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Non-simple Turning Points and Cusps

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Stimulated by a problem in the theory of thermal ignition, we prove some results on non-simple turning points and corresponding cusps for two parameter-dependent non-linear problems. These results provide a theoretical basis for the numerical computation of non-simple turning points or cusps. The numerical procedure is illustrated for the thermal ignition problem.

0. Introduction

THIS PAPER is concerned with the computation of a special kind of bifurcation point which may arise in non-linear problems of the form

$$f(\lambda, \mu, x) = 0, \tag{0.1}$$

where $\lambda, \mu \in \mathbf{R}$, $x \in \mathbf{X}$, a Banach space, and f is a C^3 mapping from $\mathbf{R} \times \mathbf{R} \times \mathbf{X} \to \mathbf{X}$. Our interest in such equations was stimulated by a problem in the theory of thermal ignition discussed in Fradkin & Wake (1977) and Bazley & Wake (1979). They consider non-linear problems of the form

$$\begin{aligned} Lx &= h(\lambda, \mu, x), \\ Bx &= 0, \end{aligned} \tag{0.2}$$

where L is a uniformly elliptic differential operator, B is a boundary operator, λ is a rate parameter, μ is related to the activation energy, and h has the form

$$h(\lambda, \mu, x) = \lambda \exp\,(x/(1+\mu x)).$$

The solution x is the dimensionless temperature and the typical solution behaviour is shown in Fig. 3(a) below, where, for $\mu \leqslant \mu_0$, the curves exhibit turning point (or limit point) behaviour. Of particular interest are the values λ_0 and μ_0 which correspond to the loss of criticality in the exothermic reaction described by (0.2) (see Boddington, Gray & Robinson, 1979). As can be seen from Figs 1(a), (b) and 3(a) these values correspond to the point where two "simple" turning points coalesce to produce a "non-simple" turning point. (These terms will be made precise by definition 1.2.)

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Two parameter problems arise in many physical applications. One example, closely related mathematically to (0.2), is the model of the steady-state behaviour of the continuously stirred Tank Reactor described in Ray (1977). A different example is discussed by Keller & Szeto (1980) who provide extensive computations of the Navier–Stokes equations for the steady viscous flow of an incompressible fluid between two rotating discs. The two parameters involved in this problem represent the Reynolds number and the disc speed ratio.

Simple turning points are well analysed in many papers, Amann (1976), Anselone & Moore (1966), Brezzi, Rappaz & Raviart (1981), Crandall & Rabinowitz (1973), Decker & Keller (1982), Keller (1977), Moore & Spence (1980, 1981), Werner (1980), and numerical methods for continuation through or the computation of such points are well developed and can now be regarded as standard operations. However, the numerical computation of non-simple turning points seems to be rarely considered.

The major aim of this paper is to present an approach for the stable computation of non-simple turning points. The main idea is that, in a sense to be made precise in Section 3, the non-simple turning point is a simple turning point of a larger "extended system", provided certain conditions are satisfied. Hence we can use our standard methods for simple turning points on this larger problem to give the required non-simple turning point. We also explore the connection between the non-simple turning point and the cusp curve in the λ, μ plane.

The plan of the paper is as follows. In Section 1 we give a brief treatment of the theory of turning points of one parameter problems. The approach follows that given in Crandall & Rabinowitz (1973) and Werner (1980). Section 2 contains a discussion about "extended systems" used originally by Keener & Keller (1973). The main results of our paper are contained in Section 3 where the analysis of two parameter problems is presented. The key theorem which provides the theoretical basis for our numerical approach, Theorem 3.1, is proved, and also the link between non-simple turning points and cusps is made explicit. Numerical results for an equation of the form (0.2) are given in Section 4.

1. Analysis of Turning Points

In this section we recall some of the main results about turning points of non-linear problems depending on a parameter. Specifically let $\mathbf{X}$ be a Banach space and consider the C^3 mapping

$$g: \begin{cases} \mathbf{R} \times \mathbf{X} \to \mathbf{X} \\ (\lambda, x) \to g(\lambda, x). \end{cases}$$

We denote by $g_\lambda(a)$, $g_x(a)$, $g_{\lambda\lambda}(a)$, $g_{\lambda x}(a)$, $g_{xx}(a)$, $g_{xxx}(a), \ldots$, the partial (Frechet-) derivatives of g at $a = (\lambda, x) \in \mathbf{R} \times \mathbf{X}$. We shall use the simple notation, ψx, to denote the dual pairing of $x \in \mathbf{X}$ and $\psi \in \mathbf{X}'$.

Definition 1.1 A zero $a_0 = (\lambda_0, x_0)$ of g is called a *turning point* of g with respect to λ if the following properties hold

$$\operatorname{Ker} g_x(a_0) = \{\alpha\phi_0 \mid \alpha \in \mathbf{R}\}, \quad \phi_0 \in \mathbf{X}, \quad \phi_0 \neq 0, \tag{1.1}$$

$$\text{Range } g_x(a_0) = \{y \in \mathbf{X} \mid \psi_0 y = 0\}, \quad \psi_0 \in \mathbf{X}', \quad \psi_0 \neq 0, \tag{1.2}$$

$$g_\lambda(a_0) \notin \text{Range } (g_x(a_0)), \tag{1.3}$$

λ_0 is called the corresponding *critical parameter*. For convenience we shall write $g_x^0, g_\lambda^0, \ldots,$ for $g_x(a_0), g_\lambda(a_0), \ldots.$

From (1.1)–(1.2), a turning point is a (simple) *critical* point in the sense that g_x^0 is not a topological isomorphism of **X**.

Locally, at a turning point, the zero set is a smooth curve. This well-known result, stated in Lemma 1.1, is easily proved by decomposing

$$\mathbf{X} = \text{Ker } g_x^0 \oplus V \tag{1.4}$$

and applying the implicit function theorem.

LEMMA 1.1 *There is a neighbourhood U of the turning point a_0 such that*

$$g^{-1}(0) \cap U = \{(\lambda(s), x(s)) : |s - s_0| \leqslant \delta\},$$

where δ is positive and $\lambda(.)$, $x(.)$ are C^3 mappings satisfying $\lambda(s_0) = \lambda_0$, $x(s_0) = x_0$, $|\lambda'(s)| + \|x'(s)\| > 0$ and $x(s) = s\phi_0 + v(s)$, $v(s) \in V$.

In the sequel we have to differentiate the identity $g(\lambda(s), x(s)) \equiv 0$ up to three times with respect to s. Instead of $g_\lambda(\lambda(s), x(s)), \ldots, g_{xxx}(\lambda(s), x(s))$, we shall write $g_\lambda^s, \ldots, g_{xxx}^s$. Then we have

$$g_\lambda^s \lambda'(s) + g_x^s x'(s) \equiv 0, \qquad |s - s_0| < \delta. \tag{1.5}$$

Thus, by (1.2) and (1.3),

$$\lambda'(s_0) = 0, \tag{1.6}$$

$$x'(s_0) = \phi_0, \tag{1.7}$$

and the following definition makes sense:

Definition 1.2 The turning point $a_0 \in \mathbf{R} \times \mathbf{X}$ is called *simple* (or *non-degenerate*) iff $\lambda''(s_0) \neq 0$. Otherwise a_0 is *non-simple*. In particular a_0 is *double* (or a *non-degenerate hysteresis point*) iff $\lambda''(s_0) = 0$, $\lambda'''(s_0) \neq 0$. [See Figs 1(a) and 1(b).]

Another differentiation of (1.5) yields

$$g_{\lambda\lambda}^s \lambda'(s)^2 + 2g_{\lambda x}^s \lambda'(s) x'(s) + g_\lambda^s \lambda''(s) + g_{xx}^s x'(s) x'(s) + g_x^s x''(s) \equiv 0, \tag{1.8}$$

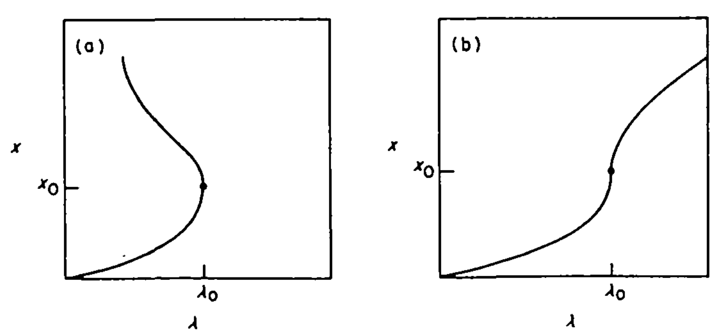

FIG. 1.

and hence, using (1.6), (1.2) and (1.3),

$$\lambda''(s_0) = -\psi_0 g_{xx}^0 \phi_0 \phi_0 / \psi_0 g_\lambda^0, \tag{1.9}$$

$$g_x^0 x''(s_0) = -g_{xx}^0 \phi_0 \phi_0 - \lambda''(s_0) g_\lambda^0, \quad x''(s_0) \in V. \tag{1.10}$$

From (1.9) follows

Proposition 1.1 The turning point $a_0 = (\lambda_0, x_0)$ is simple iff $\psi_0 g_{xx}^0 \phi_0 \phi_0 \neq 0$. Differentiating (1.8) at $s = s_0$ yields

$$3g_{\lambda x}^0 \lambda''(s_0) x'(s_0) + g_\lambda^0 \lambda'''(s_0) + 3g_{xx}^0 x'(s_0) x''(s_0) + g_{xxx}^0 x'(s_0) x'(s_0) x'(s_0) + g_x^0 x'''(s_0) = 0. \tag{1.11}$$

Assume now that a_0 is a non-simple turning point. Then from (1.9), (1.10), (1.11), (1.2) and (1.3),

$$\lambda'''(s_0) = -\psi_0(3g_{xx}^0 \phi_0 v_0 + g_{xxx}^0 \phi_0 \phi_0 \phi_0)/\psi_0 g_\lambda^0, \tag{1.12}$$

$$g_x^0 v_0 = -g_{xx}^0 \phi_0 \phi_0, \quad v_0 \in V, \tag{1.13}$$

$$x''(s_0) = v_0. \tag{1.14}$$

Now, from (1.12) we have

Proposition 1.2 A turning point $a_0 = (\lambda_0, x_0)$ is double iff

$$\psi_0 g_{xx} \phi_0 \phi_0 = 0 \tag{1.15}$$

and

$$\psi_0(3g_{xx}^0 \phi_0 v_0 + g_{xxx}^0 \phi_0 \phi_0 \phi_0) \neq 0, \tag{1.16}$$

where v_0 is given by (1.13).

We close this section with a simple example which shows the connection between double turning points and cusp points (see the cusp catastrophe example in Poston & Stewart, 1978, p. 174). Let $\mathbf{X} = \mathbf{R}$, $g(\lambda, x) := x^3 - \mu x + \lambda$, where μ is a fixed constant. For $\mu > 0$ there are two simple turning points (λ_0, x_0), $\lambda_0 = \pm 2(\mu/3)^{3/2}$, $x_0 = \pm(\mu/3)^{1/2}$, while $(0, 0)$ is a double turning point for $\mu = 0$. The critical parameter λ_0 is related to μ by

$$27\lambda_0^2 = 4\mu^3 \tag{1.17}$$

and (1.17) describes a cusp curve (Fig. 2).

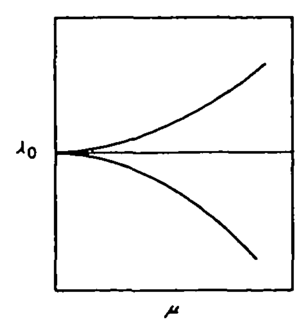

FIG. 2.

2. The Extended System

Assume (λ_0, x_0) is a turning point of g. Choose $l \in \mathbf{X}'$ such that $l\phi_0 = 1$. Then $V := \{v \in \mathbf{X} : lv = 0\}$ is a suitable complement of $\operatorname{Ker} g_x^0$ [see (1.4)]. We introduce the mapping

$$G: \begin{cases} \mathbf{R}\times\mathbf{X}\times\mathbf{X} \to \mathbf{R}\times\mathbf{X}\times\mathbf{X} \\ (\lambda, x, \phi) \mapsto \begin{pmatrix} l\phi - 1 \\ g(\lambda, x) \\ g_x(\lambda, x)\phi \end{pmatrix}. \end{cases} \tag{2.1}$$

Then

$$G(\lambda_0, x_0, \phi_0) = 0. \tag{2.2}$$

We call (2.1) [equivalently (2.2)] an *extended system* of $g(\lambda, x) = 0$. Extended systems, of various forms, have been used by several authors (Keener & Keller, 1973; Moore & Spence, 1980, 1981; Seydel, 1979; Weber, 1979) both to prove theoretical results in bifurcation theory and to compute turning points and bifurcation points. In this paper we use (2.1) in both its roles. First we discuss the question of whether or not the solutions of (2.2) are isolated, i.e. whether or not

$$DG^0 \; [:= DG(\lambda_0, x_0, \phi_0)] \in L(\mathbf{R}\times\mathbf{X}\times\mathbf{X})$$

is an isomorphism. We have

$$DG^0 \begin{bmatrix} \mu \\ u \\ v \end{bmatrix} = \begin{bmatrix} lv \\ \mu g_\lambda^0 + g_x^0 u \\ \mu g_{\lambda x}^0 \phi_0 + g_{xx}^0 \phi_0 u + g_x^0 v \end{bmatrix}. \tag{2.3}$$

Let $(\mu, u, v) \in \operatorname{Ker} DG^0$. Then $\mu g_\lambda^0 + g_x^0 u = 0$ and, by (1.2), (1.3), $\mu = 0$, $u = \alpha\phi_0$, $\alpha \in \mathbf{R}$. From the first and last row of (2.3) one obtains

$$\alpha g_{xx}^0 \phi_0 \phi_0 + g_x^0 v = 0. \tag{2.4}$$

Thus

$$\operatorname{Ker} DG^0 = \{(0, \alpha\phi_0, v) : \alpha \in \mathbf{R},\ v \in V \text{satisfy (2.4)}\}. \tag{2.5}$$

THEOREM 2.1 (*a*) *Let (λ_0, x_0) be a simple turning point of g. Then DG^0 is a linear isomorphism of* $\mathbf{R}\times\mathbf{X}\times\mathbf{X}$, *i.e.* $\operatorname{Ker} DG^0 = \{0\}$ *and* $\operatorname{Range} DG^0 = \mathbf{R}\times\mathbf{X}\times\mathbf{X}$.

(*b*) *Let (λ_0, x_0) be a non-simple turning point of g. Then the kernel (range) of DG^0 has dimension 1 (codimension 1). The kernel is spanned by $\Phi_0 := (0, \phi_0, v_0)$, where v_0 is given by $g_x^0 v_0 = -g_{xx}^0\phi_0\phi_0$, $lv_0 = 0$, and*

$$\operatorname{Range} DG^0 = \{Y \in \mathbf{R}\times\mathbf{X}\times\mathbf{X} : \Psi_0 Y = 0\},$$

where

$$\Psi_0 = (0, \zeta_0, \psi_0) \in \mathbf{R}\times\mathbf{X}'\times\mathbf{X}'$$

and ζ_0 is given by

$$\zeta_0 g_\lambda^0 = -\psi_0 g_{\lambda x}^0 \phi_0, \qquad \zeta_0 g_x^0 = -\psi_0 g_{xx}^0 \phi_0. \tag{2.6}$$

Proof. The claimed properties of $\operatorname{Ker} DG^0$ in (a) and (b) can easily be proved using (2.5) and the fact that $g_{xx}^0\phi_0\phi_0$ is not in the range of g_x^0 for simple turning points. Now we come to the properties of Range DG^0. Let

$$lv = \sigma, \tag{2.7}$$

$$\mu g_\lambda^0 + g_x^0 u = w, \tag{2.8}$$

$$\mu g_{\lambda x}^0 \phi_0 + g_{xx}^0 u\phi_0 + g_x^0 v = z, \tag{2.9}$$

such that $(\sigma, w, z) \in$ Range DG^0. From (2.8),

$$\mu = \psi_0 w/(\psi_0 g_\lambda^0), \qquad u = \alpha\phi_0 + \hat{v} \quad (\hat{v} \in V) \tag{2.10}$$

is uniquely determined up to a constant α. The (unique) existence of v in (2.7) and (2.9) is guaranteed by

$$\psi_0 y = 0, \qquad y := z - \mu g_{\lambda x}^0 \phi_0 - g_{xx}^0 u\phi_0. \tag{2.11}$$

In the case of a simple turning point, (2.11) can always be satisfied by a suitable choice of α. In the case of a non-simple turning point, (2.11) is equivalent to

$$\psi_0 z + \zeta_0(\mu g_\lambda^0 + g_x^0 u) = \psi_0 z + \zeta_0 w = \Psi_0 Y = 0.$$

Here we have made use of (2.6). Notice that $\zeta_0 \in \mathbf{X}'$ in (2.6) is uniquely determined.

As we now show, the converse of Theorem 2.1(a) is also true.

THEOREM 2.2 *Let (λ_0, x_0, ϕ_0) be an isolated solution of* (2.2) *i.e. DG^0 is a linear isomorphism of $\mathbf{R} \times \mathbf{X} \times \mathbf{X}$. Then (λ_0, x_0) is a simple turning point.*

Proof. To show (1.1) we assume that $g_x^0\phi_1 = 0$, $\phi_1 \in V$. Then from (2.5), $(0, 0, \phi_1) \in \operatorname{Ker} DG^0$ and $\phi_1 = 0$. From $\operatorname{Ker} DG^0 = \{0\}$ and (2.4)–(2.5) one easily obtains

$$p := g_{xx}^0 \phi_0 \phi_0 \notin \text{Range } g_x^0. \tag{2.12}$$

Using Proposition 1.1 it remains to show (1.2) and (1.3). Assume that $g_\lambda^0 \in$ Range g_x^0. Since (2.8) is solvable for each w, it follows that Range $g_x^0 = X$ in contradiction to (2.12). It remains to show (1.2). We shall prove

$$X = \text{Range } g_x^0 + \{\alpha g_{xx}^0 \phi_0 \phi_0 \mid \alpha \in \mathbf{R}\}.$$

Let $\sigma = 0$, $w = 0$ and z be arbitrary in (2.7)–(2.9). Then $\mu = 0$, $u = \alpha\phi_0$ and there is exactly one solution $(\alpha, v) \in R \times V$ of

$$\alpha g_{xx}^0 \phi_0 \phi_0 + g_x^0 v = z.$$

Theorems 2.1 and 2.2 imply that simple turning points correspond to isolated solutions of the extended system (2.2) in a unique way (provided $l \in \mathbf{X}'$ is suitably chosen). Other critical points (for example, bifurcation points) can never be isolated solutions of (2.2). A convergence analysis of approximate methods for the computation of turning points is given by Brezzi *et al.* (1981), Moore & Spence (1981). In particular we note that non-simple turning points are sensitive to perturbation and will probably be destroyed by discretization. Thus a direct approach on $g(\lambda, x) = 0$ or $G(\lambda, x, \phi) = 0$ will probably fail.

We close this section with the following theorem:

THEOREM 2.3 *Let (λ_0, x_0) be a simple turning point of g. Then there is a neighbourhood*

U of (λ_0, x_0) such that all zeros of g in U are non-critical points of g with the exception of (λ_0, x_0).

Proof. Assume that there is a sequence $(\lambda_n, x_n, \phi_n) \in \mathbf{R} \times \mathbf{X} \times \mathbf{X}$ with

$$\lambda_n \to \lambda_0, \quad x_n \to x_0, \quad \|\phi_n\| = 1 \quad \text{and} \quad g_x(\lambda_n, x_n)\phi_n = 0.$$

Write

$$\phi_n = \alpha_n \phi_0 + v_n, \quad \alpha_n \in \mathbf{R}, \quad v_n \in V.$$

Since $g_x^0 \phi_n \to 0$ it follows from the continuity of the pseudo-inverse of g_x^0 that $v_n \to 0$. Normalizing ϕ_n by $l\phi_n = 1$ it follows that $\phi_n \to \phi_0$ in contradiction to Theorem 2.1(a).

3. Two-parameter Problems, Double Turning Points and Cusp Points

We now consider non-linear problems which depend on two parameters. Assume that

$$f: \begin{cases} \mathbf{R} \times \mathbf{R} \times \mathbf{X} \to \mathbf{X} \\ (\lambda, \mu, x) \to f(\lambda, \mu, x) \end{cases}$$

is a C^3 mapping and that for a fixed μ_0

$$g(\lambda, x) = f(\lambda, \mu_0, x) \tag{3.1}$$

has a turning point (λ_0, x_0) with respect to λ according to definition 1.1. We also assume that g given by (3.1) satisfies (1.1)–(1.3) and we use a notation similar to that in Sections 1 and 2:

$$f(\lambda_0, \mu_0, x_0) = 0,$$
$$f_x^0 \phi_0 = 0, \qquad l\phi_0 = 1,$$
$$\psi_0 f_x^0 = 0, \qquad \psi_0 f_\lambda^0 \neq 0, \ldots, \text{etc.}$$

There should be no misunderstanding if we say that (λ_0, μ_0, x_0) is a turning point of f with respect to λ. The analogue of Lemma 1.1 is

LEMMA 3.1 *There is a neighbourhood U of (λ_0, μ_0, x_0) in $\mathbf{R} \times \mathbf{R} \times \mathbf{X}$ such that $f^{-1}(0) \cap U$ is a two-dimensional C^3 manifold.*

We introduce the extended system of $f(\lambda, \mu, x) = 0$ (cf. (2.1)).

$$F: \begin{cases} \mathbf{R} \times \mathbf{R} \times \mathbf{X} \times \mathbf{X} \to \mathbf{R} \times \mathbf{X} \times \mathbf{X} \\ (\lambda, \mu, x, \phi) \to \begin{pmatrix} l\phi - 1 \\ f(\lambda, \mu, x) \\ f_x(\lambda, \mu, x)\phi \end{pmatrix}. \end{cases} \tag{3.2}$$

Then

$$F(\lambda_0, \mu_0, x_0, \phi_0) = 0. \tag{3.3}$$

For convenience we introduce $\mathbf{Y} = \mathbf{R} \times \mathbf{X} \times \mathbf{X}$, $y = (\lambda, x, \phi) \in \mathbf{Y}$, $y_0 = (\lambda_0, x_0, \phi_0)$ and write $F(\mu, y)$ instead of $F(\lambda, \mu, x, \phi)$. Note that $F(\mu_0, \cdot) = G$ where G is given by (2.1) and g by (3.1).

Thus

$$\begin{aligned} F(\mu_0, y_0) &= 0, \\ \operatorname{Ker} F_y^0 &= \operatorname{Ker} DG^0. \end{aligned} \tag{3.4}$$

Consider now the cases of f having simple and non-simple turning points.

Case I

Assume (λ_0, μ_0, x_0) is a simple turning point of f with regard to λ. Then, by Theorem 2.1, F_y^0 is a linear isomorphism of $\mathbf{Y}$, and the implicit function theorem implies the existence of a neighbourhood U of (μ_0, y_0) such that $U \cap F^{-1}(0)$ is a smooth curve which can be parameterized by μ, i.e.

$$U \cap F^{-1}(0) = \{(\mu, y(\mu)) : |\mu - \mu^0| < \delta\}.$$

We remark that Sewell (1966) uses precisely this result in his discussion of the "equilibrium surface" in the theory of the stability of elastic structures. From Theorem 2.2 we see that every point $(\lambda(\mu), \mu, x(\mu), \phi(\mu))$ of this curve corresponds to a simple turning point $(\lambda(\mu), \mu, x(\mu))$ of f.

Our main interest will be in the second case.

Case II

Assume (λ_0, μ_0, x_0) is a non-simple turning point of f with regard to λ. Then, again using Theorem 2.1, (1.1) and (1.2) are satisfied with $\mathbf{X}$ replaced by $\mathbf{Y}$, g by F, (λ_0, x_0) by (μ_0, y_0), ϕ_0 by Φ_0 and ψ_0 by Ψ_0. To guarantee that (μ_0, y_0) is a turning point of F with regard to μ we must assume [cf. (1.3)]

$$F_\mu^0 \notin \operatorname{Range} DG^0 \tag{3.5}$$

which is equivalent to $\Psi_0 F_\mu^0 \neq 0$, i.e.

$$\zeta_0 f_\mu^0 + \psi_0 f_{\mu x}^0 \phi_0 \neq 0 \tag{3.6}$$

using (2.6). The significance of this condition is plained in Theorem 3.3. We now state our main theorem.

THEOREM 3.1 *Assume* (3.5) *holds. A double turning point* (λ_0, μ_0, x_0) *of f with regard to* λ *corresponds to a simple turning point* $(\lambda_0, \mu_0, x_0, \phi_0)$ *of F with regard to* μ.

Proof. From case II above we proved that $(\lambda_0, \mu_0, x_0, \phi_0)$ is a turning point of F with regard to μ. To show it is a simple turning point we have to prove

$$\Psi_0 F_{yy}^0 \Phi_0 \Phi_0 \neq 0.$$

Let F_1, F_2, F_3 be the components of F. Then $F_{j,yy}^0 \Phi_0 \Phi_0$, $j = 1, 2, 3$, are the components of $F_{yy}^0 \Phi_0 \Phi_0$, and by (2.6)

$$\Psi_0 F_{yy}^0 \Phi_0 \Phi_0 = \zeta_0 F_{2,yy}^0 \Phi_0 \Phi_0 + \psi_0 F_{3,yy}^0 \Phi_0 \Phi_0.$$

It is straightforward to show, using $\Phi_0 = (0, \phi_0, v_0)$,

$$\begin{aligned} F_{2,yy}^0 \Phi_0 \Phi_0 &= f_{xx}^0 \phi_0 \phi_0 \\ F_{3,yy}^0 \Phi_0 \Phi_0 &= f_{xxx}^0 \phi_0 \phi_0 \phi_0 + 2 f_{xx}^0 \phi_0 v_0. \end{aligned}$$

Hence

$$\Psi_0 F^0_{yy}\Phi_0\Phi_0 = \zeta_0 f^0_{xx}\phi_0\phi_0 + 2\psi_0 f^0_{xx}\phi_0 v_0 + \psi_0 f^0_{xxx}\phi_0\phi_0\phi_0. \tag{3.7}$$

By (2.6), (1.13) we have

$$\zeta_0 f^0_x = -\psi_0 f^0_{xx}\phi_0, \qquad f^0_x v_0 = -f^0_{xx}\phi_0\phi_0.$$

Hence

$$\zeta_0 f^0_x v_0 = -\psi_0 f^0_{xx}\phi_0 v_0 = -\zeta_0 f^0_{xx}\phi_0\phi_0$$

and (3.7) gives

$$\Psi_0 F^0_{yy}\Phi_0\Phi_0 = 3\psi_0 f^0_{xx}\phi_0 v_0 + \psi_0 f^0_{xxx}\phi_0\phi_0\phi_0 \tag{3.8}$$

which is non-zero by (1.16).

Since a simple turning point (λ_0, μ_0, x_0) of f with regard to λ corresponds to a non-critical point $(\lambda_0, \mu_0, x_0, \phi_0)$ of F with regard to μ and vice versa (use Theorem 2.2) we can use the results of Theorem 2.3 and Theorem 3.1 to prove:

THEOREM 3.2 *Let (λ_0, μ_0, x_0) be a double turning point of f with regard to λ. Under the assumption* (3.6) *there exists a neighbourhood U of (λ_0, μ_0, x_0) such that all zeros of f in U are simple turning points of f with regard to λ with the exception of the double turning point (λ_0, μ_0, x_0).*

Theorems 3.1 and 3.2 are important practically as well as theoretically, since they indicate clearly a procedure to be followed for the calculation of the double turning point (λ_0, μ_0, x_0), namely, calculate the simple turning point of F. The details of an implementation of this procedure applied to a mildly non-linear differential equation arising from a problem in thermal ignition are given in the next section.

In the rest of this section we discuss the geometrical connection between a double turning point and a cusp point (see Fig. 2). This connection is predicted by elementary cusp catastrophe models.

In Fig. 3 a typical situation is described. Figure 3(a) shows curves $f(\cdot, \mu, \cdot)^{-1}(0)$ which possess two simple turning points for $\mu < \mu_0$, a non-simple turning point for $\mu = \mu_0$, and no turning points for $\mu > \mu_0$.

Figure 3(b) shows the projection of the turning point set on to the μ, λ plane and it is natural to ask if this cusp-type geometrical behaviour will always occur under the

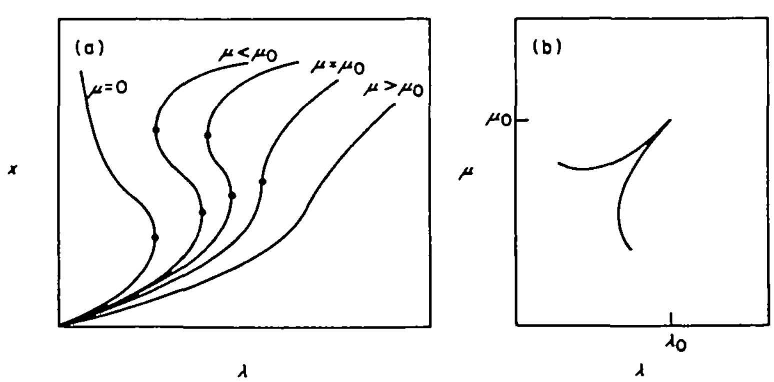

FIG. 3.

conditions of Theorem 3.1. To prove that this is indeed the case we first apply a Lyapunov–Schmidt decomposition to f and then use results from catastrophe theory.

Define $(\bar{\lambda}, \bar{\mu}, \bar{x}) \in \mathbf{R}^3$ by

$$(\lambda, \mu, x) = (\lambda_0+\bar{\lambda}, \mu_0+\bar{\mu}, x_0+\bar{x}\phi_0+v), \quad v \in V.$$

Locally, $f(\lambda, \mu, x) = 0$ is equivalent to the bifurcation (reduced) equation

$$H(\bar{\lambda}, \bar{\mu}, \bar{x}) = \psi_0 f(\lambda_0+\bar{\lambda}, \mu_0+\bar{\mu}, x_0+\bar{x}\phi_0+v(\bar{\lambda}, \bar{\mu}, \bar{x})) = 0,$$

where $v(\bar{\lambda}, \bar{\mu}, \bar{x}) \in V$ is uniquely determined by

$$Qf(\lambda_0+\bar{\lambda}, \mu_0+\bar{\mu}, x_0+\bar{x}\phi_0+v) = 0,$$

with Q a projection on Range f_x^0, which can be defined by $Q := I-P$,

where
$$\begin{aligned} Py &= (\psi_0 y)w, \\ X &= \text{Range } f_x^0 \oplus \{\alpha w \mid \alpha \in \mathbf{R}\}. \end{aligned} \tag{3.9}$$

For the partial derivatives of H w.r.t., $\bar{\lambda}, \bar{\mu}, \bar{x}$ one obtains (see Chow, Hale & Mallet-Paret, 1975, p. 183 f)

$$H(0) = 0, \tag{3.10}$$
$$H_{\bar{x}}(0) = \psi_0 f_x^0 \phi_0 = 0, \tag{3.11}$$
$$H_{\bar{x}\bar{x}}(0) = \psi_0 f_{xx}^0 \phi_0\phi_0 = 0, \tag{3.12}$$
$$H_{\bar{x}\bar{x}\bar{x}}(0) = \psi_0 f_{xxx}^0 \phi_0\phi_0\phi_0 + 3\psi_0 f_{xx}^0 \phi_0 v_0 \neq 0, \tag{3.13}$$
$$H_{\bar{\lambda}}(0) = \psi_0 f_\lambda^0, \tag{3.14}$$
$$H_{\bar{\mu}}(0) = \psi_0 f_\mu^0, \tag{3.15}$$
$$H_{\bar{\lambda}\bar{x}}(0) = \psi_0 f_{\lambda x}^0 \phi_0 + \psi_0 f_{xx}^0 \phi_0 v_1, \quad f_x^0 v_1 = -Qf_\lambda^0, \quad v_1 \in V, \tag{3.16}$$
$$H_{\bar{\mu}\bar{x}}(0) = \psi_0 f_{\mu x}^0 \phi_0 + \psi_0 f_{xx}^0 \phi_0 v_2, \quad f_x^0 v_2 = -Qf_\mu^0, \quad v_2 \in V. \tag{3.17}$$

The catastrophe theory of Thom (see Chow *et al.*, 1975, theorem 10.1 and section 11, p. 176 f) yields the following result:

Under the conditions (3.10)–(3.13) there exists a smooth change of co-ordinates

$$\tilde{\lambda} = \eta_1(\bar{\lambda}, \bar{\mu}), \quad \tilde{\mu} = \eta_2(\bar{\lambda}, \bar{\mu}), \quad \tilde{x} = \xi(\bar{\lambda}, \bar{\mu}, \bar{x}) \tag{3.18}$$

such that H has the normal form of the *cusp catastrophe*

$$\tilde{H}(\tilde{\lambda}, \tilde{\mu}, \tilde{x}) = \tilde{x}^3 + \tilde{\mu}\tilde{x} + \tilde{\lambda},$$

provided that the generic condition

$$D := \begin{vmatrix} H_{\bar{\lambda}}(0) & H_{\bar{\lambda}\bar{x}}(0) \\ H_{\bar{\mu}}(0) & H_{\bar{\mu}\bar{x}}(0) \end{vmatrix} \neq 0 \tag{3.19}$$

is satisfied. In this case we call (λ_0, μ_0, x_0) a *cusp point* of f (see the example in Section 1).

Thus it only remains to prove:

THEOREM 3.3 *Let (λ_0, μ_0, x_0) be a double turning point (non-degenerate hysteresis point) of f w.r.t. λ. Then (3.6) is equivalent to (3.19), i.e. (λ_0, μ_0, x_0) is a cusp point of f if (3.6) holds.*

Proof. Using (2.6) and (3.9) one obtains

$$H_{\bar{\lambda}\bar{x}}(0) = -\zeta_0 f_\lambda^0 - \zeta_0 f_x^0 v_1 = \zeta_0(Qf_\lambda^0 - f_\lambda^0) = \zeta_0 P f_\lambda^0 = (\zeta_0 w)(\psi_0 f_\lambda^0),$$

$$H_{\bar{\mu}\bar{x}}(0) = \psi_0 f_{\mu x}^0 \phi_0 - \zeta_0 f_x^0 v_2 = \psi_0 f_{\mu x}^0 \phi_0 + \zeta_0 f_\mu^0 + \zeta_0(Qf_\mu^0 - f_\mu^0)$$

$$= \beta + (\zeta_0 w)(\psi_0 f_\mu^0),$$

with

$$\beta := \psi_0 f_{\mu x}^0 \phi_0 + \zeta_0 f_\mu^0 \quad [\text{cf. } (3.6)].$$

Thus $D = (\psi_0 f_\lambda^0)\cdot\beta \neq 0$ iff $\beta \neq 0$, since $\psi_0 f_\lambda^0 \neq 0$ in the case of a turning point. ∎

The above theory proves the existence of a cusp curve in the $\bar{\lambda}$, $\bar{\mu}$ plane and we note that the change of co-ordinates (3.18) will not destroy the cusp character of the projection on to the $\bar{\lambda}$, $\bar{\mu}$ and λ, μ planes [see Fig. 3(b)].

Remark. It is instructive to consider also the connection with the singularity theory of Golubitsky & Schaeffer (1979). Under the conditions (3.10)–(3.13) and $\psi_0 f_\lambda^0 \neq 0$ one can show that $H(\bar{\lambda}, 0, \bar{x})$ is contact equivalent to $\bar{x}^3 + \bar{\lambda}$ and that, if (3.6) also holds, $H(\bar{\lambda}, \bar{\mu}, \bar{x})$ is contact equivalent to $\bar{x}^3 + \bar{\mu}\bar{x} + \bar{\lambda}$. Thus $H(\bar{\lambda}, \bar{\mu}, \bar{x})$ is a universal unfolding of $H(\bar{\lambda}, 0, \bar{x})$ and, hence, $f(\lambda, \mu, x)$ is a universal unfolding of $f(\lambda, \mu_0, x)$. We note that the unfolding parameter μ occurs naturally in the problem so the results of catastrophe theory adequately describe the situation. This is not always the case. (See Golubitsky & Schaeffer, section 1.c.) The relationships between the singularity theory of Golubitsky & Schaeffer and the numerical approximation of singular points of non-linear equations is discussed by Brezzi & Fujii (1982). They consider perturbations of various types of bifurcation point by analysing the bifurcation (reduced) equation obtained from $f(\lambda, \mu, x) = 0$ using the Lyapunov–Schmidt decomposition. Their analysis shows clearly the role played by the parameters λ, μ in the non-linear problem and enables one to predict the effect of discretization on a bifurcation point. Although there are theoretical links with the paper of Brezzi & Fujii, this paper differs from their paper in that the direct approach described here suggests clearly the numerical method actually used to compute a cusp point (λ_0, μ_0, x_0). Also the computable quantities, which can be used to confirm the geometrical behaviour, for example (1.15), (1.16) and (3.6), appear naturally in the theoretical analysis.

4. Example

The equation

$$f(\lambda, \mu, x) \equiv x'' + \lambda e^{x/(1+\mu x)}, \qquad x(0) = x(1) = 0, \tag{4.1}$$

which describes an exothermic chemical reaction in an infinite slab (Fradkin & Wake, 1977) is discretized on the mesh $t_j = jh$, $j = 0, 1, 2, \ldots, n$ using

$$x(t_{j-1}) - 2x(t_j) + x(t_{j+1}) - \frac{h^2}{12}[x''(t_{j-1}) + 10x''(t_j) + x''(t_{j+1})] = O(h^6).$$

The discretized form of (4.1) is

$$\mathbf{A}\mathbf{x} + \mathbf{E}(\lambda, \mu, \mathbf{x}) = 0, \quad x_0 = x_n = 0, \quad \mathbf{x} \in \mathbf{R}^{n-1}, \tag{4.2}$$

where A is a tridiagonal matrix and

$$E_i = \frac{h^2}{12}\lambda\left[\exp\left(\frac{x_{i-1}}{1+\mu x_{i-1}}\right)+10\exp\left(\frac{x_i}{1+\mu x_i}\right)+\exp\left(\frac{x_{i+1}}{1+\mu x_{i+1}}\right)\right],$$
$$i = 1, 2, \ldots, n-1.$$

Solutions of (4.2) have the form described in Fig. 3(a), (b) (see Boddington *et al.*, 1979) and we wish to find the *cusp* (λ_0, μ_0, x_0). The extended system has the form

$$\begin{aligned} l\boldsymbol{\phi}-1 &= 0 \\ \mathbf{A}\mathbf{x}+\mathbf{E}(\lambda, \mu, \mathbf{x}) &= 0 \\ [\mathbf{A}+\mathbf{E}_x(\lambda, \mu, \mathbf{x})]\boldsymbol{\phi} &= 0 \end{aligned} \tag{4.3}$$

which we write as

$$\mathbf{F}(\mu, \mathbf{y}) = 0 \tag{4.4}$$

[recall (3.3), (3.4)].

To compute solutions of (4.3) the method described in Moore & Spence (1980) is used. The functional l is chosen as

$$l\boldsymbol{\phi} = \phi_m, \qquad m = \frac{n}{2},$$

and the method involves the solution of

$$\mathscr{A}\mathbf{z}_i = \mathbf{w}_i, \quad i = 1, \ldots, 4, \tag{4.5}$$

where $\mathscr{A}$ is A with its middle column replaced by E_m. Clearly $\mathscr{A}$ does not inherit the pure diagonal structure of A but an efficient method for solving the Equations (4.5) in $O(n)$ operations is given in Chu & Spence (1980).

To compute the turning point of $\mathbf{F}(\mu, \mathbf{y})$ the method described in Keller (1977) is used. We introduce the normalization

$$N(\mu, \mathbf{y}, s) = x_m - c + s, \qquad c = \text{constant}, \quad m = \frac{n}{2}, \tag{4.6}$$

(recall $\mathbf{y} = (\lambda, \mathbf{x}, \boldsymbol{\phi})$) and solve the system

$$\begin{aligned} \mathbf{F}(\mu, \mathbf{y}) &= 0, \\ N(\mu, \mathbf{y}, s) &= 0. \end{aligned}$$

The turning point is found by using the method of false position to compute the zero of det $\{F_y(\mu, \mathbf{y})\}$. The method of Keller (1977) involves the solution of two sets of equations of the form

$$F_y(\mu, y)\mathbf{z}_j = \mathbf{w}_j, \quad j = 1, 2. \tag{4.7}$$

However, both equations in (4.7) can be solved by (4.5), with suitable $\mathbf{z}_i, \mathbf{w}_i$, $i = 1, \ldots, 4$, and so, at each step, eight sets of linear equations with the same coefficient matrix need to be solved. The numerical results are given in Table 1.

Note in particular that conditions (1.1), (1.3), (1.15), (1.16) and (3.6) are seen to hold and so the presence of a cusp is confirmed. It is worth noting that the "cusp character" is not destroyed by the perturbation, i.e. the projection of the

TABLE 1

	$n = 10$	$n = 20$	$n = 40$
λ_0	5·2293707955	5·2294859595	5·2294937243
μ_0	0·2457998185	0·2457815854	0·2457804986
$x_0(t_{n/2})$	4·8969119462	4·8965672063	4·8965490193
$\psi_0 f_\lambda^0$	0·919 $E-1$	0·231 $E-1$	0·579 $E-2$
$\psi_0 f_\mu^0$	-2·009	-0·505	-0·127
det $\{f_x^0\}$	0·158 $E-15$	-0·148 $E-14$	0·387 $E-15$
$\psi_0 f_{xx}^0 \phi_0 \phi_0$	0·844 $E-13$	0·781 $E-13$	0·378 $E-13$
$\psi_0\{3f_{xx}^0 \phi_0 v_0 + f_{xxx}^0 \phi_0 \phi_0 \phi_0\}$	-0·455 $E-2$	-0·116 $E-2$	-0·291 $E-3$
det $\{F_y\}$	0·775 $E-14$	-0·184 $E-14$	-0·219 $E-15$
$\Psi_0 F_\mu^0$ [see (3.6)]	-0·812	-0·204	-0·512 $E-1$

approximating solution on the λ, μ plane will give a cusp as in Fig. 3(b). This follows from the fact that the approximating extended system (4.4) has a simple turning point (Moore & Spence, 1981, theorem 12). The quantities $\psi_0 f_\lambda^0, \psi_0 f_\mu^0$, $\psi_0(3f_{xx}^0 \phi_0 v_0 + f_{xxx}^0 \phi_0 \phi_0 \phi_0)$ and $\psi_0 F_\mu^0$ all show $O(h^2)$ behaviour. This is because of the h^2 term in E defined by (4.2). To estimate $\psi_0 f_\lambda^0, \ldots$, one need only remove this h^2 dependence.

The example was solved for three values of n. The convergence theory in Moore & Spence (1981) shows that since (μ_0, y_0) is a simple turning point of (4.4) the computed values $\lambda_0^{(n)}$, $\mu_0^{(n)}$, $x_0^{(n)}(t_{n/2})$ should show $O(h^4)$ convergence because of the discretization. (Note that, for convenience, the dependence on n is indicated by a superscript.) The theoretical results are

$$\lambda_0 - \lambda_0^{(n)},\ \mu_0 - \mu_0^{(n)},\ x_0(t_{n/2}) - x_0^{(n)}(t_{n/2}) = O(h^4)$$

and these are confirmed by the numerical results given in Table 2 where the differences $\lambda_0^{(n)} - \lambda_0^{(2n)}, \ldots$, are given. If more accurate estimates of λ_0, μ_0, for (4.1) are required then one can use h^4 extrapolation on the λ_0, μ_0 values for $n = 20, 40$, to give

$$\lambda_0 \doteq 5{\cdot}2294942419, \qquad \mu_0 \doteq 0{\cdot}24578042616.$$

It is remarkable that Boddington *et al.* (1979) obtained almost the same numbers (in their notation: $\mu_0 = \varepsilon_{tr}$, $x_0(t_{n/2}) = \theta_{m,tr}$, $\lambda_0 = 4\delta_{tr}$). They used an analytical method which is restricted to the simple slab geometry of (4.1) while our method applies to general problems.

TABLE 2

n	$\lambda_0^{(n)} - \lambda_0^{(2n)}$	Ratio	$\mu_0^{(n)} - \mu_0^{(2n)}$	Ratio
10	-0·115 $E-3$	14·8	0·183 $E-4$	16·8
20	-0·776 $E-5$		0·109 $E-5$	
n	$x_0^{(n)}(t_{n/2}) - x_0^{(2n)}(t_n)$	Ratio		
10	0·345 $E-3$	19·0		
20	0·182 $E-4$			

A detailed discussion of the numerical methods used to solve system (4.7) and hence to compute turning points and cusps is beyond the scope of this paper. The method used for the above example was chosen because an efficient technique for solving the Equations (4.5) was found. For other equations different numerical methods may be more efficient.

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