta) \frac{d\hat{P}}{dz}, \quad z_0 \leq z \leq z_1.$$

#### 4. Asymptotic solution of the first exit problem in the normal case.

**4.1. Normal type dynamical systems.** The reduced ( $\varepsilon = 0$ ) deterministic system corresponding to equation (2.10)

$$(4.1) \quad \dot{x}^i = b^i(x)$$

is assumed to have three steady states,  $P_0, P_1$ , and  $P_2$ . Let  $B_k = (b_{ij}^k)|_{P_k}$  denote the matrix obtained by linearizing  $b(x)$  and evaluating the result at  $P_k$ . We assume that  $B_0$  and  $B_2$  have two negative real eigenvalues and that  $P_0$  and  $P_2$  are bounded away from the separatrix tube. The matrix  $B_1$  has one real positive and one real negative eigenvalue. The eigenvector corresponding to the negative eigenvalue has positive slope. A deterministic system satisfying the above postulates will be structurally similar to the one sketched in Fig. 1.

It is assumed that  $a(x)$  is bounded above and is positive definite on the deterministic separatrix.

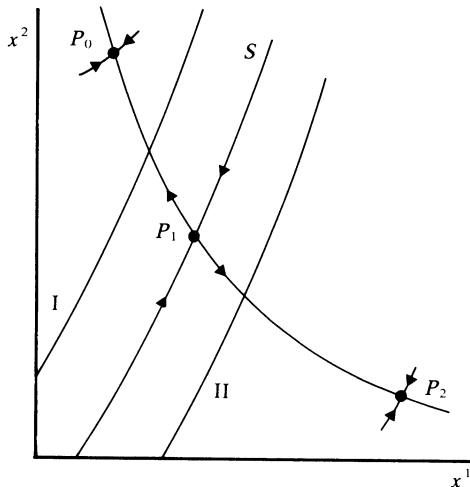


FIG. 1. The first exit problem in a dynamical system with multiple steady states (the normal type dynamical system is shown). One wishes to calculate the probability that a phase point initially in the tube defined by boundaries I, II exists through boundary II.

**4.2. The asymptotic solution.** The analysis of the one dimensional problem in § 3 indicates that a possible formal solution of the backward equation is

$$(4.2) \quad u(x) = \sum \varepsilon^n g^n(x) E(\psi(x)/\sqrt{\varepsilon}) + \varepsilon^{n+1/2} h^n(x) E'(\psi/\sqrt{\varepsilon}).$$

In (4.2),  $E(z)$  is the error integral:

$$(4.3) \quad E''(z) = -zE'(z), \quad z_0 \leq z \leq z_1.$$

The limits  $z_0, z_1$  are chosen so that (4.2) will satisfy the boundary conditions to within asymptotically small correction terms. The ansatz (4.2) was used by Mangel and Ludwig (1977). The theory of that paper is a special case of the theory presented in this section.

When derivatives of  $u(x)$  are evaluated, equation (4.3) is used to replace  $E''$  and  $E'''$  by products of  $E'$  and  $\psi/\sqrt{\varepsilon}$ . After derivatives are evaluated and substituted into (2.10) terms are collected according to powers of  $\varepsilon$ . We obtain

$$(4.4) \quad \begin{aligned} 0 = \sum_{n=0} \varepsilon^{n-1/2} (g^n - \psi h^n) & \left( b^i \psi_i - \frac{a^{ij}}{2} \psi_i \psi_j \psi \right) E'(\psi/\sqrt{\varepsilon}) \\ & + \varepsilon^n \left( b^i g_i^n + \frac{a^{ij}}{2} g_{ij}^{n-1} + c^i g_i^{n-1} \right) E(\psi/\sqrt{\varepsilon}) \\ & + \varepsilon^{n+1/2} \left\{ b^i h_i^n + a^{ij} g_i^n \psi_j + \frac{a^{ij}}{2} g^n \psi_{ij} + g^n c^i \psi_i - c^i h^n \psi_i \psi + c^i h_i^{n-1} - \psi a^{ij} h_i^n \psi_j \right. \\ & \left. + \frac{a^{ij}}{2} h_{ij}^{n-1} - \frac{a^{ij}}{2} h^n ((\psi \psi_i)_i) \right\}. \end{aligned}$$

In equation (4.4), if the superscript of  $g^n$  or  $h^n$  is less than zero, that term is set equal to zero. The leading term,  $n = 0$ , is composed of three parts and vanishes if

$$(4.5) \quad b^i \psi_i - \frac{a^{ij}}{2} \psi_i \psi_j \psi = 0,$$

$$(4.6) \quad b^i g_i^0 = 0,$$

$$(4.7) \quad b^i h_i^0 + \frac{a^{ij}}{2} g^0 \psi_{ij} + a^{ij} g_i^0 \psi_j - h_i^0 a^{ij} \psi \psi_j + g^0 c^i \psi_i - c^i h^0 \psi \psi_i - \frac{a^{ij}}{2} h^0 ((\psi \psi_i)_i) = 0.$$

Equation (4.5) is analogous to the eikonal equation of optics. It is obtained independently of  $g^n(x)$  and  $h^n(x)$ . Since  $b^i = dx^i/dt$ , equation (4.6) indicates that

$$(4.8) \quad \frac{dg^0}{dt} = 0.$$

Thus  $g^0$  is constant on trajectories. In § 4.3 we show that the constant is the same on all trajectories. Once  $\psi$  and  $g^0$  are known,  $h^0$  can be calculated from equation (4.7). Here we explicitly treat equations (4.5)–(4.7). Higher order terms are treated in an analogous fashion (Mangel (1977)).

### 4.3. Determination of $\psi$ and $g^0$ : Contours of probability.

**4.3.1. Determination of  $\psi(x)$ .** The transformation  $\phi = -\frac{1}{2}\psi^2$  converts equation (4.5) to

$$(4.9) \quad b^i \phi_i + \frac{a^{ij}}{2} \phi_i \phi_j = 0.$$

Equation (4.9) is the Hamilton–Jacobi equation or eikonal equation (see also Cohen

and Lewis (1967), Ventcel and Freidlin (1970)). It corresponds to a Hamiltonian

$$(4.10) \quad H(x, p) = \frac{1}{2} a^{ij} p_i p_j + b^i p_i,$$

and Lagrangian

$$(4.11) \quad L(x, \dot{x}) = \frac{1}{2} a_{ij} (\dot{x}^i - b^i)(\dot{x}^j - b^j),$$

where  $(a_{ij}) = (a^{ij})^{-1}$  and

$$(4.12) \quad H(x, p) + L(x, \dot{x}) = \dot{x}^i p_i.$$

According to Hamilton–Jacobi theory,  $\phi(x)$  is the minimum value of the integral of the Lagrangian taken over all paths joining  $x_0$  and  $x$ . If  $x_0$  is the saddle point, then  $\phi \equiv 0$  on the separatrix, since  $L(x, \dot{x}) \equiv 0$  if  $\dot{x}^i = b^i$ . Thus  $\phi = \psi = 0$  on the separatrix  $\mathcal{S}$ .

Since equation (4.9) is nonlinear, it may have solutions in which  $\phi(x)$  is nonzero on the separatrix. Consequently, by setting  $\phi = \psi = 0$  on  $\mathcal{S}$ , we are imposing an extra condition on  $\psi(x)$ . This condition can not be determined directly from equation (4.5) or (4.9). If  $\psi$  is nonzero on  $\mathcal{S}$ , then the first derivatives of  $\psi$  must vanish on  $\mathcal{S}$ . In this case, it is not possible to construct a solution that approaches zero on one side of the separatrix and one on the other side.

Equations (4.5) and (4.9) with initial data on  $\mathcal{S}$  represent singular characteristic initial value problems. We will show that the singularity (the saddle point) allows the unique determination of  $\psi(x)$ . Elsewhere, we give an existence proof for this type of initial value problem (Mangel (1977a)).

The most interesting experiments begin in the vicinity of the separatrix. Consequently, we will now determine  $\psi(x)$  by a Taylor expansion, for points near  $\mathcal{S}$ . Elsewhere, we show how  $\psi(x)$  can be calculated in the entire plane by the method of characteristics (Mangel (1977a)).

When equation (4.5) is differentiated and evaluated on  $\mathcal{S}$ , we obtain

$$(4.13) \quad \frac{d\psi_k}{dt} + b^i_{,k} \psi_i - \frac{a^{ij}}{2} \psi_i \psi_j \psi_k = 0, \quad k = 1, 2,$$

where  $d\psi_k/dt = b^i \psi_{ik}$ . Since  $\psi$  is constant on  $\mathcal{S}$ , the tangential derivative of  $\psi$  vanishes. Then equation (4.13) can be used to derive an equation for the normal derivative of  $\psi$ :

$$(4.14) \quad \frac{d\psi_n}{dt} + \hat{b} \psi_n - \frac{\hat{a} \psi_n^3}{2} = 0 \quad \text{on } \mathcal{S}.$$

In equation (4.14)

$$(4.15) \quad \hat{b}(t) = [(b^2)^2 b^1_{,1} - b^1 b^2 (b^2_{,1} + b^1_{,2}) + (b^1)^2 b^2_{,2}] / ((b^1)^2 + (b^2)^2)$$

$$(4.16) \quad \frac{\hat{a}}{2} = [a^{11}((b^2)^4 + (b^1)^2(b^2)^2) - 2a^{12}((b^1)^3 b^2 + b^1(b^2)^3) + a^{22}((b^1)^2(b^2)^2 + (b^1)^4)] / (((b^1)^2 + (b^2)^2)^2).$$

Equation (4.14) is a version of Abel's equation (Davis (1962, p. 75)) and is solved by introducing  $z(t)$  defined by

$$(4.17) \quad \psi_n = [B(t)z(t)]^{-1},$$

where  $B'(t) = \hat{b}B$ . The solution of (4.14) is

$$(4.18) \quad \psi_n(t) = \left\{ \int_t^\infty \hat{a}(s) \exp \left[ -2 \int_t^s \hat{b}(s') ds' \right] ds \right\}^{-1/2}.$$

Equation (4.18) satisfies the condition

$$(4.19) \quad \psi_n(\infty) = \sqrt{\frac{2\hat{b}(\infty)}{\hat{a}(\infty)}},$$

which is consistent with (4.14) at the saddle point (where  $t = \infty$  and  $d\psi_n/dt = 0$ ). The higher derivatives of  $\psi$ , up to order  $r$  can be calculated in an analogous fashion, if deterministic equations are  $C^r$ .

**4.3.2. Determination of  $z_0, z_1$  and  $g^0$ .** We first suppose that the boundaries I and II are level curves of  $\psi(x)$ , say  $\psi = \psi_I$  on I and  $\psi = \psi_{II}$  on II. We set  $z_0 = \psi_I$  and  $z_1 = \psi_{II}$  in (4.3). To leading order  $u = 0$  on boundary I, and  $u = 1$  on boundary II if

$$(4.20) \quad g^0 = \frac{1}{E(\psi_{II}/\sqrt{\varepsilon})}.$$

In light of (4.8),  $g^0 = 1/E(\psi_{II}/\sqrt{\varepsilon})$  on all trajectories that intersect boundary II. Since all trajectories in the lower half plane intersect at  $P_2$ ,  $g^0 = 1/E(\psi_{II}/\sqrt{\varepsilon})$  on all those trajectories. In particular,  $g^0$  has the above value on the trajectory from  $P_1$  to  $P_2$ . Thus,  $g_0$  has the above value on the trajectory from  $P_1$  to  $P_0$ . If this were not so, equation (4.8) would be violated when  $t$  is replaced by  $-t$ . Since all trajectories in the upper half plane intersect at  $P_0$ ,  $g^0 = 1/E(\psi_{II}/\sqrt{\varepsilon})$  on all of these trajectories. Thus,  $g^0$  is constant in the entire phase plane.

If  $\psi(x)$  is not constant on I and II, then  $u(x)$  will not be 0 or 1 on the boundaries, but will be close to 0 or 1. Let  $\psi_I^0, \psi_I^1$  be the minimum and maximum values of  $\psi$  on I. We set  $z^0 = \psi_I^0$ . Then on I,  $u(x)$  is not zero, but

$$(4.21) \quad u(x) \leq g^0 E(\psi_I^1/\sqrt{\varepsilon}) = g^0 \int_{\psi_I^0/\sqrt{\varepsilon}}^{\psi_I^1/\sqrt{\varepsilon}} e^{-s/2} ds.$$

An integration by parts yields

$$(4.22) \quad u(x) \leq \sqrt{\varepsilon} \left[ \frac{e^{-(\psi_I^0)^2/\varepsilon}}{\psi_I^0} - \frac{e^{-(\psi_I^1)^2/\varepsilon}}{\psi_I^1} \right] g^0 + O(\varepsilon^{3/2}).$$

Thus, if  $\psi_I^0$  and  $\psi_I^1$  are bounded away from 0,  $u(x)$  will be exponentially small on boundary I. This restriction is an implicit assumption about the boundaries. (Also see Appendix B for an alternative treatment.)

If  $\psi_{II}^1$  is the maximum value of  $\psi$  on II, we set

$$(4.23) \quad g^0 = \frac{1}{E(\psi_{II}^1/\sqrt{\varepsilon})}.$$

An argument similar to the one above shows that on boundary II:

$$(4.24) \quad |1 - u(x)| \leq \sqrt{\varepsilon} \left[ \frac{e^{-(\psi_{II}^0)^2/\varepsilon}}{\psi_{II}^0} - \frac{e^{-(\psi_{II}^1)^2/\varepsilon}}{\psi_{II}^1} \right] g^0 + O(\varepsilon^{3/2}),$$

where  $\psi_{II}^0$  is the minimum value of  $\psi(x)$  on boundary II.

With the above choices of  $z_0, z_1$  and  $g^0$ , the ansatz (4.2) will satisfy the boundary conditions to within exponentially small correction terms.

**4.3.3. Contours of probability.** Once  $\psi$  and  $g^0$  are known, the leading term in the expansion of  $u(x)$  is

$$(4.25) \quad u(x) \sim g^0 E(\psi(x)/\sqrt{\varepsilon}) + O(\varepsilon^{1/2}).$$

Since  $\psi_t$  vanishes on the separatrix, in a vicinity of the separatrix

$$(4.26) \quad \psi(x) = \psi_n(x_s) \delta n + O(\delta n^2)$$

where  $x_s$  is a point on the separatrix and  $\delta n$  is the distance from  $x_s$  to  $x$ .

Contours of equal probability are obtained when  $\psi(x)$  is a constant. Thus, to leading order, we obtain contours at distances  $\delta n = 1/\psi_n$  from the separatrix.

**4.4. Completion of the first term: Evaluation of  $h^0$ .** Since  $\psi = 0$  on the separatrix, equation (4.7) becomes

$$(4.27) \quad \frac{dh^0}{dt} - \frac{a^{ij}}{2} h^0 \psi_i \psi_j = -\frac{a^{ij}}{2} \psi_{ij} g^0 - g^0 c^i \psi_i.$$

At the saddle point,  $dh^0/dt$  vanishes. Equation (4.27) can then be solved for  $h^0(P_1)$ :

$$(4.28) \quad h^0(P_1) = \frac{a^{ij} \psi_{ij} g^0 + 2g^0 c^i \psi_i}{a^{ij} \psi_i \psi_j} \Big|_{P_1} \equiv K.$$

The solution of (4.28) which satisfies (4.29) is

$$(4.29) \quad h^0(t) = \frac{\int_t^\infty p(s) [(a^{ij}/2) \psi_{ij} + c^i \psi_i] g^0 ds + K}{p(t)},$$

where

$$(4.30) \quad \rho(s) = \exp \left[ \int_s^\infty \frac{a^{ij}}{2} \psi_i \psi_j dt' \right]$$

and  $K$  is given by equation (4.28).

Once  $h^0(t)$  is known on  $\mathcal{S}$ , equation (4.7) can be used to calculate  $h^0$  in the plane. Since the separatrix is a characteristic curve of (4.7), the problem as posed is a characteristic initial value problem. Elsewhere, we show how the above problem can be converted to a noncharacteristic initial value problem and  $h^0$  calculated everywhere in the plane. The existence proof for solutions of (4.7), with initial data on the separatrix is analogous to the existence proof given in Mangel (1977a). In a vicinity of the separatrix,  $h^0$  can be calculated by a Taylor expansion exactly as  $\psi(x)$  was calculated.

## 5. Asymptotic solution of the first exit problem in the marginal case.

**5.1. Marginal type dynamical systems.** The deterministic evolution of the macrovariable is governed by

$$(5.1) \quad \dot{x} = b(x, \eta)$$

where  $\eta \in R^1$  is a parameter. Equation (5.1) may have three steady states,  $Q_0(\eta)$ ,  $Q_1(\eta)$  and  $P_2$ . Let  $B_k$  be the matrix  $(b_{ij}')$  evaluated at  $Q_0$ ,  $Q_1$  or  $P_2$ ,  $k = 0, 1, 2$ . We assume that:

1) For all values of  $\eta$ ,  $B_2$  has two real negative eigenvalues. Although  $P_2$  may depend upon  $\eta$ ,  $P_2$  is always bounded away from the separatrix tube.

2) As  $\eta \downarrow 0$ , the distance between  $Q_0(\eta)$  and  $Q_1(\eta)$  decreases. When  $\eta = 0$ ,  $Q_0$  and  $Q_1$  coalesce and annihilate each other (i.e. when  $\eta < 0$ , (5.1) has one real and two complex steady states).

3) When  $\eta > 0$ ,  $B_0$  has two real negative eigenvalues and  $B_1$  has one real positive and one real negative eigenvalue. When  $\eta = 0$ ,  $B_0 = B_1$  has one zero and one real negative eigenvalue. The eigenvector corresponding to the negative eigenvalue has positive slope. The double point  $Q_0(0)/Q_1(0)$  is called a saddle node (Andronov et al. (1973)).

A deterministic system satisfying the above assumptions will be structurally similar to the system sketched in Fig. 2.

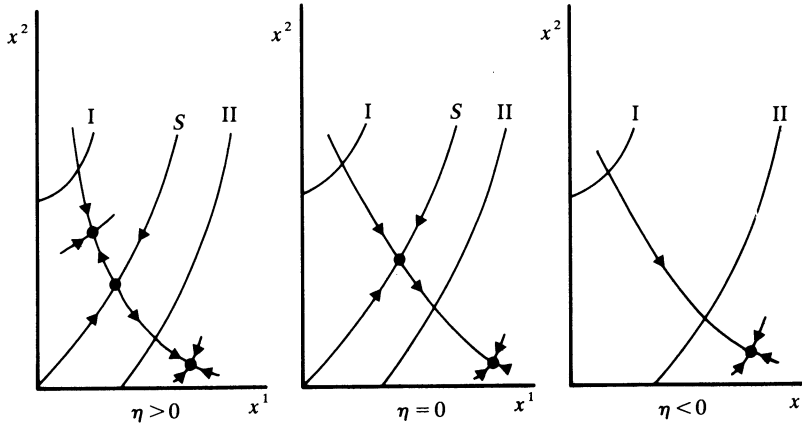


FIG. 2. The marginal type dynamical system. When  $\eta > 0$ , there are two steady states in the separatrix tube. As  $\eta \downarrow 0$ , the two steady states approach each other and coalesce at  $\eta = 0$ . When  $\eta < 0$ , the two steady states in the tube are annihilated.

The above conditions can be reformulated by a change of coordinates. Define the  $y^1$  axis in the direction of the eigenvector of the nonnegative eigenvalue of  $B_1$ . The  $y^2$  axis is in the direction of the eigenvector of the negative eigenvalue of  $B_1$ , with the origin at  $Q_1$ . Then

$$(5.2) \quad \dot{y} = \tilde{b}(y, \eta)$$

is the deterministic system in the new coordinates. The system is of the marginal type if:

$$(5.3) \quad \begin{aligned} 1) & \det(b_{ij}^1(Q_1, 0)) = 0, \\ 2) & \tilde{b}_{1,1}^1(Q_1, 0) = \tilde{b}_{1,1}^2(Q_1, 0) = 0, \\ 3) & \tilde{b}_{2,2}^2(Q_1, 0) \neq 0, \\ 4) & \tilde{b}_{1,1}^1(Q_1, 0) - \tilde{b}_{1,1}^2(Q_1, 0) \neq 0. \end{aligned}$$

## 5.2. The asymptotic solution.

**5.2.1. Breakdown of the error approximation.** If one wishes to use the theory of § 4 to solve the backward equation, then  $\psi(x)$ , the argument of the error integral, must satisfy

$$(5.4) \quad b^i \psi_i - \frac{a^{ij} \psi_i \psi_j}{2} \psi = 0.$$

In the marginal case,  $b(x)$  vanishes at two points  $Q_0$  and  $Q_1$ . In § 4.3 we showed that  $\psi(Q_1) = 0$ . It is clear that  $\psi(Q_0)$  must be less than  $\psi(Q_1)$ . Thus, at  $Q_0$ , the  $\psi_i$  must vanish or be infinite and  $\psi(x)$  is no longer a regular function. If  $\psi(x)$  is to be regular, the error integral must be replaced by a more complicated special function.



**5.2.2. Uniform solution in terms of the Airy integral.** The analysis presented in § 3 indicates that the uniform solution of the backward equation in the marginal case can be given in terms of the Airy integral and its derivative. In analogy to § 4.2 we seek a formal solution of (2.10) of the form

$$(5.5) \quad u(x) = \sum \varepsilon^n g^n(x) A(\psi/\varepsilon^{1/3}, \alpha/\varepsilon^{2/3}) + \varepsilon^{n+2/3} h^n(x) A'(\psi/\varepsilon^{1/3}, \alpha/\varepsilon^{2/3}).$$

In equation (5.5), the parameter  $\alpha$  and functions  $\psi(x)$ ,  $g^n(x)$  and  $h^n(x)$  are to be determined. The function  $A(z, \beta)$  is the Airy integral and satisfies

$$(5.6) \quad \frac{d^2 A}{dz^2} = -(z^2 - \beta) \frac{dA(z, \beta)}{dz}, \quad z_0 \leq z \leq z_1.$$

When the derivatives of  $u(x)$  are evaluated, equation (5.6) is used to replace  $A''$  by products of  $A'$  and  $(\psi^2 - \alpha)/\varepsilon^{2/3}$ . Following Lynn and Keller (1970) we assume that

$$(5.7) \quad \alpha = \sum \alpha_k \varepsilon^k.$$

After derivatives are evaluated and substituted into the backward equation (2.10), terms are collected according to powers of  $\varepsilon$ . We obtain:

$$(5.8) \quad \begin{aligned} 0 = & \sum_{n=0} \varepsilon^{n-1/3} A' (g^n - (\psi^2 - \alpha_0) h^n) \left( b^i \psi_i - (\psi^2 - \alpha_0) \frac{a^{ij}}{2} \psi_i \psi_j \right) \\ & + \sum_{n=0} \varepsilon^n A \left( b^i g_i^n + \frac{a^{ij}}{2} g_{ij}^{n-1} + c^i g_i^{n-1} \right) \\ & + \sum_{n=0} \varepsilon^{n+2/3} A' \left( b^i h_i^n + c^i g^n \psi_i - c^i \psi_i (\psi^2 - \alpha_0) h^n + c^i h_i^{n-1} + \frac{a^{ij}}{2} g^n \psi_{ij} \right. \\ & \quad \left. + a^{ij} g_i^n \psi_j + \frac{a^{ij}}{2} h_{ij}^{n-1} - (\psi^2 - \alpha_0) a^{ij} h_i^n \psi_j - h^n \frac{a^{ij}}{2} (\psi_i (\psi^2 - \alpha_0))_j \right. \\ & \quad \left. + \sum_{k=1}^{n+1} \alpha_k \left\{ h^{n+1-k} \left( b^i \psi_i - (\psi^2 - \alpha_0) \frac{a^{ij}}{2} \psi_i \psi_j \right) \right. \right. \\ & \quad \left. \left. + \frac{a^{ij}}{2} \psi_i \psi_j (g^{n+1-k} - (\psi^2 - \alpha_0) h^{n+1-k}) \right\} \right. \\ & \quad \left. + \sum_{k=1}^n \alpha_k \left( c^i \psi_i h^{n-k} + \frac{a^{ij}}{2} (2 h_i^{n-k} \psi_j + h^{n-k} \psi_{ij}) \right) + \sum_{k=2}^{n+1} \frac{a^{ij}}{2} \psi_i \psi_j h^{n-k+1} \left( \sum_{j=1}^{k-1} \alpha_j \alpha_{k-j} \right) \right). \end{aligned}$$

In equation (5.8), if a superscript is less than zero, that term is set equal to zero.

The leading term ( $n = 0$ ) is composed of three parts and will vanish if

$$(5.9) \quad b^i \psi_i - \frac{a^{ij}}{2} \psi_i \psi_j (\psi^2 - \alpha_0) = 0,$$

$$(5.10) \quad b^i g_i^0 = 0,$$

$$(5.11) \quad \begin{aligned} & b^i h_i^0 - h^0 \frac{a^{ij}}{2} ((\psi_i (\psi^2 - \alpha_0))_j) - (\psi^2 - \alpha_0) a^{ij} h_j^0 \psi_i \\ & - \alpha_1 \frac{a^{ij}}{2} \psi_i \psi_j (g^0 - (\psi^2 - \alpha_0) h^0) + \frac{a^{ij}}{2} g^0 \psi_{ij} + c^i \psi_i g^0 + c^i \psi_i h^0 (\psi^2 - \alpha_0) = 0. \end{aligned}$$

Equations (5.9, 10) were used in obtaining (5.11).

From equation (5.9) we see that  $\psi(x)$  will be a regular function of  $x$ . The field  $b(x)$  vanishes at two points  $Q_0, Q_1$ . We require that  $\psi^2 = \alpha_0$  at these two points. Since

$\psi(Q_1) > \psi(Q_0)$  for the problem as formulated, we set  $\psi(Q_0) = -\sqrt{\alpha_0}$  and  $\psi(Q_1) = \sqrt{\alpha_0}$ .

Here, we explicitly treat (5.9)–(5.11). Higher order terms can be treated in an analogous fashion (Mangel (1977a)).

**5.3. Evaluation of the parameter  $\alpha_0$ .** The substitution  $\phi = -\frac{1}{3}\psi^3 + \alpha_0\psi - \frac{2}{3}\alpha_0^{3/2}$  converts (5.9) to the eikonal equation (4.9). An argument analogous to the one in § 4.3 shows that  $\psi = \sqrt{\alpha_0}$  on the entire separatrix  $\mathcal{S}$ . The parameter  $\alpha_0$  must be determined so that (5.9) is satisfied with initial data  $\psi = \sqrt{\alpha_0}$  on the separatrix and the additional condition that  $\psi = -\sqrt{\alpha_0}$  at  $Q_0$ . The one additional condition allows the unique determination of  $\alpha_0$ .

The following iterative procedure can be used to determine  $\alpha_0$ . An initial choice of  $\alpha_0, \alpha_0^{(0)}$  is made. We set  $\psi = -\sqrt{\alpha_0^{(0)}}$  at  $Q_0$ . Equation (5.9) is then solved by the method of characteristics (Courant (1962)). When the method of characteristics is used, the phase plane is covered by a family of trajectories called rays. The rays are generated from the system of ordinary differential equations

$$(5.12) \quad \frac{dx^i}{ds} = b^i - a^{ij}p_j(\psi^2 - \alpha_0),$$

$$(5.13) \quad \frac{d\psi}{ds} = \frac{dx^i}{ds} \cdot p_i$$

$$(5.14) \quad \frac{dp_k}{ds} = -b^i_{,k}p_i + 2a^{ij}\psi p_i p_j p_k + \frac{a^{ij}_{,k}}{2}p_i p_j(\psi^2 - \alpha_0),$$

where  $p_i = \psi_i$ . Some of the rays emanating from  $Q_0$  will hit the separatrix  $\mathcal{S}$ . If  $\psi \neq \sqrt{\alpha_0^{(0)}}$  on  $\mathcal{S}$ , then  $\alpha_0^{(0)}$  must be replaced by an improved estimate of  $\alpha_0, \alpha_0^{(1)}$ . The method of false position (Dennis and More (1977)) can be used to calculate increments in  $\alpha_0$ . The above procedure can be repeated until  $\alpha_0$  is determined to any desired accuracy. As the estimates  $\alpha_0^{(n)}$  approach the true value  $\alpha_0$ , the rays will begin to bend and run parallel to the separatrix, which is itself a ray. An indication that a ray is approaching the separatrix is that  $b^i\psi_i = \psi_i \rightarrow 0$ . This criterion can be used in numerical determination of  $\alpha_0$ .

An equivalent procedure would follow rays that emanate from the saddle  $Q_1$  and approach  $Q_0$ . If  $\psi$  does not approach  $-\sqrt{\alpha_0^{(0)}}$  as the ray approaches  $Q_0$ , the estimate of  $\alpha_0^{(0)}$  must be modified. A priori it is not clear which technique is preferable. The decision must be made on the basis of practicality.

**5.4. Determination of  $\psi$  and  $g^0$ : Contours of probability.** A procedure analogous to the one in § 4.3 yields the following equation for  $\psi_n(t)$  on  $\mathcal{S}$ :

$$(5.14a) \quad \frac{d\psi_n}{dt} + \hat{b}\psi_n - \sqrt{\alpha_0} \hat{a}\psi_n^3 = 0.$$

When  $\alpha_0 > 0$ , i.e. the two points have not coalesced, equation (5.14a) can be treated exactly as (4.14) was. Elsewhere we show that the constructions given here are regular at the marginal bifurcation (Mangel (1977a)).

Similarly, the values of  $z_0, z_1$  and  $g_0$  can be determined as in § 4.3, except that the error integral is replaced by the incomplete Airy integral. When  $g^0$  is evaluated, the expansion of the Airy integral (3.19) can be used to simplify the evaluation of  $g^0$ .

Once  $\psi$  and  $g^0$  are known, the leading part of the formal expansion for the first exit probability is

$$(5.15) \quad u(x) \sim g^0 A(\psi(x)/\varepsilon^{1/3}, \alpha_0/\varepsilon^{2/3}) + O(\varepsilon^{2/3}).$$

Equation (5.15) can be used to generate contours of equal probability.

**5.5. Completion of the first term: Calculation of  $h^0$  and  $\alpha_1$ .** The function  $h^0(x)$  must satisfy equation (5.11). Since  $\psi^2 = \alpha_0$  on the separatrix, on  $\mathcal{S}$  the equation for  $h^0$  is

$$(5.16) \quad \frac{dh^0}{dt} - h^0 a^{ij} [\sqrt{\alpha_0} \psi_i \psi_j] = \left( \alpha_1 \frac{a^{ij}}{2} \psi_i \psi_j - \frac{a^{ij}}{2} \psi_{ij} - c^i \psi_i \right) g^0.$$

We assume that  $\alpha_0 > 0$ , i.e. that  $Q_0$  and  $Q_1$  are distinct. Elsewhere, we show how to calculate  $h^0$  when  $\alpha_0 = 0$  Mangel (1977a)).

Since  $d/dt = b^i \partial/\partial x^i$ , at the saddle point equation (5.16) becomes an algebraic equation, with solution

$$(5.17) \quad h^0(Q_1) = \frac{(\alpha_1 a^{ij} \psi_i \psi_j - a^{ij} \psi_{ij} - 2c^i \psi_i)}{-2\sqrt{\alpha_0} a^{ij} \psi_i \psi_j} g^0 \Big|_{Q_1}.$$

If  $p(t)$  is defined by

$$(5.18) \quad p(t) = \int_t^\infty a^{ij} \psi_i \psi_j \sqrt{\alpha_0} ds,$$

then the solution of (5.16) satisfying (5.17) is

$$(5.19) \quad h^0(t) = \frac{-\int_t^\infty \exp(p(s)) g^0 [\alpha_1 (a^{ij} \psi_i \psi_j)/2 - a^{ij} \psi_{ij}/2 - c^i \psi_i] ds + h^0(Q_1)}{\exp(p(t))}.$$

Once  $h^0(t)$  is known on the separatrix, it can be determined everywhere in the plane by the method of characteristics (Mangel (1977a)).

The parameter  $\alpha_1$  is still undetermined. It can be approximately calculated as follows. The field  $b(x)$  vanishes at  $Q_0$ , where  $\psi = -\sqrt{\alpha_0}$ . At  $Q_0$ , equation (5.16) becomes

$$(5.20) \quad h^0(Q_0) = \frac{(\alpha_1 a^{ij} \psi_i \psi_j - a^{ij} \psi_{ij} - 2c^i \psi_i)}{2\sqrt{\alpha_0} a^{ij} \psi_i \psi_j} g^0 \Big|_{Q_0}.$$

When  $Q_0$  and  $Q_1$  are close together, we determine  $h^0$  at  $Q_0$  by a Taylor expansion

$$(5.21) \quad h^0(Q_0) \approx h^0(Q_1) + v_i \delta x^i,$$

where  $v_i = \partial h^0 / \partial x^i|_{Q_1}$ . The parameter  $\alpha_1$  is chosen so that equations (5.20) and (5.21) agree.

A more exact determination of  $\alpha_1$  uses the method of characteristics, as the calculation of  $\alpha_0$  did. A manifold  $\mathcal{S}'$  can be determined on which (5.16) is not a characteristic initial value problem. Then, equation (5.16) can be solved by the method of characteristics, starting at  $Q_1$ . When a ray reaches  $Q_0$ ,  $h^0$  should have the value given in (5.20). If the value of  $h^0$  at  $Q_0$ , when calculated by the method of characteristics, is not the same as the value given in (5.20), then the estimate of  $\alpha_1$  must be modified. The method of false position can be used to calculate the iterates of  $\alpha_1$ .

## 6. Asymptotic solution of the first exit problem in the critical case.

**6.1. Critical type dynamical systems.** The macrovariables evolve according to a deterministic kinetic equation

$$(6.1) \quad \dot{x} = b(x, \eta, \delta)$$

where  $\eta, \delta$  are one-dimensional parameters. The physical systems of interest here motivate the following assumptions about the bifurcation set of (6.1):

1) For some values of  $\eta$ ,  $\delta$ , (6.1) has three steady states  $P_0(\eta, \delta)$ ,  $P_1(\eta, \delta)$  and  $P_2(\eta, \delta)$ . All three steady states are contained in the separatrix tube. If  $B_k = (b_{ij}^k)$  evaluated at  $P_k$ , then when the three steady states are distinct,  $B_0$  and  $B_2$  have real negative eigenvalues.  $B_1$  has one real negative and one real positive eigenvalue. The eigenvector corresponding to the negative eigenvalue has positive slope.

2) As  $\eta$ ,  $\delta$  vary, two of the steady states may coalesce and annihilate each other. This behavior is analogous to the marginal bifurcation.

3) As  $\eta$ ,  $\delta$  vary, all three steady states may move together and coalesce when  $\eta = \delta = 0$ . At the critical bifurcation,  $B_1 = (b_{ij}^1)$  has a zero eigenvalue. We assume that the steady state remaining after the critical bifurcation is a stable steady state.

A deterministic system satisfying the above postulates will be structurally similar to the one sketched in Fig. 3.

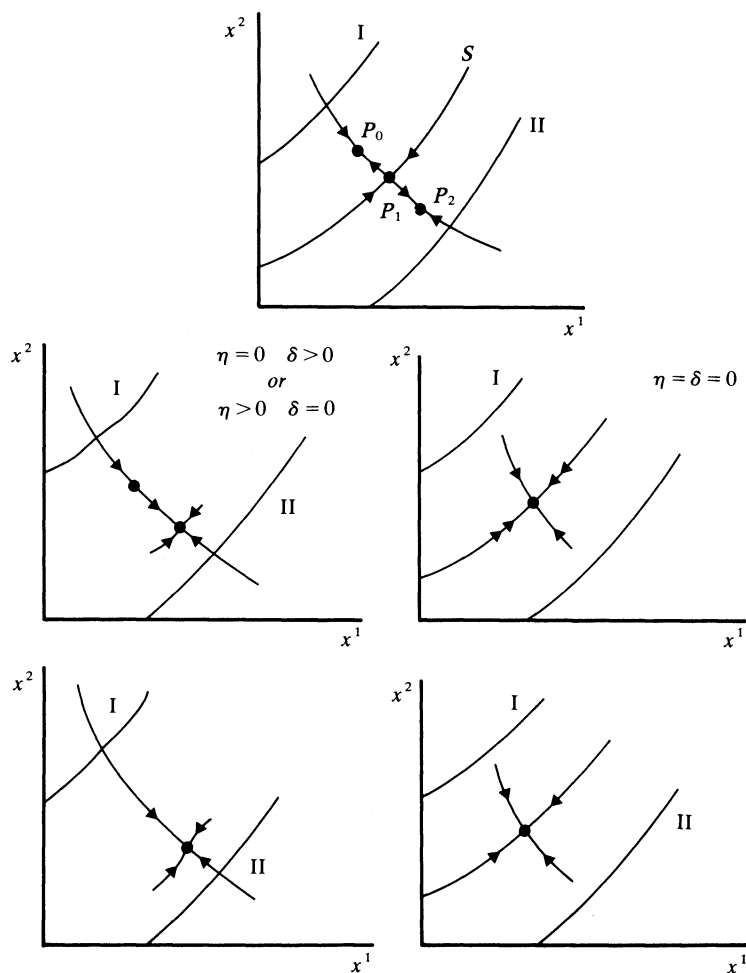


FIG. 3. The critical type dynamical system. When  $\eta$  and  $\delta$  are both greater than zero, there are three steady states in separatrix tube. When  $\eta = \delta = 0$ , the three coalesce to a weakly attracting stable steady state.

The above properties can be restated in terms of a new coordinate system as follows. The  $y^1$  axis is in the direction of the eigenvector of the nonnegative eigenvalue of  $B_1$ . The  $y^2$  axis is in the direction of the eigenvector of the negative eigenvalue, with

the origin at  $P_1$ . The deterministic evolution is then

$$(6.2) \quad \dot{y} = \tilde{b}(y, \eta, \delta).$$

A dynamical system is a critical type system if:

$$(6.3) \quad \begin{aligned} &1) \det(b^i_{,j}(P_1, 0, 0)) = 0; \\ &2) \tilde{b}^1_{,1}(P_1, 0, 0) = \tilde{b}^2_{,1}(P_1, 0, 0); \\ &\quad = \tilde{b}^1_{,11}(P_1, 0, 0) = \tilde{b}^2_{,11}(P_1, 0, 0) = 0; \\ &3) \tilde{b}^2_{,2}(P_1, 0, 0) \neq 0; \\ &4) \tilde{b}^1_{,111}(P_1, 0, 0) = \tilde{b}^2_{,111}(P_1, 0, 0) \neq 0. \end{aligned}$$

## 6.2. The asymptotic solution.

**6.2.1. Breakdown of solutions using the Airy integral.** If the theory of § 5 were used in the critical case, the argument of the Airy integral would have to satisfy

$$(6.4) \quad b^i \psi_i - \frac{a^{ij}}{2} \psi_i \psi_j (\psi^2 - \alpha_0) = 0.$$

Since the deterministic field now vanishes at three points in the separatrix tube, expression (6.4) indicates that  $\psi(x)$  will not be regular at the third steady state. If we wish to construct a solution in which  $\psi(x)$  is regular, the Airy integral must be replaced by a more complicated special function.

**6.2.2. Uniform solution in terms of the Pearcey integral.** The analysis in § 3 and results in §§ 4 and 5 indicate that a possible formal solution of the backward equation in the critical case is

$$(6.5) \quad \begin{aligned} u(x) = &\sum \varepsilon^n g^n(x) P(\psi(x)/\varepsilon^{1/4}, \alpha/\varepsilon^{1/2}, \beta/\varepsilon^{3/4}) \\ &+ \varepsilon^{n+3/4} h^n(x) P'(\psi(x)/\varepsilon^{1/4}, \alpha/\varepsilon^{1/2}, \beta/\varepsilon^{3/4}) \end{aligned}$$

where the parameters  $\alpha, \beta$  and functions  $\psi(x)$ ,  $h^n(x)$  and  $g^n(x)$  are to be determined. The function  $P(z, \alpha, \beta)$  is the Pearcey integral, satisfying

$$(6.6) \quad \frac{d^2 P}{dz^2}(z, \alpha, \beta) = (z^3 - \alpha z - \beta) \frac{dP(z, \alpha, \beta)}{dz}, \quad z_0 \leq z \leq z_1.$$

When the derivatives of  $u(x)$  are evaluated, equation (6.6) is used to replace  $P''$  by products of  $P'$  and  $(\psi^3 - \alpha\psi - \beta)/\varepsilon^{3/4}$ . We assume that  $\alpha$  and  $\beta$  have asymptotic expansions of the form

$$(6.7) \quad \alpha = \sum \varepsilon^k \alpha_k, \quad \beta = \sum \beta_k \varepsilon^k.$$

After derivatives of  $u(x)$  are evaluated and substituted into the backward equation

(2.10), terms are collected according to powers of  $\varepsilon$ . We obtain

$$\begin{aligned}
 0 = & \sum_{n=0} \varepsilon^{n-1/4} P'(g^n + h^n(\psi^3 - \alpha_0\psi - \beta_0)) \left( b^i \psi_i + \frac{a^{ij}}{2} \psi_i \psi_j (\psi^3 - \alpha_0\psi - \beta_0) \right) \\
 & + \sum_{n=0} \varepsilon^n P \left( b^i g_i^n + \frac{a^{ij}}{2} g_{ij}^{n-1} + c^i g_i^{n-1} \right) \\
 & + \sum_{n=0} \varepsilon^{n+3/4} P' \left\{ b^i h_i^n + c^i g_i^n + c^i h_i^{n-1} + h^n c^i \psi_i (\psi^3 - \alpha_0\psi - \beta_0) + a^{ij} g_i^n \psi_j \right. \\
 & \quad + \frac{a^{ij}}{2} h_{ij}^{n-1} + \frac{a^{ij}}{2} g^n \psi_{ij} + (\psi^3 - \alpha_0\psi - \beta_0) a^{ij} h_i^n \psi_j \\
 & \quad + \frac{a^{ij}}{2} h^n (\psi_i (\psi^3 - \alpha_0\psi - \beta_0))_j \\
 & \quad - \sum_{k=1}^{n+1} (\psi \alpha_k + \beta_k) \left\{ \frac{a^{ij}}{2} \psi_i \psi_j (g^{n+1-k} + h^{n+1-k} (\psi^3 - \alpha_0\psi - \beta_0)) \right. \\
 & \quad \quad \left. + h^{n+1-k} \left( b^i \psi_i + \frac{a^{ij}}{2} \psi_i \psi_j (\psi^3 - \alpha_0\psi - \beta_0) \right) \right\} \\
 & \quad + \sum_{k=2}^{n+1} \frac{a^{ij}}{2} \psi_i \psi_j h^{n-k+1} \left( \sum_{j=1}^{k-1} (\psi \alpha_j + \beta_j) (\psi \alpha_{k-j} + \beta_{k-j}) \right) \\
 & \quad - \sum_{k=1}^n (\psi \alpha_k + \beta_k) \left( c^i \psi_i h^{n-k} - \frac{a^{ij}}{2} (2h_i^{n-k} \psi_j + h^{n-k} \psi_{ij}) \right) \\
 & \quad \left. - \sum_{k=1}^n \alpha_k \frac{a^{ij}}{2} \psi_i \psi_j h^{n-k} \right\}.
 \end{aligned}
 \tag{6.8}$$

In (6.8), if a superscript is less than zero, that term is set equal to zero.

The first term in (6.8) is composed of three parts and will vanish if

$$b^i \psi_i + \frac{a^{ij}}{2} \psi_i \psi_j (\psi^3 + \alpha_0\psi - \beta_0) = 0, \tag{6.9}$$

$$b^i g_i^0 = 0, \tag{6.10}$$

$$\begin{aligned}
 & b^i h_i^0 + \frac{a^{ij}}{2} g^0 \psi_{ij} + (\psi^3 - \alpha_0\psi - \beta_0) a^{ij} h_i^0 \psi_j + \frac{a^{ij}}{2} h^0 \psi_{ij} (\psi^3 - \alpha_0\psi - \beta_0) \\
 & \quad + h^0 \frac{a^{ij}}{2} \psi_i \psi_j (3\psi^2 - \alpha_0) \\
 & \quad - (\psi \alpha_1 + \beta_1) f^0(\psi, 1) + g^0 c^i \psi_i + c^i \psi_i h^0 (\psi^3 - \alpha_0\psi - \beta_0) = 0,
 \end{aligned}
 \tag{6.11}$$

where we have denoted

$$\begin{aligned}
 f^n - (\psi, l) = & \sum_{k=l}^{n+1} \frac{a^{ij}}{2} \psi_i \psi_j (g^{n+1-k} + h^{n+1-k} (\psi^3 - \alpha_0\psi - \beta_0)) \\
 & + h^{n+1-k} \left( b^i \psi_i + \frac{a^{ij}}{2} \psi_i \psi_j (\psi^3 - \alpha_0\psi - \beta_0) \right).
 \end{aligned}
 \tag{6.12}$$

The field  $b(x)$  vanishes at  $P_0$ ,  $P_1$  and  $P_2$ . The function  $\psi(x)$  will remain regular if  $\psi^3 - \alpha_0\psi - \beta_0$  vanishes at the points where  $b(x)$  vanishes. Let  $\psi_0 \leq \psi_1 \leq \psi_2$  denote the ordered roots of

$$\psi^3 - \alpha_0\psi - \beta_0 = 0. \tag{6.13}$$

We then set  $\psi(P_0) = \tilde{\psi}_0$ ,  $\psi(P_1) = \tilde{\psi}_1$  and  $\psi(P_2) = \tilde{\psi}_2$ .

Here we treat equations (6.9)–(6.11) explicitly. Higher order terms are discussed in (Mangel (1977a)).

**6.3. Determination of the parameters  $\alpha_0$  and  $\beta_0$ .** The transformation  $\phi = \frac{1}{4}\psi^4 - \alpha_0\psi^2/2 - \beta_0\psi - \frac{1}{4}\tilde{\psi}_1^4 + \alpha_0\tilde{\psi}_1^2/2 + \beta_0\tilde{\psi}_1$  converts equation (6.9) to the eikonal equation (4.9). An argument using Hamiltonian–Jacobi theory, as in § 4.3 shows that  $\psi = \tilde{\psi}_1$  on the entire separatrix.

Equation (6.9) must be solved with initial data on the separatrix and the two extra conditions  $\psi(P_0) = \tilde{\psi}_0$  and  $\psi(P_2) = \tilde{\psi}_2$ . The two extra conditions allow the unique determination of  $\alpha_0$  and  $\beta_0$ . As in § 5.3, an iterative procedure is used to determine  $\alpha_0$  and  $\beta_0$ .

Initial estimates,  $\alpha_0^{(0)}$  and  $\beta_0^{(0)}$ , are used in (6.9). Equation (6.9) is solved by the method of characteristics, starting close to the saddle point where  $\psi = \tilde{\psi}_1$  and  $\tilde{\psi}_1$  is the middle root of

$$(6.14) \quad \psi^3 - \alpha_0^{(0)}\psi - \beta_0^{(0)} = 0.$$

Some rays emanating from  $P_1$  will approach  $P_0$ , others will approach  $P_2$ . As  $P_0$  is approached,  $\psi$  should approach  $\tilde{\psi}_0$ ; as  $P_2$  is approached  $\psi$  should approach  $\tilde{\psi}_2$ . If  $\psi(P_0)$ ,  $\psi(P_2)$  are not  $\tilde{\psi}_0$ ,  $\tilde{\psi}_2$ , then the values of the parameters must be modified. The method of false position can be used to calculate iterates of  $\alpha_0$  and  $\beta_0$ . This procedure can be repeated until  $\alpha_0$  and  $\beta_0$  are determined to any order of accuracy.

**6.4. Determination of  $\psi$  and  $g^0$ : Contours of probability.** Using the procedure outlined in § 4.3 the following equation can be derived for  $\psi_n(t)$  on the separatrix

$$(6.15) \quad \frac{d\psi_n}{dt} + \hat{b}\psi_n + \frac{\hat{a}}{2}\psi_n^3(3\tilde{\psi}_1^2 - \alpha_0) = 0.$$

We assume that the three steady states have not coalesced, so that  $\tilde{\psi}_1$  and  $\alpha_0$  are not both zero. Elsewhere we show that the constructions given here are regular at the critical bifurcation. Equation (6.15) can be treated exactly as (4.14) was treated.

Similarly,  $z_0$ ,  $z_1$  and  $g^0$  can be calculated as in § 4.2, except that the error integral is replaced by the incomplete Pearcey integral. When  $g^0$  is evaluated, the expansions (3.26) can be used to simplify numerical calculation.

Once  $\alpha_0$ ,  $\beta_0$ ,  $\psi$  and  $g^0$  are known, the leading term in the formal expansion of  $u$  is

$$(6.16) \quad u(x) \sim g^0 P(\psi/\varepsilon^{1/4}, \alpha_0/\varepsilon^{1/2}, \beta_0/\varepsilon^{3/4}) + O(\varepsilon^{3/4}).$$

Equation (6.16) can be used to generate contours of equal probability.

**6.5. Completion of the first term: Calculation of  $h^0$ ,  $\alpha_1$  and  $\beta_1$ .** The function  $h^0$  must be determined from equation (6.11). On the separatrix, where  $\psi = \tilde{\psi}_1$  and  $\psi^3 - \alpha_0\psi - \beta_0$  vanishes, (6.11) becomes

$$(6.17) \quad \frac{dh^0}{dt} + h^0 \frac{a^{ij}}{2} \psi_i \psi_j (3\tilde{\psi}_1^2 - \alpha_0) = (\tilde{\psi}_1 \alpha_1 + \beta_1) \frac{a^{ij}}{2} g^0 \psi_i \psi_j - g^0 c^i \psi_i - \frac{a^{ij}}{2} g^0 \psi_{ij}.$$

Since  $d/dt = b^i \partial/\partial x^i$ , at the saddle point  $P_1$  equation (6.17) becomes

$$(6.18) \quad h^0(P_1) = \frac{((\tilde{\psi}_1 \alpha_1 + \beta_1) a^{ij} \psi_i \psi_j - 2c^i \psi_i - a^{ij} \psi_{ij})}{(3\tilde{\psi}_1^2 - \alpha_0) a^{ij} \psi_i \psi_j} g^0 \Big|_{P_1}.$$

If  $p(t)$  is defined by

$$(6.19) \quad p(t) = \int_t^\infty (3\tilde{\psi}_1^2 - \alpha_0) \frac{a^{ij}}{2} \psi_i \psi_j ds,$$

and

$$(6.20) \quad f(t) = \left( -(\tilde{\psi}_1 \alpha_1 + \beta_1) \frac{a^{ij}}{2} \psi_i \psi_j + c^i \psi_i + \frac{a^{ij} \psi_{ij}}{2} \right) g^0,$$

the solution of (6.17) satisfying (6.18) is

$$(6.21) \quad h^0(t) = \frac{\int_t^\infty f(s) e^{-p(s)} ds + h^0(P_1)}{\exp[-p(t)]}.$$

Once  $h^0(t)$  is known on the separatrix, it can be determined everywhere in the plane, by the method of characteristics, as described in Mangel (1977a).

The parameters  $\alpha_1$  and  $\beta_1$  are still undetermined. They can be determined by using the method of characteristics, in a manner analogous to the calculation of  $\alpha_0$  and  $\beta_0$ .

A new manifold  $\mathcal{S}'$  can be constructed, with  $h^0$  known on  $\mathcal{S}'$ , so that (6.11) is not a characteristic initial value problem. Then (6.11) can be solved by the method of characteristics. Some rays emanating from  $\mathcal{S}'$  will approach  $P_0$  or  $P_2$ , where  $h^0$  must have the value

$$(6.22) \quad h^0(P_k) = \frac{((\tilde{\psi}_k \alpha_1 + \beta_1) a^{ij} \psi_i \psi_j - 2c^i \psi_i - a^{ij} \psi_{ij})}{(3\tilde{\psi}_k^2 - \alpha_0) a^{ij} \psi_i \psi_j} g^0 \Big|_{P_k}, \quad k = 0, 2.$$

If the value of  $h^0$  at  $P_k$ , when calculated by the method of characteristics, is not the same as the value determined from (6.22), then the estimates of  $\alpha_1$  and  $\beta_1$  must be improved. The method of false position can be used to calculate iterates of  $\alpha_1$  and  $\beta_1$ .

**6.6. Two complex steady states with small imaginary parts.** When  $\eta < 0$  (marginal case) or  $\eta < 0$ ,  $\delta < 0$  (critical case) only one real steady state exists. There will be two complex steady states. If the imaginary parts of the complex steady states are small, then the linear part of the deterministic equations about the real steady state will be small. Consequently, the dynamics at the steady state are almost completely nonlinear. This situation will correspond to an almost algebraic (rather than exponential) decay of perturbations to the real steady state. The error integral, which corresponds to nonvanishing linear dynamics, will not provide an adequate asymptotic solution of the first exit problem. The Pearcey integral, however, can be used to provide an adequate asymptotic solution.

When the ansatz (6.5) is used, the function  $\psi(x)$  must satisfy (6.9). In order to determine  $\alpha_0$  and  $\beta_0$  by the method of characteristics, complex rays would be needed. An easier, although less accurate, technique uses power series for  $\alpha_0$ ,  $\beta_0$ . It is possible to derive power series of the form (Mangel (1977a))

$$(6.23a) \quad \alpha_0 = \sum_{i,j}^r A_{ij} \eta^i \delta^j$$

$$(6.23b) \quad \beta_0 = \sum_{i,j}^r B_{ij} \eta^i \delta^j.$$

The power series extend up to order  $r$ , in  $\eta$  and  $\delta$ , if the deterministic equations are  $C^r$  in  $\eta$  and  $\delta$ . Since we are using power series, the results given in this section are valid only in a neighborhood of the origin in  $(\eta, \delta)$  space.



The value of  $\psi$  on the separatrix is  $\psi_r$ , where  $\psi_r$  is the real root of

$$(6.24) \quad \psi^3 - \alpha_0\psi - \beta_0 = 0.$$

Using the technique in § 6.4 we can calculate the value of  $\psi$  in a neighborhood of the separatrix by a Taylor expansion. The value of  $g^0$  can be determined as described in § 4.3. Thus, the leading term of the first exit probability is

$$(6.25) \quad u(x) \sim g^0 P(\psi(x)/\varepsilon^{1/4}, \alpha_0/\varepsilon^{1/2}, \beta_0/\varepsilon^{3/4}).$$

Our solution is approximate in the following sense. Since  $\alpha_0, \beta_0$  are only given as power series, equation (6.9) is not satisfied identically, but must be replaced by

$$b^i \psi_i + \frac{a^{ij} \psi_i \psi_j}{2} (\psi^3 - \alpha_0\psi - \beta_0) = O(\eta^{r+1} + \delta^{r+1}).$$

Let  $\mathcal{L}$  indicate the backward operator. Then, our formal result will satisfy the backward operator to an order of  $\varepsilon\eta\delta$ :

$$(6.26) \quad \mathcal{L}u = O(\varepsilon^{-1/4}(\eta^{r+1} + \delta^{r+1})).$$

The estimate (6.26) indicates how close  $\eta, \delta$  must be to the origin for our ansatz to be valid. Unlike all previous results, which were independent of  $\varepsilon$ , the validity of the extension presented in this section is dependent upon  $\varepsilon$ .

**Appendix A. Asymptotic solution of the expected time equation.** Let  $T(x)$  be defined by

$$(A.1) \quad T(x) = E\{\min t : \tilde{x}(t) \in \mathcal{R}, \tilde{x}(t') \notin \mathcal{R}, t' < t | \tilde{x}(0) = x, \tilde{x}(t) \text{ hits } \mathcal{R}\}.$$

Then  $T(x)$  is the expected amount of time it takes the process to hit  $\mathcal{R}$  starting at  $x$ . In § 2, we showed that  $T(x)$  satisfies the backward equation (Gihman and Skorohod (1972))

$$(A.2) \quad \frac{\varepsilon a^{ij}}{2} T_{ij} + b^i T_i + \varepsilon c^i T_i = -u(x).$$

In (A.2),  $u(x)$  is the probability of eventually reaching  $\mathcal{R}$ , conditioned on  $\tilde{x}(0) = x$ . Equation (A.2) is an inhomogeneous backward equation. In this appendix, we give the asymptotic solution of (A.2). The solutions are closely related to the solutions in §§ 4–6, so that only the first term will be considered. Equation (A.2) must be supplemented by boundary conditions. Let  $d$  be the distance from  $x$  to  $\mathcal{R}$ .

The first boundary condition is

$$(A.3) \quad T(x) \equiv 0, \quad x \in \mathcal{R}.$$

As a second boundary condition, we require that  $T(x)$  be bounded as  $|d| \rightarrow \infty$ . In Feller's terminology (Feller (1952)), we are requiring that  $\infty$  be an "entrance boundary". Feller's theory applies to one-dimensional systems and there is no analogous two-dimensional theory. On the other hand, the second boundary condition is in accord with intuition for the systems of interest here.

**A.1. Normal case.** The results presented in § 4 and the asymptotic analysis of a one-dimensional version of (A.2) indicate that a possible solution of (A.2) is

$$(A.4) \quad T(x) = \sum \varepsilon^n g^n F(\psi(x)/\sqrt{\varepsilon}) + \varepsilon^{n+1/2} h^n(x) F'(\psi(x)/\sqrt{\varepsilon}) + \varepsilon^n k^n(x).$$

In (A.4),  $g^n(x)$ ,  $h^n(x)$ ,  $k^n(x)$  and  $\psi(x)$  are to be determined. The function  $F(z)$  satisfies

$$(A.5) \quad \frac{d^2 F(z)}{dz^2} = -z \frac{dF}{dz} - 1, \quad z_0 \leq z \leq z_1.$$

Equation (A.5) is an inhomogeneous version of the equation that the error integral satisfies.

When derivatives are evaluated, (A.5) is used to replace  $F''$  by  $(-\psi F'/\sqrt{\varepsilon} - 1)$ . After substitution into equation (A.2), terms are collected according to powers of  $\varepsilon$ . The leading term ( $n = 0$ ) vanishes if the following equations are satisfied:

$$(A.6) \quad O(F'/\sqrt{\varepsilon}): b^i \psi_i - \frac{a^{ij}}{2} \psi_i \psi_j \psi = 0,$$

$$(A.7) \quad O(F): b^i g_i^0 = 0,$$

$$(A.8) \quad O(\varepsilon^0): b^i k_i^0 - \frac{a^{ij}}{2} \psi_i \psi_j g^0 = -u(x),$$

$$(A.9) \quad O(\varepsilon^{1/2} F'): b^i h_i^0 + \frac{a^{ij}}{2} g^0 \psi_{ij} - h_i^0 a^{ij} \psi_j \psi - h^0 c^i \psi_i \psi + g^0 c^i \psi_i - h^0 \frac{a^{ij}}{2} [(\psi \psi_i)_j] = 0.$$

Equations (A.6), (A.7), (A.9) are identical to equations (4.5)–(4.7). Thus, the constructions in § 4.3 for  $\psi$  and  $h^0$  are applicable here. Equation (A.7) indicates that  $g^0$  is constant on trajectories. The argument in § 4.3 shows that  $g^0$  has the same value on all trajectories.

At the saddle point  $P_1$ ,  $b(x)$  vanishes. Equation (A.8) becomes

$$(A.10) \quad \frac{-a^{ij}}{2} \psi_i \psi_j g^0 = -u(P_1).$$

Thus, the value of  $g^0$  is  $g^0 = 2u(P_1)/a^{ij} \psi_i \psi_j$ . Once  $g^0$  is known,  $k^0$  can be calculated by the method of characteristics if initial data are given. We assume that  $\mathcal{R}$  is not a characteristic curve, and set  $k^0 = 0$  on  $\mathcal{R}$ . (If  $\mathcal{R}$  is a characteristic curve, then the equation (A.8) must be treated by a more complicated procedure (Mangel (1977a)).)

We also assume, without losing generality, that  $\psi = \psi_0$  on  $\mathcal{R}$ . Then, we set  $z_0 = \psi_0/\sqrt{\varepsilon}$  and  $F(\psi_0/\sqrt{\varepsilon}) = F'(\psi_0/\sqrt{\varepsilon}) = 0$  in equation (A.4). With the above choices,  $T(x) \equiv 0$  if  $x \in \mathcal{R}$ . If  $\mathcal{R}$  is not a level curve of  $\psi$ , then  $T(x)$  will not identically vanish if  $x \in \mathcal{R}$  but will be exponentially small (§ 4.3).

**A.2. Marginal case.** The above solution for  $T(x)$  breaks down in the marginal case for the same reason that the solution for  $u(x)$  that used the error integral broke down (§ 5.2.1). Based on the ansatz given in § 5 and the expansion of a simpler problem, we seek a solution of (A.2) of the form

$$(A.11) \quad T(x) = \sum \varepsilon^n g^n(x) B(\psi/\varepsilon^{1/3}, \alpha/\varepsilon^{2/3}, 1/\varepsilon^{1/3}, \gamma) \\ + \varepsilon^{n+2/3} h^n(x) B'(\psi/\varepsilon^{1/3}, \alpha/\varepsilon^{2/3}, 1/\varepsilon^{1/3}, \gamma) + \varepsilon^n k^n(x).$$

In (A.11), the function  $B(z, \alpha, \gamma_1, \gamma_2)$  satisfies an inhomogeneous version of the equation that the Airy integral satisfies:

$$(A.12) \quad \frac{d^2 B(z; \alpha, \gamma_1, \gamma_2)}{dz^2} = -(z^2 - \alpha) \frac{dB}{dz} - \gamma_1 + \gamma_2 z, \quad z_0 \leq z.$$

When derivatives of  $T(x)$  are calculated, (A.12) is used to replace  $B''$  by terms involving

$B'$ ,  $\psi$ ,  $\alpha$  and  $\gamma$ . We assume that

$$(A.13) \quad \alpha = \sum \alpha_k \varepsilon^k \quad \text{and} \quad \gamma = \sum \gamma_k \varepsilon^k.$$

After derivatives of  $T(x)$  are calculated and substituted into equation (A.2), terms are collected according to powers of  $\varepsilon$ . The leading term ( $n^* = 0$ ) vanishes if

$$(A.14) \quad O(\varepsilon^{-1/3} B'): b^i \psi_i - \frac{a^{ij}}{2} \psi_i \psi_j (\psi^2 - \alpha_0) = 0,$$

$$(A.15) \quad O(\varepsilon^0 B): b^i g_i^0 = 0,$$

$$(A.16) \quad O(\varepsilon^0): b^i k_i^0 + \frac{a^{ij}}{2} \psi_i \psi_j g^0 (-1 + \psi \gamma_0) = -u(x).$$

The  $O(\varepsilon^{2/3} B')$  term vanishes if  $h^0$  satisfies equation (5.11). Equation (A.14) is identical to (5.9). Thus, the constructions for  $\psi$ ,  $\alpha_0$  and  $h^0$  in § 5 can be used here. Equation (A.15) indicates that  $g^0$  is a constant on trajectories. The argument used in § 4.3 shows that  $g^0$  has the same value on all trajectories.

In the marginal case, the vector field  $b(x)$  vanishes at two points  $Q_0, Q_1$  within the domain of interest. At these two points, (A.16) becomes

$$(A.17) \quad \frac{a^{ij} \psi_i \psi_j}{2} g^0 (-1 + \psi \gamma_0)|_{Q_k} = -u(Q_k), \quad k = 1, 2.$$

Equation (A.17) provides two equations for  $g^0$  and  $\gamma_0$ . At the marginal bifurcation, an application of l'Hôpital's rule shows that  $\gamma_0 = 0$ . Equation (A.17) still provides one equation (at the saddle-node  $Q$ ) for  $g^0$ :

$$(A.18) \quad \frac{-a^{ij} \psi_i \psi_j}{2} g^0|_Q = -u(Q).$$

Once  $g^0$  and  $\gamma_0$  are known,  $k^0$  can be calculated as described above.

We also assume that  $\mathcal{R}$  is a level curve of  $\psi$ , say  $\psi = \psi_0$  on  $\mathcal{R}$ . Then, in (A.12) we set  $z_0 = \psi_0 / \varepsilon^{1/3}$  and  $B(z_0) = B'(z_0) = 0$ . With these choices,  $T(x) \equiv 0$  on  $\mathcal{R}$ .

If  $\mathcal{R}$  is a characteristic curve, or  $\psi$  is not constant on  $\mathcal{R}$ , the remarks of the previous section apply.

**A.3. Critical case.** The solution in the previous section will break down if the domain of interest contains three steady states or the deterministic system exhibits the critical bifurcation. Based on the results in § 6 and the expansion of a simpler problem, we seek a solution of (A.2) of the form

$$(A.19) \quad T(x) = \sum \varepsilon^n g^n(x) Q(\psi / \varepsilon^{1/4}; \alpha / \varepsilon^{1/2}, \beta / \varepsilon^{3/4}, 1 / \varepsilon^{1/4}, \gamma_1, \varepsilon^{1/4} \gamma_2) \\ + \varepsilon^{n+3/4} h^n(x) Q'(\psi / \varepsilon^{1/4}; \alpha / \varepsilon^{1/2}, \beta / \varepsilon^{3/4}, 1 / \varepsilon^{1/4}, \gamma_1, \varepsilon^{1/4} \gamma_2) + \varepsilon^n k^n(x).$$

In (A.19), the function  $Q(z; \alpha, \beta, \gamma_1, \gamma_2)$  satisfies

$$(A.20) \quad \frac{d^2 Q}{dz^2} = (z^3 - \alpha z - \beta) \frac{dQ}{dz} - \gamma_1 + \gamma_2 z + \gamma_3 z^2, \quad z_0 \leq z.$$

When derivatives of  $T(x)$  are evaluated, (A.20) is used to replace  $Q''$  by terms involving  $Q'$ ,  $\alpha$ ,  $\beta$ ,  $\gamma_1$  and  $\gamma_2$ . After derivatives are evaluated and substituted into (A.2), terms are collected according to powers of  $\varepsilon$ . We assume that

$$(A.21) \quad \alpha = \sum \alpha_k \varepsilon^k, \quad \beta = \sum \beta_k \varepsilon^k, \\ \gamma_1 = \sum \gamma_{1k} \varepsilon^k, \quad \gamma_2 = \sum \gamma_{2k} \varepsilon^k.$$

The first term of the asymptotic solution vanishes if

$$(A.22) \quad O(\varepsilon^{-1/4}Q'): b^i\psi_i + \frac{a^{ij}}{2}\psi_i\psi_j(\psi^3 - \alpha_0\psi - \beta_0) = 0,$$

$$(A.23) \quad O(\varepsilon^0Q): b^i g_i^0 = 0,$$

$$(A.24) \quad O(\varepsilon^0): b^i k_i^0 + g^0(-1 + \gamma_{10}\psi + \gamma_{20}\psi^2) \frac{a^{ij}\psi_i\psi_j}{2} = -u(x).$$

The  $O(\varepsilon^{3/4}Q')$  term vanishes if  $h^0$  satisfies equation (6.11). Equation (A.22) is identical to (6.9). Thus, the constructions given in § 6 for  $\psi$ ,  $\alpha_0$ ,  $\beta_0$  and  $h^0$  are applicable here.

At the nodes  $P_0$ ,  $P_2$  and saddle point  $P_1$ ,  $b(x)$  vanishes. Equation (A.24) becomes

$$(A.25) \quad g^0(-1 + \gamma_{10}\psi(P_k) + \gamma_{20}\psi^2(P_k)) \frac{a^{ij}\psi_i\psi_j}{2} = -u(P_k), \quad k = 0, 1, 2.$$

The constants  $g^0$ ,  $\gamma_{10}$  and  $\gamma_{20}$  can be determined from (A.25). Once  $g^0$ ,  $\gamma_{10}$  and  $\gamma_{20}$  are known,  $k^0$  can be determined as described in § A.1. At the critical bifurcation  $\gamma_{10} = \gamma_{20} = 0$ . We assume that  $\mathcal{R}$  is a level curve of  $\psi$ ,  $\psi = \psi_0$  on  $\mathcal{R}$ . Then, in (A.20), we set  $z_0 = \psi_0/\varepsilon^{1/4}$  and  $Q(z_0) = Q'(z_0) = 0$ . If  $k^0 \equiv 0$  on  $\mathcal{R}$ , then  $T(x) \equiv 0$  on  $\mathcal{R}$ .

**Appendix B. Formal satisfaction of the boundary conditions.** By extending the method of Cohen and Lewis (1967, pp. 284–285), it is formally possible to satisfy the boundary conditions  $u = 0$  on I and  $u = 1$  on II exactly. The solutions constructed in §§ 3–6 will be called interior solutions. To be concrete, consider the normal case, so that the interior solution,  $u^{\text{int}}$ , is given in terms of the error integral and its derivative. We now construct boundary solutions,  $u^{\text{I}}(x)$ ,  $u^{\text{II}}(x)$  such that

$$(B.1) \quad u^{\text{int}} + u^{\text{I}}(x) = 0 \quad \text{on I,}$$

$$(B.2) \quad u^{\text{int}} + u^{\text{II}}(x) = 1 \quad \text{on II.}$$

We shall give the construction to satisfy (B.1); the construction used to satisfy (B.2) is analogous. Let  $s(x)$  measure the distance from  $x$  to I. Let  $N(s(x)) \equiv N(x)$  be a neutralizer:  $N(x)$  is a  $C^\infty$  function,  $N(0) = 1$  and  $N$  rapidly approaches zero as  $s$  increases. We construct a boundary solution of the form

$$(B.3) \quad u^{\text{I}}(x) = \sum_{n=0} \varepsilon^n g_{\text{I}}^n(x) E(\psi^{\text{I}}(x)/\sqrt{\varepsilon}) N(x) + \sum_{n=0} \varepsilon^{n+1/2} h_{\text{I}}^n(x) E'(\psi^{\text{I}}(x)/\sqrt{\varepsilon}) N(x).$$

In (B.3),  $\psi^{\text{I}}(x)$ , the  $g_{\text{I}}^n(x)$  and  $h_{\text{I}}^n(x)$  are to be determined. Substitution of (4.2) and (B.3) into (B.1) yields:

$$(B.4) \quad \begin{aligned} & \sum_{n=0} \varepsilon^n g_{\text{int}}^n E(\psi^{\text{int}}(x)/\sqrt{\varepsilon}) + \varepsilon^{n+1/2} h_{\text{int}}^n(x) E'(\psi^{\text{int}}(x)/\sqrt{\varepsilon}) \\ & + \varepsilon^n g_{\text{I}}^n(x) E(\psi^{\text{I}}(x)/\sqrt{\varepsilon}) N(x) + \varepsilon^{n+1/2} h_{\text{I}}^n(x) E'(\psi^{\text{I}}(x)/\sqrt{\varepsilon}) N(x) = 0. \end{aligned}$$

for  $x \in \text{I}$ .

From (B.4), we set

$$(B.5) \quad \psi^{\text{I}}(x) = \psi^{\text{int}}(x) \quad \text{for } x \in \text{I},$$

$$(B.6) \quad g_{\text{int}}^n + N(x) g_{\text{I}}^n(x) = 0 \quad \text{for } x \in \text{I},$$

$$(B.7) \quad h_{\text{int}}^n + N(x) h_{\text{I}}^n(x) = 0 \quad \text{for } x \in \text{I}.$$

Since  $u^{\text{I}}(x)$  must satisfy the backward equation (2.10), we can derive the equations that  $\psi^{\text{I}}$ ,  $g_{\text{I}}^n$  and  $h_{\text{I}}^n$  satisfy by using the procedure in § 4. Equations (B.5)–(B.7) are then used to provide initial data when the ray equations are integrated.

An analogous procedure is followed at boundary II, and in the marginal and critical cases.

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