SIAM J. NUMER. ANAL.
Vol. 28, No. 3, pp. 809-832, June 1991

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THE NUMERICAL SOLUTION OF NONLINEAR EQUATIONS HAVING SEVERAL PARAMETERS. PART III: EQUATIONS WITH Z_2-SYMMETRY*

A. D. JEPSON†, A. SPENCE‡, AND K. A. CLIFFE§

Abstract. The computation of symmetry-breaking bifurcation points of nonlinear multiparameter problems with Z_2 (reflectional) symmetry is considered. The numerical approach is based on recent work in singularity theory, which is used to construct systems of equations and inequalities characterising various types of symmetry-breaking bifurcation points. Numerical continuation methods are then used to follow paths of symmetry-breaking bifurcations, and hence compute regions in parameter space for which a problem has qualitatively similar bifurcation diagrams.

The power of the numerical approach is illustrated by computations of axisymmetric flows in the finite Taylor problem.

Key words. bifurcation, symmetry, singularity theory, Navier–Stokes

AMS(MOS) subject classifications. 58C27, 65J15, 65N30

1. Introduction. We consider nonlinear equations of the form

$$F(x, \lambda, \alpha)=0, \qquad F: X\times R\times R^p \to Y, \tag{1.1}$$

where $x \in X$, a Banach space, $\lambda \in R$ is a distinguished (or bifurcation) parameter, $\alpha \in R^p$ is a vector of control parameters, and F is a nonlinear mapping from $X\times R\times R^p$ to Y, a Banach space. There has been much recent interest in the computation of singular points of (1.1), i.e., the points $(x_0, \lambda_0, \alpha_0)$, say, at which $F_x^0 \equiv F_x(x_0, \lambda_0, \alpha_0)$ is singular, because of their importance in understanding nonlinear phenomena (see, for example, [12], [20], [23]). The conference proceedings [18] reflects this interest and provides a good survey of numerical methods for the calculation of singular points of (1.1). For convenience throughout this paper we shall refer to the case $X = Y = R$ as the *scalar* problem and all other cases as *vector* problems, irrespective of whether or not X is finite dimensional.

In [14] the application of singularity theory by Golubitsky and Schaeffer [12] was used to derive numerically convenient defining equations and inequalities for singularities arising in scalar problems of the form (1.1). These defining conditions were used to organize singular points into a "hierarchy of singularities." This allowed a straightforward, unified explanation of a numerical approach to the computation of regions in the control parameter space within which the bifurcation diagrams of (1.1) were qualitatively similar.

The aim of the paper is to extend the ideas presented in [14] to vector problems of the form (1.1), where, in addition, F satisfies a reflectional symmetry (or Z_2-covariance) condition, commonly written in the form $SF(x, \lambda, \alpha)=F(Sx, \lambda, \alpha)$, $S^2=I$, $S\neq I$. To do this two distinct steps must be made which we now outline.

* Received by the editors December 15, 1986; accepted for publication (in revised form) June 1, 1990.

† Department of Computer Science, University of Toronto, Toronto, Ontario, Canada M5S 1A4. This research was supported by Natural Sciences and Engineering Research Council of Canada, the British Council, and the University of Toronto.

‡ School of Mathematics, University of Bath, Claverton Down, Bath BA2 7AY, United Kingdom. This research was supported by Natural Sciences and Engineering Research Council of Canada and Science and Engineering Research Council of the United Kingdom.

§ Theoretical Physics Division, AERE Harwell, Oxfordshire OX11 0RA, United Kingdom. This research is part of the longer-term research carried out within the Underlying Program of the United Kingdom Atomic Energy Authority.

First, in § 2, the results in [14] are extended to cover the Z_2-symmetric case $f(-x, \lambda, \alpha) = -f(x, \lambda, \alpha)$, $x \in R$. A new Z_2-hierarchy of singularities is given which shows considerable differences from the nonsymmetric hierarchy. However, once this Z_2-hierarchy is derived, much of the discussion in [14] on the numerical implementation applies with at most minor and obvious differences. Thus we omit all of the general discussion of how to move up and down the hierarchy, how to compute bifurcation diagrams for given values of α, or how to compute regions in control parameter space for which the problem has qualitatively similar bifurcation diagrams. However, many of these ideas are mentioned with respect to the example calculations in § 6.

The second step is to show how the results in § 2 can be applied to vector problems satisfying the symmetry condition and the condition that dim Null $(F_x^0) = 1$. This is done in § 3 using a generalisation of the Lyapunov–Schmidt reduction [2], [15], by which a vector problem is reduced to an equivalent scalar problem satisfying the Z_2-symmetry condition. The reduction process can be reversed to great effect. All of the numerically useful results in § 2 for the scalar problem are shown to apply to the vector problem. Also various types of extended systems for the calculation of symmetry-breaking bifurcation points can be derived, and it is shown that they all inherit the useful numerical properties of the conditions for the scalar problem. For example, under a general stability assumption, it is shown that these extended systems are *regular* at the bifurcation points. Section 4 contains a short discussion on the implementation of one particular extended system.

To illustrate the applicability and power of the numerical approach we consider in §§ 5 and 6 the calculation of axisymmetric flows in the Taylor problem. The nonlinear equations are the Navier–Stokes equations in a cylindrical annulus. A finite element method is used to derive a discretized form like (1.1), where $p = 2$ and the number of equations is roughly 10^3. For reasons of space we omit most of the detail of the discretization and refer the reader to [8] for a complete account including the utilization of the symmetry. Bifurcation diagrams and control parameter space plots are given (cf. [14]) and an especially interesting high-order singularity (the Z_2-codimension 3* singularity in [11]) is computed.

This paper is the third in a series on the application of ideas from singularity theory to nonlinear multiparameter problems. The first paper [14] describes the basic approach, and the second [16] discusses vector problems without symmetry. Finally, we make two remarks. Through the Z_2-symmetry is common in applications, much more complicated symmetries also arise with a correspondingly more complex bifurcation phenomena (see, for example, [12], [21]) and the ideas in this paper can also be applied in such cases (see [1]). Second, we are grateful to a referee for pointing out that the assumption $X \subset Y$ is an unnecessary restriction, since provided a Z_2-action is defined on X and Y and F is Z_2-covariant then we can always assume $X = Y$.

2. Singularity theory for Z_2-symmetry functions. In this section we discuss the case of x being a scalar state variable in the multiparameter nonlinear problem

$$f(x, \lambda, \alpha) = 0, \qquad f: R \times R \times R^p \to R, \tag{2.1a}$$

subject also to the Z_2-symmetry condition

$$f(-x, \lambda, \alpha) = -f(x, \lambda, \alpha). \tag{2.1b}$$

We assume f is smooth, that is, C^∞ in a neighbourhood of zero. Clearly $x = 0$ is a solution of (2.1) for all λ, α and it can be shown [12, Chap. VI] that f can be written in the form

$$f(x, \lambda, \alpha) = a(z, \lambda, \alpha)x \tag{2.2}$$

for $z=x^2$ and some smooth a. (Note that a is not unique (see [12, p. 249]) but that this causes no difficulty since the theory produces defining conditions in terms of derivatives of a which are uniquely determined in terms of derivatives of f.) We are interested in the values of λ, α such that $(0, \lambda, \alpha)$ is a *singular* point of (2.1); that is,

$$f_x(0, \lambda, \alpha)=0 \tag{2.3}$$

or, equivalently,

$$a(0, \lambda, \alpha)=0. \tag{2.4}$$

In § 2.1, we present the classification of singular points of (2.1) in a form that is suitable for numerical computation. The important numerical properties of this classification are then discussed in § 2.2.

2.1. The Z_2-hierarchy. The results in this section are essentially given in [11] and [12, Chap. VI]; we refer the reader to these references for more detail of the theory. The aim of this section is to describe a numerical strategy for (2.1a, b) based on that theory. As in [14] we introduce a graph, which we call the *Z_2-hierarchy*, in which the singularities of Z_2-codimension less than 4 are arranged. The graph, Fig. 1, is structured to emphasise the relationships between the singularities and to illustrate the systematic nature of our numerical approach. The (q, j)-singularity is defined to be the singularity which the polynomial at the (q, j)-node has at $(x, \lambda)=(0, 0)$. A (q, j)-singularity has Z_2-codimension q. The node labelled $(3^*, 0)$ represents a one-parameter family (called a modal family) of codimension-3 singularities, and will be discussed further below. The numeric labels above the nodes in the hierarchy ($\nu=1, \cdots, 11$) correspond to the numbering used in Table 5.1 of [12, p. 263]. In the sequel we drop the Z_2 and refer simply to the hierarchy, codimension, etc.

The defining conditions given in Proposition 3.47 in [11] can also be recovered from the hierarchy. As in [14] we write the defining conditions in the form of an extended system

$$H_{q,j}(0, \lambda, \alpha)=0 \in R^{q+1} \tag{2.5a}$$

and nondegeneracy conditions (or side-constraints)

$$C^k_{q,j}(0, \lambda, \alpha) \neq 0, \qquad k=1, \cdots, K_{q,j}. \tag{2.5b}$$

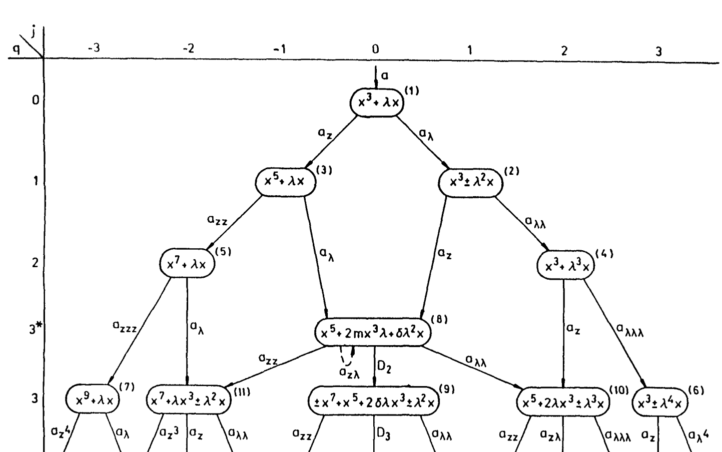

FIG. 1. *Z_2-Hierarchy. Here* $\delta=\pm 1$, $m=a_{z\lambda}/|a_{zz}a_{\lambda\lambda}|^{1/2}$, $D_2=a_{z\lambda}^2-a_{zz}a_{\lambda\lambda}$, *and* $D_3=-a_{zzz}a_{z\lambda}a_{\lambda\lambda}+2a_{zz\lambda}a_{zz}a_{\lambda\lambda}-2a_{z\lambda\lambda}a_{z\lambda}a_{zz}+a_{\lambda\lambda\lambda}a_{zz}^2$.

For a particular (q,j)-singularity, $(q,j)\neq(3^*,0)$, system (2.5a) is formed by choosing a path from the top of the hierarchy down to the (q,j)-node. Equation (2.5a) is then just the restriction that all the labels beside branches on this path must vanish (all paths give equivalent $H_{q,j}$'s). For example,

$$H_{2,-2}(z,\lambda,\alpha)\equiv(a, a_z, a_{zz}). \tag{2.6a}$$

The side-constraints (2.5b) are obtained by requiring that the labels on all the branches leaving the (q,j)-node must not vanish. In particular, for the $(2,-2)$-singularity we have

$$C^1_{2,-2}\equiv a_{zzz}\neq 0, \qquad C^2_{2,-2}\equiv a_\lambda\neq 0. \tag{2.6b}$$

The derivatives of a can, of course, be rewritten in terms of f and x (e.g., $a_{z\lambda}$ becomes $f_{xxx\lambda}$). The one exception to these rules for constructing defining conditions is for the $(3^*,0)$-modal family.

The normal form

$$x^5+2m\lambda x^3+\delta\lambda^2 x=0, \qquad \delta=\pm1, \qquad m^2\neq\delta \tag{2.7}$$

given in the $(3^*,0)$-node of the hierarchy represents a family of *inequivalent* codimension-3 singularities. That is, two different values of m in (2.7) produce two polynomials that are not equivalent. The parameter m is called a modal parameter. The conditions

$$A_{3^*,0}(0,\lambda,\alpha)\equiv(a, a_z, a_\lambda)=0, \tag{2.8a}$$

$$C^1_{3^*,0}\equiv a_{zz}\neq 0, \quad C^2_{3^*,0}\equiv D_2\neq 0, \quad C^3_{3^*,0}\equiv a_{\lambda\lambda}\neq 0, \tag{2.8b}$$

which can be obtained in the hierarchy using the method described above, are necessary and sufficient conditions (see Theorem 2.13 below) for f to be equivalent to *some member* of the $(3^*,0)$-family. It is convenient to denote the member having modal parameter m as the $(3^*,0,m)$-singularity. In order to get defining conditions for this singularity we must append another equation, namely,

$$M_{3^*,0}(0,\lambda,\alpha;m)=0, \tag{2.9}$$

to (2.8a). Here,

$$M_{3^*,0}(x,\lambda,\alpha;m)\equiv a_{z\lambda}/|a_{zz}a_{\lambda\lambda}|^{1/2}-m, \tag{2.10a}$$

or

$$M_{3^*,0}(x,\lambda,\alpha;m)\equiv(a_{z\lambda})^2 w-a_{zz}a_{\lambda\lambda}, \qquad w\equiv\frac{\operatorname{sign}(a_{zz}a_{\lambda\lambda})}{m^2}, \tag{2.10b}$$

and sign (m) is to be taken equal to sign $(a_{z\lambda})$. These two forms are equivalent in that their use in (2.9) leads to the same value of m. However, in numerical computations, (2.10a) is more convenient for $|m|\ll 1$ while (2.10b) is better for $|m|\gg 1$. Therefore the $(3^*,0,m)$-extended system is

$$H_{3^*,0}(x,\lambda,\alpha;m)\equiv\begin{pmatrix} A_{3^*,0}(x,\lambda,\alpha)\\ M_{3^*,0}(x,\lambda,\alpha;m)\end{pmatrix}. \tag{2.11}$$

An additional type of side-constraint appears with the $(3^*,0)$-family, namely,

$$C_{3^*,0}(0,\lambda,\alpha)\equiv a_{z\lambda}\neq 0, \tag{2.12}$$

which is obtained from the label on the dotted branch in the hierarchy. The meaning of the additional side-constraint is rather subtle, and we only sketch its significance here. If in Definition 3.2 of [11] the condition that S, X, and Λ be C^∞ functions is replaced with $S, X, \Lambda \in C$ (which provides topological Z_2-equivalence), then the range of the model parameter m breaks up into two ($\delta = -1$) or four ($\delta = +1$) pieces. In particular, if $a_{zz}a_{\lambda\lambda} < 0$ then the two ranges are $m > 0$ and $m < 0$, otherwise for $a_{zz}a_{\lambda\lambda} > 0$ the four ranges are $m \varepsilon (-\infty, -1)$, $(-1, 0)$, $(0, 1)$, and $(1, \infty)$. In each of these ranges the $(3^*, 0, m)$-singularities and their unfolding behaviour are *topologically* equivalent. The boundaries of these regions are of interest. The points of $m = \pm\infty$ are signaled by one of the side constraints a_{zz} or $a_{\lambda\lambda}$ vanishing, and the points are $m = \pm 1$ are given by D_2 vanishing. These points are called connector points and correspond to transitions out of the $(3^*, 0)$-family to the $q = 3$ level, or below. The remaining endpoint, at $m = 0$, is called a regular distinguished point and corresponds to a particular member within the $(3^*, 0)$-family. It occurs when the label on the dotted branch (i.e., $a_{z\lambda}$ or, equivalently, m) vanishes.

The fact that the above conditions are defining conditions for f to have a (q, j)-singularity is the content of the following theorem.

THEOREM 2.13. *With* $0 \leqq q \leqq 3$, *assume that*

$$H_{q,j}(0, \lambda, \alpha; m) = 0 \tag{2.13a}$$

is the extended system derived from the Z_2*-hierarchy, and that*

$$C^k_{q,j} \neq 0, \qquad k = 1, \cdots, k_{q,j}, \tag{2.13b}$$

are the corresponding side-constraints.

Then for $(q, j) \neq (3^*, 0)(= (3^*, 0)$, respectively), (2.13a), (2.13b) are satisfied if and only if $(0, \lambda, \alpha)$ is a (q, j)-singularity ($(3^*, 0, m)$-singularity) for (2.1a). Moreover, for $(q, j) = (3^*, 0)$, conditions (2.8a) and (2.8b) are satisfied if and only if f is Z_2-equivalent to a member of the $(3^*, 0)$-family.

Proof. There are only minor differences between the current theorem and [11, Prop. 3.47]. First, we have allowed the contact transformations in Definition 3.2 of [11] to reverse the signs of f, x, and λ. This eliminates endless $\pm$ signs in the normal forms and simplifies the presentation. However, we note that in order to obtain an appropriate bifurcation diagram these reflections must be taken into account (i.e., undone)! Second, we have chosen an explicit form for the side-constraint, $D_3 \neq 0$, of the $(3, 0)$-singularity. The form of D_3 used here can be obtained by setting the vector v in Proposition 3.47 to be $v = (-a_{z\lambda}, a_{zz})/(a_{zz})^{1/3}$. The details of this are trivial and are omitted. □

The defining conditions discussed above solve the "recognition problem" for Z_2-singularities having codimension $q \leqq 3$. That is, given any f with a singular point at $(0, \lambda, \alpha)$, the Z_2-hierarchy can be used to determine if the codimension of the singularity is less than 4 and, if it is, the particular singularity type. The idea is simple: starting at the top of the Z_2-hierarchy we descend any branch having label that vanishes at $(0, \lambda, \alpha)$. We end up either below the $q = 3$ level, in which case (2.1a) has a singularity of codimension larger than 3, or at a (unique) node with nonzero labels on all the descending branches emanating from this node. From Theorem 2.13 we can conclude that f is contact equivalent to the polynomial inside this node (with, in the case of the $(3^*, 0)$-node, the particular value of m satisfying (2.9)).

The direct numerical implementation of this recognition process would very likely be a disaster. The presence of roundoff errors would mean that the criteria that a label is "zero at $(0, \lambda, \alpha)$" must be replaced by "nearly zero at $(0, \lambda, \alpha)$". Unfortunately, precise and reliable criteria for how near is near enough depend critically on the nature of f near $(0, \lambda, \alpha)$. The defining conditions can, however, be used to great advantage in a different way. Given a point (x, λ, α) (not necessarily a solution of (2.1a)), we ask if there is a singular point of a specified type nearby. In particular we seek a solution of the extended system (2.13a). This is a nonlinear system of $q+1$ equations in terms of the $p+1$ unknowns (λ, α).

If $p=q$ then, given a sufficiently good initial guess, and that

$$\frac{\partial H_{q,j}}{\partial(\lambda, \alpha)}(0, \lambda, \alpha; m) \text{ is nonsingular} \tag{2.14}$$

at the root, standard numerical algorithm can be reliably used. Our general approach of descending and ascending the hierarchy, discussed in [14] can often be used to provide good initial guesses; in the next section we show that (2.14) can also be expected to hold (except at isolated points).

2.2. Regularity of the defining conditions. Recall that the notion of a versal unfolding [12, p. 258] is used to capture the intuitive idea of structural stability. Suppose f satisfies (2.1) and is a versal unfolding for a singularity at $(0, \lambda_0, \alpha_0)$. Consider small perturbations of f given by

$$\hat{f}(x, \lambda, \alpha, \varepsilon) \equiv f(x, \lambda, \alpha) + \varepsilon g(x, \lambda, \alpha),$$

where g is a smooth function satisfying (2.1b). The behaviour of (2.1a) near $(x, \lambda, \alpha) = (0, \lambda_0, \alpha_0)$ is essentially unaltered by these small perturbations since the versal unfolding property of f ensures

$$\hat{f}(x, \lambda, \alpha, \varepsilon) = T(x, \lambda, \alpha, \varepsilon) f(X(x, \lambda, \alpha, \varepsilon), \Lambda(\lambda, \alpha, \varepsilon), B(\alpha, \varepsilon))$$

for $(x, \lambda, \alpha, \varepsilon)$ near $(0, \lambda_0, \alpha_0, 0)$. Here T, X, Λ, B are smooth functions which satisfy [11, Def. 3.2] and

$$T(x, \lambda, \alpha, 0) = 1, \quad X(x, \lambda, \alpha, 0) = x, \quad \Lambda(\lambda, \alpha, 0) = \lambda, \quad B(\alpha, 0) = \alpha.$$

In particular, $\hat{f}$ has a singular point at $(0, \Lambda(\lambda_0, \alpha_0, \varepsilon), B(\alpha_0, \varepsilon))$ of exactly the same type as the original singularity of f at $(0, \lambda_0, \alpha_0)$. Thus the singularity of f can be said to be structurally stable. Given that errors are inherent in the development of mathematical models, and in numerical computations, it is reasonable to restrict our attention to structurally stable phenomena.

The connection between versal unfoldings and property (2.14) is given in the following theorem.

THEOREM 2.15. *Let* $0 \leqq q \leqq 3$. *Suppose* $H_{q,j}(0, \lambda, \alpha, m)$ *is the* (q, j)*-extended system obtained from the* Z_2*-hierarchy and* $(0, \lambda_0, \alpha_0, m)$ *satisfies* (2.13a) *and* (2.13b). *Then* $f(x, \lambda, \alpha)$ *is a versal unfolding of* $f(x, \lambda, \alpha_0)$ *if and only if*

$$\operatorname{rank}\left[\frac{\partial H_{q,j}}{\partial(\lambda, \alpha)}(0, \lambda_0, \alpha_0; m)\right] = q+1, \tag{2.15}$$

that is, for $p=q$, $(0, \lambda_0, \alpha_0)$ *is a regular solution of* $H_{q,j}=0$.

The proof of this result is rather technical, is not needed to understand the remainder of this paper, and is relegated to the Appendix. We note that the proof for the cases $q \leqq 2$ and $q = 3^*$, along with the necessary tools for the remaining cases, are developed in [11].

Clearly Theorem 2.15 is an extremely useful result. In particular, continuation methods readily compute paths of regular points and so paths of singular points can be computed by continuation. If the side-constraints are also monitored, then higher-order singular points can be detected. In [14, §§ 4, 5] a method is described for computing regions in parameter space R^p which have "qualitatively similar" bifurcation diagrams, and for moving up and down the hierarchy for nonsymmetric problems. A similar procedure applies in the Z_2-symmetric case, and is illustrated in § 6 by an example.

In applying this procedure it is often convenient to treat the $(3^*, 0)$-family as if it were a codimension-2 singularity (e.g., when topological equivalence is sufficient). Recall from Theorem 2.13 that membership in the $(3^*, 0)$-family is defined by (2.8). As we show below, (2.8a) can be expected to have regular solutions and therefore the same path-following techniques can be applied.

COROLLARY 2.16. *Suppose that, for some some* $m \in R$, $(0, \lambda_0, \alpha_0)$ *is a versally unfolded* $(3^*, 0, m)$*-singularity. Then* $(0, \lambda_0, \alpha_0)$ *is a solution of* (2.8a) *and* i_1, $i_2 \in \{1, \cdots, p\}$ *can be chosen such that*

$$\frac{\partial A_{3^*,0}}{\partial(\lambda, \alpha_{i_1}, \alpha_{i_2})}(0, \lambda_0, \alpha_0) \text{ is nonsingular.} \tag{2.16}$$

Proof. The result follows by noting that $A_{3^*,0}$ can be obtained from $H_{3^*,0}$ by deleting the last row, and then applying Theorems 2.13 and 2.15. □

The following corollary discusses the fact that, in the process of taking one step up or one step down, the hierarchy usually presents no numerical difficulties (cf. [14, Thm. 5.8]).

COROLLARY 2.17. *Suppose* $1 \leqq q \leqq 3$, $p = q$, *and* $(0, \lambda_0, \alpha_0)$ *is either*:

(i) *a universally unfolded* (q, j)*-singularity of* (2.1a) *with* $(q, j) \neq (3^*, 0)$; *or*

(ii) *a* $(3^*, 0, m)$*-singularity with* (2.16) *satisfied for* $(i_1, i_2) = (1, 2)$. *Let* (q', j') *be such that the* (q', j')*-node appears above the* (q, j)*-node, with a single branch connecting the two.*

Then for $(q', j') \neq (3^*, 0)(= (3^*, 0)$, *respectively*) $(0, \lambda_0, \alpha_0)$ *is either a regular point or a simple turning point of the system*

$$H_{q',j'}(0, \lambda, \alpha) = 0 \qquad (A_{3^*,0}(0, \lambda, \alpha) = 0). \tag{2.17}$$

Proof. The hypotheses imply that the extended system for the (q', j')-node can be obtained by crossing one element out of the system for the (q, j)-node, and that the Jacobian of the (q, j)-system is nonsingular. Therefore the Jacobian for the (q', j')-system must have full rank at $(0, \lambda_0, \alpha_0)$. □

Finally we have a result which indicates that one of the side-constraints changes sign as a path of singularities crosses a higher-order singularity, which proves to be useful for the numerical detection of these higher-order singularities.

COROLLARY 2.18. *Suppose* p, (q, j), (q', j') *and* $(0, \lambda_0, \alpha_0)$ *are as in Corollary* 2.17. *Let* $(0, \lambda(s), \alpha(s))$ *be a smooth parameterization of the solution path of* (2.17) *with* $\lambda(0) = \lambda_0$, $\alpha(0) = \alpha_0$, *and* $(\dot\lambda(0), \dot\alpha(0))((d\lambda/ds)(0), (d\alpha/ds)(0)) \neq 0$. *Finally, let* $C(0, \lambda, \alpha)$ *be the label on the branch connecting the* (q', j')*-node with the* (q, j)*-node. Then*

$$\frac{d}{ds} C(0, \lambda(s), \alpha(s))|_{s=0} \neq 0. \tag{2.18}$$

Proof. Let

$$H(0, \lambda, \alpha) = 0 \tag{2.19a}$$

denote the extended system for the (q', j')-node. Then, as in Corollary 2.17,

$$\begin{pmatrix} H(0, \lambda, \alpha) \\ C(0, \lambda, \alpha) \end{pmatrix} = 0 \tag{2.19b}$$

is the extended system for the (q, j)-node. Since $(\lambda(s), \alpha(s))$ is a solution path for (2.19a), we have

$$\frac{\partial H}{\partial(\lambda, \alpha)}(0, \lambda_0, \alpha_0)\begin{pmatrix}\dot{\lambda}(0)\\ \dot{\alpha}(0)\end{pmatrix}=0. \tag{2.20}$$

However, by assumption,

$$\frac{\partial}{\partial(\lambda, \alpha)}\begin{pmatrix}H\\ C\end{pmatrix}\Bigg|_{(\lambda_0,\alpha_0)} \text{ is nonsingular.}$$

In particular, $(\dot{\lambda}(0), \dot{\alpha}(0))$ cannot be a null vector for this Jacobian, and from (2.20), we see that (2.18) must be satisfied. □

Clearly, the success of the numerical approach relies on the results of Theorems 2.13, 2.15 and of Corollaries 2.16–2.18. It is convenient to group these ideas into one concept, namely, that of an extended system with side-constraints being *well formulated.* This could be done now for $H_{q,j}$ and $C^k_{q,j}$, but since the concept has more general applicability we leave the actual statement until § 3.2.

3. Vector problems with Z_2-symmetry. In this section we describe how the results in § 2 can be extended to cover vector problems satisfying a Z_2-symmetry condition. The process relies on a generalisation of the well-known Lyapunov–Schmidt reduction. This section is split into three subsections. In the first we outline the theory of the generalised reduction in the presence of symmetry, and derive an equivalent scalar equation (the reduced equation). In the second subsection, by essentially reversing the reduction process, defining conditions are constructed for the vector problem which inherit the desirable properties discussed in § 2. Finally in the third subsection we derive suitable extended systems for the actual numerical calculation of symmetry-breaking bifurcation points.

3.1. The generalised reduction with Z_2-symmetry. Consider

$$F(x, \lambda, \alpha)=0, \qquad F: X\times R\times R^p\to Y, \tag{3.1}$$

where X, Y are Banach spaces with $X\subset Y$. Assume $u_0 := (x_0, \lambda_0, \alpha_0)$ is a solution of (3.1) satisfying

(3.2a) $F^0_x := F_x(u_0)$ is a Fredholm operator of index zero, (see [22]);

(3.2b) $N(F^0_x] = \text{span}\,\{\varphi_0\}, \qquad N[(F^0_x)^*] = \text{span}\,\{\psi^*_0\}$,

where $(F^0_x)^*$ is the adjoint operator associated with F^0_x.

In addition we assume that (3.1) satisfies the following symmetry condition: there exists a linear operator $S: Y\to Y$ such that

$$S\neq I, \qquad S^2=I \quad \text{on } Y, \tag{3.3a}$$

$$S\neq I, \qquad S^2=I \quad \text{on } X(\subset Y), \tag{3.3b}$$

$$F(Sx, \lambda, \alpha)=SF(x, \lambda, \alpha). \tag{3.3c}$$

The mapping S induces splittings of X and Y into symmetric and antisymmetric subspaces

$$X = X_s\oplus X_a, \qquad Y=Y_s\oplus Y_a, \tag{3.4a}$$

where

$$x\in X_s \Leftrightarrow Sx=x, \qquad x\in X_a\Leftrightarrow Sx=-x, \tag{3.4b}$$

with similar definitions for Y_s and Y_a. By differentiating (3.3c) it follows that

(3.5) $$SF_x(x, \lambda, \alpha) = F_x(x, \lambda, \alpha)S \quad \text{for } x \in X_s.$$

Therefore, for $x_0 \in X_s, N[F_x^0]$ is invariant under S, and it follows that either $\phi_0 \in X_s$ or $\phi_0 \in X_a$. Also, (3.3c) implies that F satisfies $F: X_s \times R^{p+1} \to Y_s$. Therefore, if $\phi_0 \in X_s$, the analysis can proceed entirely within X_s and Y_s, and the symmetry is unimportant. Hence, for the rest of this paper we restrict our attention to the *symmetry-breaking case*

(3.6a) $$\phi_0 \in X_a.$$

In this case we also require

(3.6b) $$F_x^0 \in \text{Isom}(X_s, Y_s),$$

which gives

(3.6c) $$F_x^0 : X_a \to Y_a \qquad \text{is Fredholm with index zero.}$$

Then it follows from (3.5) that

(3.6d) $$\psi_0^* Y_s = 0.$$

In the application we are considering the point $(x_0, \lambda_0, \alpha_0)$, and hence the null vectors ϕ_0 and ψ_0^*, are not known a priori. Indeed, the accurate location of a suitable $(x_0, \lambda_0, \alpha_0)$ is a goal of the computation. However, initial guesses $\tilde{\phi}$ and $\tilde{\psi}^*$ for both ϕ_0 and ψ_0^* will be generally available, and it is these approximations we use to perform the reduction.

We choose subspaces X_1, X_2, Y_1, and Y_2 and projections P and Q as in [16, eqns. (3.4), (3.5), respectively] but, in addition, we assume

(3.7) $$SX_i = X_i, \quad SY_i = Y_i, \quad i = 1, 2$$

and define projections P^s, P^a, Q^s, and Q^a by

(3.8a) $$P^s : X \to X, \quad R[P^s] = X_s, \quad N[P^s] = X_a, \quad P^a = I - P^s,$$

(3.8b) $$Q^s : Y \to Y, \quad R[Q^s] = Y_s, \quad N[Q^s] = Y_a, \quad Q^a = I - Q^s.$$

Also we assume (2.6) of [15]

(3.9) $$N[P] \cap N[(I - Q)F_x^0] = \{0\},$$

which ensures [15, Thm. 2.10]:

(3.10) $$(I - Q)F_x^0(I - P) : X_1 \to Y_1 \text{ is nonsingular.}$$

In addition we have the following lemma.

LEMMA 3.11. *Suppose φ_0, ψ_0^* satisfy (3.6) and P, Q, P^s, Q^s are as above. Let $u = (x, \lambda, \alpha) \in X_s \times \mathbf{R} \times \mathbf{R}^p$, then*

(3.11a) $$S\tilde{\phi} = -\tilde{\phi}, \qquad \tilde{\psi}^* S = -\tilde{\psi}^*,$$

(3.11b) $$PP^s = P^s P = 0, \qquad QQ^s = Q^s Q = 0,$$

(3.11c) $$F_x(u) = L^s(u) + L^a(u), \quad L^s := Q^s F_x P^s, \quad L^a := Q^a F_x P^a.$$

Moreover, for u sufficiently close to u_0,

(3.12a) $$L^s(u) : X_s \to Y_s \text{ is nonsingular,}$$

(3.12b) $$L^a(u) : X_a \to Y_a \text{ is Fredholm of index zero,}$$

(3.12c) $$N[L^a(u_0)] = \text{span}\{\phi_0\}, \qquad R[L^a(u_0)] = \{y \in Y_a \mid \psi_0^* y = 0\}.$$

Proof. From (3.7) it follows that P and Q commute with S. Therefore $P(Q)$ commutes with $P^s(Q^s$, respectively), and $R[P]$ is invariant under S. Now we obtain from (3.3b) that $S\tilde{\phi} = \pm\tilde{\phi}$. However, $S\tilde{\phi} = \tilde{\phi}$ can be shown to imply $P\varphi_0 = 0$, which contradicts (3.9), and therefore $S\tilde{\phi} = -\tilde{\phi}$. A similar argument can be used to show $\tilde{\psi}^* S = -\tilde{\psi}^*$, and therefore we have (3.11a). The relations in (3.11b) follow from the commutativity noted above and (3.11a).

To prove (3.11c) we use (3.4b) and (3.5) to show that the cross terms $Q^a F_x P^s$ and $Q^s F_x P^a$ both vanish. Finally, (3.12) is an easy consequence of (3.2), (3.6), and (3.11c). □

The reduction process proceeds by writing (3.1) as

$$(I - Q)F(\Omega, \lambda, \alpha) = 0, \qquad P\Omega = \varepsilon\tilde{\phi}; \tag{3.13a}$$

$$QF(\Omega, \lambda, \alpha) = 0, \tag{3.13b}$$

where $\varepsilon \in R$. The Implicit Function Theorem and (3.10) ensure the existence and local uniqueness of a solution

$$\Omega(\varepsilon, \lambda, \alpha) \equiv x_0 + x_1(\varepsilon, \lambda, \alpha) + \varepsilon\tilde{\phi}, \qquad Px_1 = 0, \tag{3.13c}$$

of (3.13a) for $(\varepsilon, \lambda, \alpha)$ near $(0, \lambda_0, \alpha_0)$ with $x_1(0, \lambda_0, \alpha_0) = 0$. Substitution of this solution into (3.13b) provides the *reduced equation*

$$h(\varepsilon, \lambda, \alpha) := \tilde{\psi}^* Q^a F(\Omega(\varepsilon, \lambda, \alpha), \lambda, \alpha) = 0. \tag{3.14}$$

(Here we have used $\tilde{\psi}^* Q = \tilde{\psi}^* Q^a$, which can be obtained from (3.7), (3.8), and (3.11).)

An important consequence of requiring that the reduction process respect the Z_2-symmetry (i.e., requiring (3.7)) is that the reduced function, h, inherits the reflectional symmetry of F (see, for example, [12, p. 306]). This is easily shown after noting that $S\Omega(\varepsilon, \lambda, \alpha) = \Omega(-\varepsilon, \lambda, \alpha)$ and is stated as

$$h(-\varepsilon, \lambda, \alpha) = -h(\varepsilon, \lambda, \alpha). \tag{3.15}$$

Lemma 3.11 motivates the following definition.

DEFINITION 3.16. Let F and h be as above, and suppose $a(z, \lambda, \alpha)$ satisfies $h(\varepsilon, \lambda, \alpha) = \varepsilon a(\varepsilon^2, \lambda, \alpha)$. Then $(x_0, \lambda_0, \alpha_0)$ is said to be a (q, j)-singularity (i.e., a (q, j)-Z_2-symmetry-breaking bifurcation point) of (3.1) if $a(z, \lambda, \alpha)$ satisfies the scalar defining conditions (2.13a, b) at $(0, \lambda_0, \alpha_0)$. Similarly, the $(3^*, 0)$-family and the $(3^*, 0, m)$-singularity are defined in terms of $a(z, \lambda, \alpha)$ and the conditions listed in § 2. Moreover, F is said to be a versal (universal) unfolding of the singularity at $(x_0, \lambda_0, \alpha_0)$ if h is a versal (universal, respectively) unfolding about $(0, \lambda_0, \alpha_0)$.

Some effort is required to show that this definition is consistent. In particular, it must be shown that any suitable choice of P and Q in the reduction process leads to a reduced function having the same type of singularity and unfolding behaviour at $(0, \lambda_0, \alpha_0)$. This is done for the nonsymmetric case in [15], and the result for the Z_2-symmetric case follows with minor modifications. The required setting is quite technical and therefore we omit the details.

3.2. Defining conditions for vector problems. Definition 3.16 indicates that defining conditions for (3.1) to have a (q, j)-singularity (which we take to include the $(3^*, 0, m)$-singularity) can be obtained directly from the reduced equation and the conditions derived in § 2. However, a direct application of this approach does not lead to a computationally efficient scheme. The source of the difficulty is that the reduced function $h(\varepsilon, \lambda, \alpha)$ is only defined on the solution set of (3.13a). If an iterative procedure is used to solve the (q, j)-extended system applied to h, then, for each iteration, (3.13a) must be solved for $\Omega(\varepsilon, \lambda, \alpha)$. A more efficient approach can be obtained by extending the definition of h to include points not on the solution set of (3.13a). The following treatment is an extension of that in [16, § 4] to the Z_2-symmetric case.

Let $w=(\varepsilon, \lambda, \alpha, c) \in R \times R \times R^p \times Y_s$ and define $\Omega(w)$ to be the solution of

(3.17a) $$Q^s F(\Omega, \lambda, \alpha) = c \in Y_s,$$

(3.17b) $$(I-Q)Q^a F(\Omega, \lambda, \alpha) = 0, \qquad PP^a\Omega = \varepsilon\tilde{\phi},$$

for w near $w_0 := (0, \lambda_0, \alpha_0, 0)$, with

(3.17c) $$\Omega(w_0) = x_0.$$

The particular form of (3.17a, b) has been chosen to be especially convenient for the discussion in § 3.3. We note that Lemma 3.11 and the Implicit Function theorem ensure the existence and local uniqueness of $\Omega(w)$. The corresponding reduced function,

(3.18) $$\tilde{h}(\varepsilon, \lambda, \alpha, c) := \tilde{\psi}^* Q^a F(\Omega(w), \lambda, \alpha),$$

can easily be shown to satisfy

(3.19a) $$h(\varepsilon, \lambda, \alpha) = \tilde{h}(\varepsilon, \lambda, \alpha, 0),$$

(3.19b) $$\tilde{h}(-\varepsilon, \lambda, \alpha, c) = -\tilde{h}(\varepsilon, \lambda, \alpha, c).$$

In the sequel we drop the tilde from $\tilde{h}$.

Let $H_{q,j}(w)$ and $C^k_{q,j}(w)$ be the extended system and side-constraint functions (defined in § 2) applied to $h(\varepsilon, \lambda, \alpha, c)$. It now follows from Definition 3.16 that $u_0 = (\Omega(w_0), \lambda_0, \alpha_0)$ is a (q, j)-singularity of (3.1) if and only if (λ_0, α_0) satisfies

(3.20a) $$G_{q,j}(0, \lambda_0, \alpha_0, 0) = 0, \qquad G_{q,j}(w) := \begin{pmatrix} c \\ H_{q,j}(w) \end{pmatrix} \in Y_s \times R^{q+1},$$

(3.20b) $$C^k_{q,j}(0, \lambda_0, \alpha_0, 0) \neq 0, \qquad k = 1, \cdots, K_{q,j}.$$

Finally, as we show below, we can apply a change of coordinates to write (3.20) in terms of (x, λ, α) for x in a X_s-neighbourhood of x_0.

LEMMA 3.21. (Inheritance). *Let $u = (x, \lambda, \alpha)$, $x \in X_s$, and $\bar{w}(u) := (\lambda, \alpha, Q^s F(u))$. Define*

(3.21) $$F_{q,j}(u) := G_{q,j}(0, \bar{w}(u)).$$

Then, for u in a $X_s \times R \times R^p$-neighbourhood of u_0, a smooth inverse mapping $(\bar{w})^{-1}$: $R \times R^p \times Y_s \to X_s \times R \times R^p$ exists. Moreover, for $w_0 := (0, \bar{w}(u_0)) = (0, \lambda_0, \alpha_0, 0)$,

$$\frac{\partial H_{q,j}}{\partial(\lambda, \alpha)}(w_0) \colon R \times R^p \to R^{q+1}$$

is surjective (nonsingular for $p = q$) if and only if

$$\frac{\partial F_{q,j}}{\partial u}(u_0) \colon X_s \times R \times R^p \to Y_s \times R^{q+1}$$

is surjective (nonsingular for $p = q$).

The proof follows the lines of that for [16, Thm. 4.11] and is omitted.

Given this result, defining conditions for (3.1) to have a (q, j)-singularity at u are

(3.22a) $$F_{q,j}(u) = \begin{pmatrix} Q^s F(u) \\ H_{q,j}(0, \bar{w}(u)) \end{pmatrix} = 0 \in Y_s \times R^{q+1},$$

(3.22b) $$C^k_{q,j}(0, \bar{w}(u)) \neq 0, \qquad k = 1, \cdots, K_{q,j}.$$

Moreover, from the Lemma it easily follows that all results about the suitability of the defining conditions (2.13a, b) for the scalar problem (2.1), namely, Theorems 2.13, 2.15, and Corollaries 2.16–2.18, carry directly over to the vector case (3.1) through the use of the defining conditions given in (3.22a, b). A brief summary of these results follows:

(i) *Specificity.* Conditions (3.22a, b) are satisfied at $u_0 = (x_0, \lambda_0, \alpha_0)$ if and only if u_0 is a (q, j)-singular point of (3.1).

(ii) *Regularity.* Suppose u_0 satisfies (3.22a, b). Then $F(x, \lambda, \alpha)$ is a versal unfolding if and only if $\partial F^0_{q,j}/\partial u$ is surjective.

(iii) *Transversality of side-constraints.* Let (q', j') and (q, j), with $q' < q$, correspond to a pair of nodes in the hierarchy that are connected by a single branch. Then if u_0 is a universally unfolded (q, j)-singularity and $u(s)$ is a path of (q', j')-singularities with $u(0) = u_0$, $u(0) \neq 0$, then the side-constraint corresponding to the label on the (q', j')-(q, j) branch switches sign as s passes through zero. (Here we have given a rough statement; the precise formulation must deal with the $(3^*, 0)$-family, as done in Corollary 2.18.)

These three properties are important for the numerical implementation of the approach described in [14]. We refer to a set of defining conditions that have these three properties as *well formulated.*

In addition we have the following.

(iv) *Well behaved at degeneracies.* Let (q', j') and (q, j) be as in property (iii) above (or, more precisely, as in Corollary 2.17). Suppose u_0 is a uniformly unfolded (q, j)-singularity of (3.1) (and, if $(q, j) = (3^*, 0)$, appropriate α_1 and α_2 are chosen according to Corollary 2.17). Then u_0 is either a regular point or a simple turning point in the path of (q', j')-singularities passing through u_0.

We remark that property (iv) is not included in the concept of well-formulated defining conditions since it does not generalise (e.g., in the nonsymmetric case, a path of pitchfork bifurcation points ($q = 2$) undergoes a bifurcation at a universally unfolded hilltop bifurcation point ($q = 3$); [12]). It is expected that the other three properties do generalise, in particular, that well-formulated defining conditions can always be found. Finally we note that, when new singularities are considered, we need only develop the defining conditions for the low-dimensional reduced equation. If these conditions can be shown to be well formulated then the inheritance lemma provides the same properties for the defining conditions induced for the full problem. This represents a considerable technical improvement over the direct approach (see [7], [13]).

3.3. Computational forms. It remains to show how the vector defining conditions (3.22a, b) can be evaluated at a given point $(x, \lambda, \alpha) \in X_s \times R \times R^p$. In this section we show how (3.22a) can be rewritten into several different, mathematically equivalent forms. The different forms are not *computationally* equivalent, however, and the choice of a particular one depends on the relative costs of various matrix–vector computations. This is further illustrated by the application to the Taylor problem considered in the subsequent sections.

We assume that Q^s and P^s are known explicitly, and F is written in the form

$$F(u) = \begin{pmatrix} F^s(u) \\ F^a(u) \end{pmatrix} = \begin{pmatrix} Q^s F(u) \\ Q^a F(u) \end{pmatrix}. \tag{3.23}$$

Then (3.21) becomes

$$F_{q,j}(u) := \begin{pmatrix} F^s(u) \\ H_{q,j}(0, \bar{w}(u)) \end{pmatrix}, \tag{3.24}$$

and we are left with computing $H_{q,j}(0, \bar{w}(u))$. To do this we differentiate (3.18). For example,

$$a(w) := h_\varepsilon(w) = \tilde{\psi}^* L^a \Omega_\varepsilon, \tag{3.25a}$$

$$a_\lambda(w) := h_{\varepsilon\lambda}(w) = \tilde{\psi}^*[L^a \Omega_{\varepsilon\lambda} + F^a_{xx}\Omega_\varepsilon \Omega_\lambda + F^a_{x\lambda}\Omega_\varepsilon], \tag{3.25b}$$

where $L^a := L^a(u)$ is as in (3.11c), and the derivatives of Ω are evaluated at $w = (0, \bar{w}(u)) = (0, \lambda, \alpha, F^s(u))$. At this point Ω_ε and Ω_λ are not yet known, although linear equations for them can be obtained by differentiating (3.17a, b). In particular, we obtain

$$L^s(u)\Omega_\varepsilon(w) = 0, \quad (I-Q)L^a(u)\Omega_\varepsilon = 0, \quad PP^a\Omega_\varepsilon = \phi.$$

By writing $\Omega_\varepsilon = \Omega^s_\varepsilon + \Omega^a_\varepsilon$ (in the obvious notation), we find $\Omega^s_\varepsilon \equiv 0$ (see (3.12a)) and

$$\mathscr{L}^a(u)\Omega^a_\varepsilon(u) = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \in (Y_1 \cap Y_a) \times R, \tag{3.26}$$

where

$$\mathscr{L}^a(u) := \begin{pmatrix} (I-Q)L^a(u) \\ \tilde{\phi}^* PP^a \end{pmatrix} : X_a \to (Y_1 \cap Y_a) \times R, \tag{3.27a}$$

$$\tilde{\phi}^* : X_a \to R \quad \text{with } \tilde{\phi}^*\tilde{\phi} = 1. \tag{3.27b}$$

By using (3.10) and Lemma 3.11 it is not difficult to show that

$$\mathscr{L}^a(u) : X_a \to (Y_1 \cap Y_a) \times R \text{ is nonsingular;} \tag{3.28}$$

hence (3.26) has a unique solution. Similarly, $\Omega_\lambda = \Omega^s_\lambda + \Omega^a_\lambda$, and $\Omega_{\varepsilon\lambda}$ are uniquely defined by

$$F^s_x(u)\Omega^s_\lambda(u) = -(I-Q)F^s_\lambda(u), \qquad \Omega^a_\lambda = 0, \tag{3.29a}$$

$$\mathscr{L}^a(u)\Omega^a_{\varepsilon\lambda}(u) = \begin{pmatrix} -(I-Q)[F^a_{xx}\Omega^s_\lambda + F^a_{x\lambda}]\Omega^a_\varepsilon \\ 0 \end{pmatrix}, \qquad \Omega^s_{\varepsilon\lambda} = 0. \tag{3.29b}$$

Finally, through the use of the (scalar)Z_2-hierarchy, we obtain

$$F_{0,0}(u) := \begin{pmatrix} F^s \\ h_\varepsilon \end{pmatrix} = \begin{pmatrix} F^s \\ \tilde{\psi}^* L^a \Omega^a_\varepsilon \end{pmatrix} = O \in X_s \times R, \tag{3.30a}$$

$$F_{1,1}(u) := \begin{pmatrix} F^s \\ h_\varepsilon \\ h_{\varepsilon\lambda} \end{pmatrix} = \begin{pmatrix} F^s \\ \tilde{\psi}^* L^a \Omega^a_\varepsilon \\ \tilde{\psi}^*[L^a\Omega^a_{\varepsilon\lambda} + F^a_{xx}\Omega^a_\varepsilon\Omega^s_\lambda + F^a_{x\lambda}\Omega^a_\varepsilon] \end{pmatrix} = 0 \in X_s \times R^2. \tag{3.30b}$$

Here, as in (3.25), L^a and the derivatives of F, Ω are evaluated at u, with the derivatives of Ω given by (3.26) and (3.29). Similar manipulations provide expressions for the other derivatives of h required to form the side-constraints and the other (q, j)-extended systems. As in the above examples, only the solutions of linear systems are required to obtain $F_{q,j}(u)$ and $C^k_{q,j}(u)$.

We note that, after the solution $u = u_0$ is found, (3.9), (3.11), (3.26), and (3.27) provide

$$\Omega^a_\varepsilon(0, \tilde{w}(u_0)) = \xi\phi_0 \in N[F^0_x] \tag{3.31}$$

for some $\xi \in R\backslash\{0\}$. If, as is usually the case, a continuation method is being used to compute solutions of $F_{q,j}(u)=0$, then the computed null vector Ω_ε^a (suitably normalized) can be used as the approximate null vector ϕ for the next step. In order to use the form (3.30a) or (3.30b) we also require an approximate "left null vector" ($\tilde{\psi}^*$) for the next step. For example, we might use ψ_0^*, the left null vector associated with the current solution u_0. It is easy to check that $\psi_0^*=\tilde{\psi}^*(u_0)$, where $\tilde{\psi}^*(u)$ satisfies

$$(v^*, \beta)\mathscr{L}^a(u) = -QL^a(u), \tag{3.32a}$$

$$\tilde{\psi}^*(u) = (v^*(I-Q)+Q)Q^a, \tag{3.32b}$$

and $v^*: Y_1 \cap Y_a \to R$, $\beta \in R$. The left vector $\tilde{\psi}^*(u)$ for $u \neq u_0$ can also be used to advantage in the evaluation of the extended system. We do not pursue this here, but refer the interested reader to [16] for similar calculations.

In the example computations discussed in the subsequent sections it was inconvenient to solve transposed systems of the form (3.32a). We end this section by considering another form for $F_{q,j}$ which does not require the solution of transposed systems. The idea is to treat the necessary derivatives of Ω as independent variables, appending their defining conditions to the extended system. The details of similar manipulations are given in [16, § 5] and so we merely state that (3.30a) and (3.30b) are equivalent to

$$F_{0,0}(u, \phi_a) := \begin{pmatrix} F^s(u) \\ F_x^a(u)\phi_a \\ l^*\phi_a - 1 \end{pmatrix} = 0, \tag{3.33a}$$

$$F_{1,1}(u, \phi_a, v_s, w_a) := \begin{pmatrix} F^s(u) \\ F_x^a(u)\phi_a \\ l^*\phi_a - 1 \\ F_x^s(u)v_s + F_\lambda^s(u) \\ F_x^a(u)w_a + F_{xx}^a\phi_a v_s + F_{x\lambda}^a\phi_a \\ l^*w_a - 1 \end{pmatrix} = 0, \tag{3.33b}$$

respectively, with $\phi_a, w_a \in X_a$, $v_s \in X_s$ (see [7]). Similar expressions can be developed for the other types of singularities (see § 4). We note that the regularity of solutions of (3.33a), (3.33b), or indeed any other system derived in this way, is a direct consequence of the regularity of the original system (3.22a). The side-constraints can also be monitored without using ψ^*, as is discussed in the next section.

4. Numerical implementation. In this section we discuss briefly some of the main points in the numerical implementation of the systems given in § 3 for the computation of singular points. In that section it was shown that there are at least two different choices for the (0, 0)-extended system, namely, (3.30a) and (3.33a), and that by taking different choices for the projection Q in (3.8) there are other, mathematically equivalent, extended systems (cf. [16] for the nonsymmetric case). The choice of extended system depends very much on the details of the implementation for any specific problem. In the example on the Taylor problem in § 5, $X = R^n$, where $n \approx 10^3$, F arises from a finite element discretisation of the Navier–Stokes equations, and the methods for the calculation of the symmetry-breaking bifurcation points are designed to fit into a large general purpose finite element code for two-dimensional partial differential equations including incompressible flow problems. Thus decisions on the choice of method are not made purely with respect to the Taylor problem.

There are many aspects to the numerical implementation of any method but for this discussion there are two points which should be mentioned. First a direct method based on the frontal method [10] is used to compute LU factors of matrices arising from the finite element discretisation. For problems of moderate size, say, having a few thousand unknowns, it is acceptable to alter the structure of the Jacobian F_x by replacing one column by another column to ensure the resulting matrix is nonsingular. This modification to the matrix structure does not adversely affect the efficiency of the frontal method since the variable corresponding to the extra column is simply held in the active matrix throughout the decomposition. Second, at the time the software was written the system (3.30a) had not been analysed by the authors. When (3.30a) did become available it was not used because the frontal method software was at an early developmental stage and could not easily produce the LU factors of F_x^T. A second assembly and factorisation would have been required to produce this information, and would have been too expensive. At present this is no longer a limitation of the software and either system could now be used, but for our application (3.30a) does not produce savings sufficient to warrant recording the algorithms.

Such considerations lead us to use methods based on systems like (3.33a) and (3.33b) even though at first sight they may appear unsuitable because of the inclusion of the unknowns φ, u, etc., in the systems. The solution procedure is based on that described in [7] and [24] and is not repeated here. We merely note that, to check a side constraint, $\psi^* d \neq 0$, say, after the nonlinear solver has converged, it is sufficient to solve

$$\begin{pmatrix} F_x^a & b \\ l^* & 0 \end{pmatrix} \begin{pmatrix} w \\ \alpha \end{pmatrix} = \begin{pmatrix} d \\ 0 \end{pmatrix}. \tag{4.1}$$

Then $\alpha \neq 0 \Rightarrow \psi^* d \neq 0$. Note that matrices like (4.1) arise in the solution procedure described in [24] and so little extra work is required.

It is worth mentioning that for the finite element method used in § 5 the evaluation of terms like $F_{xx}\varphi_a u_s$ (which arise in the Jacobians of the extended systems) is no more complicated than the evaluation of F. Hence there is no reason not to use high-order derivative terms. This is particularly important in the consideration of the singularities of codimension 1, 2, and 3*, which involve several such terms.

Finally, for convenience, we outline how to set up extended systems for the $(1, -1)$ and the $(3^*, 0, m)$-singularities corresponding to (3.33b). The approach is similar to that described in § 3.3 to derive (3.33a, b) and so we omit all details. The condition $a_z(w) := h_{\varepsilon\varepsilon\varepsilon}(w) = 0$ (cf. (3.25a, b)) leads to the following equations where $u = (x, \lambda, \alpha)$:

$$\begin{gathered} F_x^s(u) z_s + F_x^a \phi_a \phi_a = 0, \\ F_x^a(u) q_a + F_{xx}^a \phi_a z_s + \tfrac{1}{3} F_{xxx}^a \phi_a \phi_a \phi_a = 0, \\ l^* q_a = 0 \end{gathered} \tag{4.2}$$

and these are appended to (3.33a) to compute a $(1, -1)$-singularity. To compute a $(3^*, 0, m)$-singularity, append (4.2) to (3.33b).

5. The Taylor problem. In this section we are concerned with the application of the systems developed in § 3 to the problem of calculating steady axisymmetric flows in the Taylor problem [6]. The experimental situation we have in mind consists of two concentric circular cylinders. The inner cylindrical wall rotates and the outer cylinder and both ends are stationary. The annular gap between the cylinders is filled with a fluid, and it is the motion of this fluid that is studied. One of the ends consists of a movable annular collar so that the length of the annulus may be adjusted. Benjamin [2] and Benjamin and Mullin [3] have carried out several experimental investigations of flow in the above apparatus and have discovered an interesting variety of bifurcation phenomena. The apparatus has two parameters which may be adjusted: namely, the speed of the inner cylinder (in nondimensional form the Reynolds number, R) and the length of the annulus (in nondimensional form the aspect ratio, Γ); the apparatus is mirror symmetric about the midplane of the annulus. (The apparatus also possesses a symmetry about the axis of the cylinders, but since this symmetry is not broken by the computed solutions it is not important for our analysis (recall the discussion leading to (3.6a).)

A discrete model of this boundary value problem was obtained using a finite element method and numerical solutions obtained using standard continuation methods (e.g., the pseudo-arclength approach of [17]) in conjuction with the extended systems described in this paper. The equations are given in [6]-[8] and are not reproduced here. It is sufficient to know that after nondimensionalisation, the unknowns are the primitive variables (u_r, u_ϕ, u_z) and p, with (r, ϕ, z) the polar coordinates in the region $D=\{(r, z)\,|\,0\leqq r\leqq 1, -0.5\leqq z\leqq 0.5\}$.

The boundary conditions are that u_r and u_z are zero on the entire boundary of D, and that u_ϕ is zero on the outer cyclinder ($r=1$) and 1 on the inner cylinder ($r=0$). On the ends ($z=\pm 0.5$) u_ϕ is zero except near the inner cylinder, where it increases smoothly to 1 over a small distance, ε. The exact value of ε and the variation of u_ϕ will depend on the details of the experiment; however, provided $\varepsilon<0.05$, we have found the results to be insensitive to the precise value of ε. We note that ε must be positive because when $\varepsilon=0$ the rate of dissipation of energy in the fluid becomes infinite [3]. The Z_2-symmetry in the equations can be expressed as [7], [8]

$$
\begin{aligned}
(5.1)\qquad & S\{u_r(r, z), u_\phi(r, z), u_z(r, z), p(r, z)\} \\
& \quad =\{u_r(r, -z), u_\phi(r, -z), -u_z(r, -z), p(r, -z)\}
\end{aligned}
$$

and clearly $S\neq I$, $S^2=I$.

The finite element method involves covering the region D with a mesh of nine-node, isoparametric quadrilateral elements and approximating the velocities (u_r, u_z, u_ϕ) by piecewise biquadratic functions and the pressure by piecewise linear functions, which are, in general, discontinuous across element boundaries. The meshes used to obtain the results given in § 6 were uniform in the r- and z-directions except near the corners where the inner cylinder meets the ends, where local refinement was used (see [6]). A typical mesh is shown in Fig. 2. For the calculation of symmetric flows and symmetry-breaking singular points, only half the region D need be discretized, whereas for asymmetric flows and other types of singular point the whole of D must be discretized.

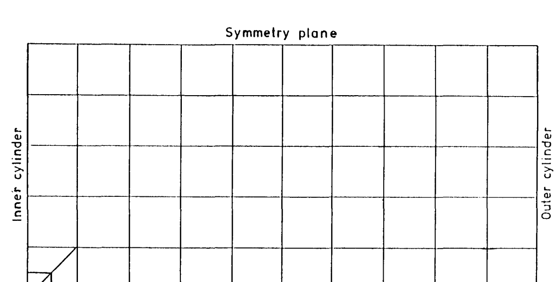

FIG. 2. *The finite element mesh.*

The meshes for the full region may be characterized by the triple (NR, NZ, NC), where NR and NZ are the numbers of elements in the r- and z-directions and the mesh has $2NC-1$ elements in each of the two corners where there is local refinement. A mesh for one half of the region D will be denoted by (NR, NZ, NC, S) and is essentially equivalent to that part of an $(NR, 2NZ, NC)$ mesh with $z \leqq 0$. The total number of degrees of freedom on an (NR, NZ, NC) mesh is $3(2NR+1)(2NZ+1)+60(NC-1)+3NR.NZ+12(NC-1)$ and $3(2NR+1)(2NZ+1)+30(NC-1)+3NR.NZ+6(NC-1)$ on an (NR, NZ, NC, S) mesh. The calculations presented in § 6 were done on $(10, 10, 5)$ and $(10, 5, 5, S)$ meshes having 1878 and 987 degrees of freedom, respectively.

Further details of the finite element implementation can be found in [8]. We merely state that the resulting finite-dimensional system may be written as

$$F(x, R, \Gamma, \eta)=0, \tag{5.2}$$

where x represents the motion of the fluid, R is the Reynolds number, Γ is the aspect ratio, and η the radius ratio. Also F satisfies the Z_2-symmetry condition for an appropriate discretişation of (5.1). Finally, we remark that we do not discuss any questions of the convergence of the numerical scheme in this paper, but refer the reader to [5], [19] for preliminary results on this topic.

6. Results. In this section we present some numerical results for the finite Taylor problem obtained with the techniques described in this paper. The physical situation we are concerned with is when the length of the annular region is comparable to the separation of the cylinders, so that the aspect ratio is near 1. Under these conditions the flows have either one or two Taylor cells. The two-cell flows may be symmetric about the mid-plane or asymmetric. (The single-cell flows are, in fact, highly asymmetric two-cell flows with one cell so weak as to be barely observable [6].) At sufficiently low Reynolds number all the flows are symmetric and have two cells because the Navier-Stokes equations have a unique solution at low Reynolds number.

At aspect ratio 1 and radius ratio 0.615 (i.e., the situation studied in [3]), symmetric two-cell branch was computed, on a symmetric grid, using standard continuation techniques. The presence of the symmetry-breaking bifurcation, which leads to the development of the single-cell flows, was detected by monitoring the sign of the determinant of the antisymmetric Jacobian matrix. This requires an LU decomposition of the antisymmetric Jacobian matrix after the solution has been obtained, and since each solution requires about five Newton steps, this increases the computational cost by approximately 20%. The path of symmetry-breaking bifurcations passing through the detected point, with radius ratio fixed at 0.615, was then computed. The side-constraints for the $(0, 0)$-singularity were monitored along the path and a change in sign indicated the presence of a $(1, -1)$- and a $(1, 1)$-singularity. The paths of these two singularities were computed using system (3.33b) for the $(1, 1)$-singularity and the corresponding system for the $(1, -1)$-singularity (see § 4). The paths of these singularities in the Γ-η plane are shown in Fig. 3. Along each singular path the side-constraints were monitored, which indicated a $(2, -2)$-singularity on the path of $(1, -1)$-singular points and $(3^*, 0, m)$-singularity where the $(1, -1)$ and $(1, 1)$ paths touch. Also two paths of nonsymmetric codimension-1 singularities are given. A path of nondegenerate hysteresis points on the asymmetric part of the solution emanates from the $(2, -2)$-singularities. Similarly, a path of nonsymmetric transcritical bifurcation points emanates from the $(3^*, 0, m)$-singularity. These paths were calculated using systems for nonsymmetric singularities analogous to (3.33) (see [16]).

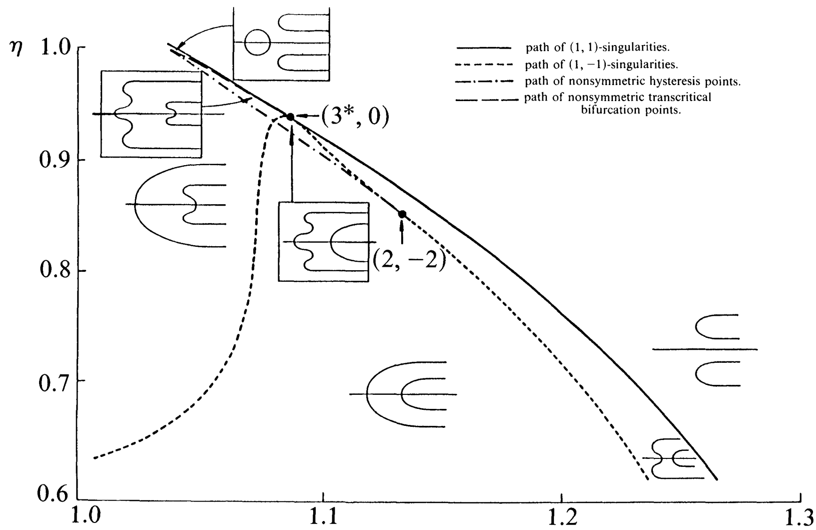

FIG. 3. *Γ-η parameter space. The lines represent paths of codimension one singularities. The parameter space is divided into open regions by the paths and representative bifurcation diagrams are given for each region.*

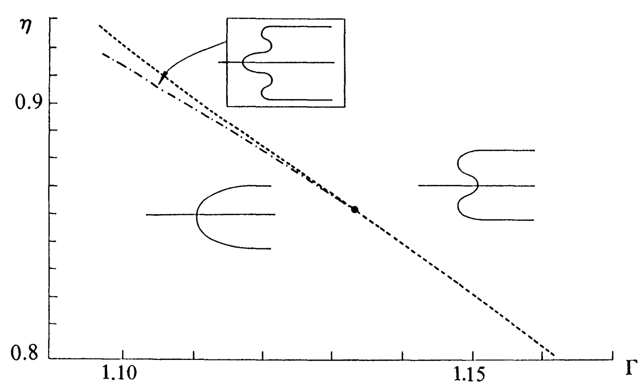

FIG. 4. *Parameter space near the* $(2, -2)$*-singularity.*

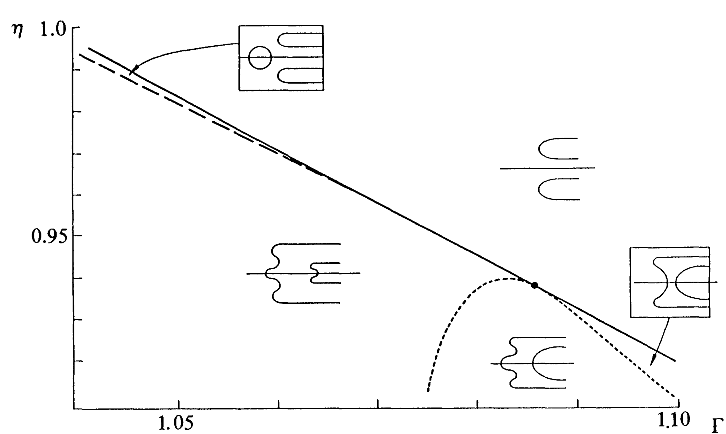

FIG. 5. *Parameter space near the* $(3, 0)$*-singularity.*

Figure 3 shows the parameter space Γ-η divided up into disjoint regions, by the paths of singularities. In each region the bifurcation diagrams are qualitatively similar and the forms of the diagrams are indicated on the figure. Figures 4 and 5 show expanded forms of the regions near the $(2, -2)$- and $(3^*, 0)$-singularities, respectively. Figure 4 should be compared with the diagram of the canonical form and its unfolding (transition set) in [12, p. 269]. (Note that there is a minor error in that figure—the path of hysteresis points should be tangential to the path of $(1, -1)$-singularities at the $(2, -2)$-singularity.) Figure 5 also should be compared with the canonical form in [12, p. 276] since $a_{\lambda\lambda}a_{zz} < 0$. We note that the case $m > 0$ is simply a reflection in λ of the $m < 0$ case.

Finally it should be mentioned that much of the interesting structure near the $(2, -2)$- and $(3^*, 0)$-singularities is not experimentally observable. The reason for this is that at the larger radius ratios the transition to time-dependent nonaxisymmetric flow occurs at a lower Reynolds number than the singularities in question.

Appendix.

Proof of Theorem 2.15. We apply a separate analysis for each singularity having codimension less than 4. We begin by sketching a general approach which can be used for all the singularities. However, simpler proofs are often available for any particular type of singularity, and these are not pursued here.

Let (q, j), $q \leqq 3$, denote one of the singularities for (2.1) (including the $(3^*, 0, m)$-singularity). Suppose $u_0 = (x_0, \lambda_0, \alpha_0) = 0$ is a (q, j)-singularity of (2.1). Let $H_{q,j}(u; f)$ denote the extended system obtained from the Z_2-hierarchy as applied to f (see § 2). Therefore

$$H_{q,j}(0; f) = 0 \in R^{q+1}. \tag{A.1}$$

In the sequel we omit the subscripts q, j from $H_{q,j}$.

The first step of the proof is to show that the rank of $(\partial H/\partial(\lambda, \alpha))(0; f)$ is invariant under contact transformation. In particular, we have the following lemma.

LEMMA A.1. *Suppose* $p = q$ *and*

$$\frac{\partial H}{\partial(\lambda, \alpha)}(0; f) \textit{ is nonsingular.} \tag{A.1}$$

Define

$$g(x, \lambda, \alpha) := T(x^2, \lambda) f(X(x, \lambda), \Lambda(\lambda), \alpha), \tag{A.2a}$$

where

$$X(x, \lambda) = x\mathscr{H}(x^2, \lambda), \qquad \mathscr{H}(0, 0) \neq 0, \tag{A.2b}$$

$$\Lambda(0) = 0, \qquad \Lambda_\lambda(0) \neq 0, \qquad T(0, 0) \neq 0. \tag{A.2c}$$

That is, (A.2a) *is a* Z_2*-equivalence relation. Then in the obvious notation, the extended system applied to g satisfies*

$$\frac{\partial H}{\partial(\lambda, \alpha)}(0; g) \textit{ is nonsingular.} \tag{A.3}$$

This lemma is also proved using a case-by-case analysis, for which we provide a general outline below. For the moment we assume that Lemma A.1 has been proven, and consider the remainder of the proof of Theorem 2.15.

Lemma A.1 ensures that we need only consider functions f that have been put into normal form. That is, we can take

$$f(x, \lambda, \alpha) = h(x, \lambda) + x\left\{\sum_{i=1}^{q} \alpha_i p_i(z, \lambda, \alpha)\right\} \tag{A.4a}$$

with $z = x^2$ and

$$h(x, \lambda) = xa(z, \lambda), \tag{A.4b}$$

given by the *polynomial* in the (q, j)-node of the hierarchy. Using the notation in [12, Chap. VI], it now remains to show that (A.1) is equivalent to (see, [12, Thm. 3.3, p. 259])

$$\vec{\mathscr{E}}_{x,\lambda}(Z_2) = T(h, Z_2) + R\{xp_i(z, \lambda, 0) \mid i = 1, \cdots, q\}. \tag{A.5}$$

(For brevity, we assume here that the reader is familiar with the material in [12].) This final computation is significantly aided by the explicit expressions for $T(h, Z_2)$ for each of the singularities in question, provided in Table 5.2 of [12]. Below we provide an example of this last calculation for the $(3^*, 0, m)$-singularity.

Let $h(x, \lambda)$ be the normal form for the $(3^*, 0, m)$-singularity, that is, (A.4b) is satisfied with

$$a(z, \lambda) = (z^2 + 2mz\lambda + \delta\lambda^2), \qquad \delta = \pm 1, \quad m \in R. \tag{A.6}$$

Given any germ $xb(z, \lambda) \in \vec{\mathscr{E}}_{x,\lambda}(Z_2)$ we write out the coefficients of the Taylor expansion for $b(z, \lambda)$ about $(0, 0)$ in a vector

$$v := (b_{00}, b_{10}, b_{11}, b_{20}, b_{21}, b_{22})^T, \tag{A.7a}$$

where

$$b(z, \lambda) = \sum_{i,j} b_{ij} z^{i-j} \lambda^j. \tag{A.7b}$$

(In general, the coefficients of the nonomials that are *not* higher-order terms, that is, not in the module $P(h, Z_2)$ given in Table 5.2 of [12], are included in the vector v.) Next a matrix is formed by writing down a basis for a complementary space of $P(h, Z_2)$ in $T(h, Z_2)$, and appending terms obtained from the unfolding. In particular, for the $(3^*, 0, m)$-singularity we obtain

$$M = \begin{pmatrix} 0 & 0 & 0 & a_\alpha \\ 0 & 0 & m & a_{z\alpha} \\ 0 & 0 & \delta & a_{\lambda\alpha} \\ 1 & 1 & 0 & \frac{1}{2}a_{zz\alpha} \\ 2m & m & 0 & a_{z\lambda\alpha} \\ \delta & 0 & 0 & \frac{1}{2}a_{\lambda\lambda\alpha} \end{pmatrix} \in R^{6\times 6}, \qquad \alpha \in R^3, \quad \delta = \pm 1. \tag{A.8}$$

The first column of M corresponds to $z^2 + 2m\lambda + \lambda^2$, which is a germ in $T(h, Z_2)$. The condition that f in (A.4) is a universal unfolding (i.e., that (A.5) is satisfied) is equivalent to

$$\det M \neq 0 \tag{A.9}$$

(see [11, Prop. 3.48], $\nu = 7$, where the same construction has been used).

By multiplying the last three rows of M by the matrix

$$V := \frac{1}{2}\begin{pmatrix} -m & 1 & -m\delta \\ 2 & 0 & 0 \\ 0 & 0 & -2\delta \end{pmatrix} \tag{A.10}$$

we obtain

(A.11a)
$$\hat{M} = \begin{pmatrix} I & 0 \\ 0 & V \end{pmatrix} M = \begin{pmatrix} 0 & \hat{M}_{12} \\ \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix} & \hat{M}_{22} \end{pmatrix},$$

(A.11b)
$$\hat{M}_{12} = \begin{pmatrix} 0 & a_\alpha \\ m & a_{z\alpha} \\ \delta & a_{\lambda\alpha} \\ 0 & r_\alpha \end{pmatrix} \in R^{4\times 4},$$

(A.11c)
$$r_\alpha = \tfrac{1}{4}(2a_{z\lambda\alpha} - m[a_{zz\alpha} + \delta a_{\lambda\lambda\alpha}]).$$

It is clear from (A.10) and (A.11) that (A.9) is equivalent to

(A.12)
$$\det \hat{M}_{12} \neq 0.$$

Moreover, it is trivial to check that

(A.13)
$$r_\alpha = \frac{\partial}{\partial\alpha} M_{3^*,0,m}(0), \qquad r_\lambda = \frac{\partial}{\partial\lambda} M_{3^*,0,m}(0) = 0,$$

where $M_{3^*,0,m}$ is as in (2.10a) (a similar result can be shown for $M_{3^*,0,m}$ given by (2.10b) when $m \neq 0$). It now follows from (A.11b) and (A.13) that

(A.14)
$$\frac{\partial H_{3^*,0,m}}{\partial(\lambda, \alpha)}(0) = \hat{M}_{12},$$

and the desired equivalence results follow from (A.12).

The same approach can be used for the other (q, j)-singularities; we omit the details. We are left with the following proof.

Proof of Lemma A.1. We begin by eliminating the trivial case of scaling, that is, for transformations (A.2a) with

(A.15)
$$T = T_0, \quad X = X_0 x, \quad \Lambda = \Lambda_0 \lambda.$$

Here, T_0, X_0, and Λ_0 are nonzero constants. In this case a straightforward computation can be used to show (A.3). For the remainder of the proof it is convenient to assume that f has already been rescaled so that the transformation (A.2) also satisfies

(A.16a)
$$T(0,0) = 1, \qquad \mathcal{X}(0,0) = 1,$$

(A.16b)
$$\Lambda(\lambda) = \lambda + l_2\lambda^2 + O(\lambda^3).$$

A second simplification results from the fact that we need only consider infinitesimal contact transformations. The argument for this is common to any particular type of singularity, and goes as follows. Let T, X, Λ be as in (A.2) with (A.16) satisfied. Define

(A.17a)
$$T(x, \lambda; t) = tT(x, \lambda) + (1-t),$$

(A.17b)
$$X(x, \lambda; t) = tX(x, \lambda) + (1-t)x,$$

(A.17c)
$$\Lambda(\lambda; t) = t\Lambda(\lambda) + (1-t)\lambda,$$

(A.17d)
$$h(x, \lambda, \alpha; t) := T(x, \lambda; t) f(X(x, \lambda; t), \Lambda(\lambda; t), \alpha)$$

for $t \in [0, 1]$. Then it follows that the transformation (A.17d) is a Z_2-equivalence relation with (A.16) satisfied for all t. In the obvious notation, define

(A.18)
$$J(t) = \frac{\partial H(0; t)}{\partial(\lambda, \alpha)}, \qquad t \in [0, 1].$$

If it can be shown that

$$\frac{dJ}{dt}(t)=A(t)J(t), \qquad t\in[0,1], \tag{A.19}$$

then the lemma follows from the relation (see [9, Thm. 7.3, p. 28])

$$\det J(1)=\left\{\int_0^1 tr[A(s)]\,ds\right\}\det J(0) \tag{A.20}$$

and the fact that $J(0)=(\partial H/\partial(\lambda,\alpha))(0;f)$, $J(1)=(\partial H/\partial(\lambda,\alpha))(0;g)$.

Therefore we are left with proving (A.19). Note, however, that $h(x,\lambda,\alpha;t+\tau)$ and $h(x,\lambda,\alpha;t)$ are contact equivalent, and that the corresponding transformation satisfies (A.16). Hence (A.19) will follow if we can show that, for a general function f (with a (q,j)-singularity at $(0,0,0)$),

$$\frac{dJ}{dt}(0)=A(0)J(0), \qquad J(0):=\frac{\partial H}{\partial(\lambda,\alpha)}(0;f), \tag{A.21}$$

for $A(0)$ a smooth function of $\dot{T}$, $\dot{X}$, and $\dot{\Lambda}$. Here and in the sequel $\dot{T}=dT/dt$, etc.

The entire proof now relies on proving (A.21). We illustrate the necessary calculations by considering the $(3^*,0,m)$-singularity (the other singularities can be treated in a similar, and often simpler, way). We assume that f is of the form (A.4) with a suitable scaling so that

$$a(z,\lambda)=z^2+2m\lambda z+\delta\lambda^2+\text{hots}, \tag{A.22}$$

where hots denotes higher-order terms (that is, elements of $P(f;Z_2)$, which includes cubic and higher-order terms in z and λ).

Note that Theorem 2.13 ensures a, a_z, and a_λ all vanish at $(0,0)$. In fact, since (A.17c) satisfies (A.16) for all t, it follows that $h(x,\lambda,\alpha;t)$ is of the form (A.4) with

$$a(z,\lambda;t)=z^2+2m\lambda z+\delta\lambda^2+\text{hots}, \tag{A.23}$$

where m and δ do *not* vary with t.

We now proceed in the same manner that led to (A.8), only this time higher-order terms arise in M. In particular, we find

$$M(t)=\begin{pmatrix} 0 & 0 & 0 & a_\alpha \\ 0 & 0 & m & a_{z\alpha} \\ 0 & 0 & \delta & a_{\lambda\alpha} \\ 1 & 1 & \frac{1}{2}a_{zz\lambda} & \frac{1}{2}a_{zz\alpha} \\ 2m & m & a_{z\lambda\lambda} & a_{z\lambda\alpha} \\ \delta & 0 & \frac{1}{2}a_{\lambda\lambda} & \frac{1}{2}a_{\lambda\lambda\alpha} \end{pmatrix}\in R^{6\times 6}, \quad \alpha\in R^3, \quad m\in R, \quad \delta=\pm 1. \tag{A.24}$$

Moreover, it is easily checked that, for V as in (A.10), $\hat{M}$ and $\hat{M}_{12}$ as in (A.11a), we have

$$\hat{M}_{12}(t)=\frac{\partial H}{\partial(\lambda,\alpha)}(0;h(x,\lambda,\alpha;t))=:J(t). \tag{A.25}$$

Note that (A.10) and (A.23) show that

$$\dot{V}=0. \tag{A.26}$$

By differentiating (A.17a, b, c, d) with respect to t, and using (A.16), a straightforward calculation shows that

$$\dot{M}(0) = \mathcal{T}M(0). \tag{A.27a}$$

Here $\mathcal{T} \in \boldsymbol{R}^{6\times6}$ has the form

$$\mathcal{T} = \begin{array}{c} \begin{array}{ccc} \overbrace{}^{1} & \overbrace{}^{2} & \overbrace{}^{3} \end{array} \\ \begin{pmatrix} 0 & 0 & 0 \\ * & 0 & 0 \\ * & * & 0 \end{pmatrix} \end{array} \begin{array}{l} \\ \}1 \\ \}2, \\ \}3 \end{array} \tag{A.27b}$$

where * denotes the blocks that can be nonzero. Moreover, the nonzero elements correspond to coefficients in $\dot{T}$, $\dot{X}$, $\dot{\lambda}$.

Finally, for $\hat{M}$ defined as in (A.11a), we have

$$\begin{aligned} \frac{d\hat{M}}{dt}(0) &= \begin{pmatrix} I & 0 \\ 0 & V \end{pmatrix} \frac{dM}{dt}(0) = \begin{pmatrix} I & 0 \\ 0 & V \end{pmatrix} \mathcal{T}M(0) \\ &= \hat{\mathcal{T}} \begin{pmatrix} I & 0 \\ 0 & V \end{pmatrix} M(0) = \hat{\mathcal{T}} \begin{pmatrix} 0 & J(0) \\ \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix} & \hat{M}_{22}(0) \end{pmatrix}, \end{aligned} \tag{A.28a}$$

where

$$\hat{\mathcal{T}} = \begin{pmatrix} I & 0 \\ 0 & V \end{pmatrix} \mathcal{T} \begin{pmatrix} I & 0 \\ 0 & V^{-1} \end{pmatrix}. \tag{A.28b}$$

It is clear from (A.28b) that $\hat{\mathcal{T}}$ has the same block structure as depicted in (A.27b). Therefore it follows from (A.28) that

$$\frac{dJ}{dt}(0) = \hat{\mathcal{T}}_{11} J(0), \tag{A.29}$$

where $\hat{\mathcal{T}}_{11}$ is the principal 4×4 submatrix in $\hat{\mathcal{T}}$. This proves (A.21), and completes our proof of Lemma A.1. □

We remark that the unfolding conditions given in [11, Prop. 3.48] for $\nu = 3$ and 5 are correct only if f is in normal form. The proper conditions for general f can be obtained from Theorem 2.15.

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