SIAM J. NUMER. ANAL.
Vol. 41, No. 2, pp. 401–435

COMPUTATION OF PERIODIC SOLUTION BIFURCATIONS IN ODES USING BORDERED SYSTEMS*

E. J. DOEDEL†, W. GOVAERTS‡, AND YU. A. KUZNETSOV§

Abstract. We consider numerical methods for the computation and continuation of the three generic secondary periodic solution bifurcations in autonomous ODEs, namely the fold, the period-doubling (or flip) bifurcation, and the torus (or Neimark–Sacker) bifurcation. In the fold and flip cases we append one scalar equation to the standard periodic BVP that defines the periodic solution; in the torus case four scalar equations are appended. Evaluation of these scalar equations and their derivatives requires the solution of linear BVPs, whose sparsity structure (after discretization) is identical to that of the linearization of the periodic BVP. Therefore the calculations can be done using existing numerical linear algebra techniques, such as those implemented in the software AUTO and COLSYS.

Key words. bifurcations, periodic solutions, continuation, boundary value problems

AMS subject classifications. 65P30, 65L10, 37M20, 37G15

PII. S0036142902400779

1. Introduction.

We consider parameterized ODEs of the form

$$\frac{dx}{dt} \equiv x' = f(x, \alpha), \tag{1.1}$$

where $x \in \mathbf{R}^n$ is the *state variable*, where $\alpha \in \mathbf{R}^m$ represents *parameters*, and where $f(x, \alpha) \in \mathbf{R}^n$ is a (usually nonlinear) smooth function of x and α. Examples of systems of the form (1.1) are ubiquitous in mathematical models in physics, engineering, chemistry, economics, finance, etc.

The simplest solutions of (1.1) are the *equilibria*, that is, solutions of the equation

$$f(x, \alpha) = 0.$$

An equilibrium (x_0, α_0) is asymptotically stable if all eigenvalues of the Jacobian matrix $f_x(x_0, \alpha_0)$ have a strictly negative real part; it is unstable if there is at least one eigenvalue with a strictly positive real part. In generic one-parameter problems, i.e., when $m = 1$, eigenvalues on the imaginary axis appear in two ways: as a simple zero eigenvalue, or as a conjugate pair $\pm i\omega$, $\omega > 0$, of purely imaginary eigenvalues. The first singularity corresponds generically to a *limit point bifurcation*, where two solutions coalesce and annihilate each other under parameter variation. The second singularity corresponds generically to a *Hopf bifurcation*, from which a family of periodic solutions emerges. Early papers on the numerical computation of bifurcations of equilibria are [16], [22], and [20].

*Received by the editors January 9, 2002; accepted for publication (in revised form) October 16, 2002; published electronically April 23, 2003.
http://www.siam.org/journals/sinum/41-2/40077.html
†Applied Mathematics 217-50, California Institute of Technology, Pasadena CA 91125 (on leave from Concordia University, Montreal, Canada) (doedel@cs.concordia.ca).
‡Department of Applied Mathematics and Computer Science, University of Gent, Krijgslaan 281-S9, B-9000 Gent, Belgium (willy.govaerts@rug.ac.be).
§Mathematical Institute, Utrecht University, Budapestlaan 6, P.O. Box 80010, 3508 TA Utrecht, The Netherlands and Institute of Mathematical Problems of Biology, Russian Academy of Sciences, Pushchino, Moscow Region, 142290 Russia (kuznetsov@math.uu.nl).

Periodic solutions are solutions for which $x(T) = x(0)$ for some number $T > 0$. The minimal such T is called the *period*. In generic one-parameter problems, periodic solutions can bifurcate in several ways that can be characterized by the properties of the *monodromy matrix*. The monodromy matrix is the linearized T-shift along orbits of (1.1), evaluated at the point $x(0)$ on the periodic solution. The eigenvalues of this matrix are called the *Floquet multipliers* of the periodic solution [14], [17].

A periodic solution always has a multiplier equal to 1. If this multiplier has geometric multiplicity 1, then we call the periodic solution *regular*. The corresponding eigenvector of the monodromy matrix is the tangent vector to the periodic solution at the point where the monodromy matrix is computed. If all other multipliers are strictly inside the unit circle in the complex plane, then the periodic solution is asymptotically stable. If at least one multiplier has modulus greater than 1, then the periodic solution is unstable. In all other cases, one should take into account higher-order derivatives of the T-shift to decide whether or not the periodic orbit is stable.

Three singularities, determined by the monodromy matrix, can occur along a one-parameter family ("curve" or "branch") of periodic solutions, namely (1) *a fold singularity*, when the multiplier 1 has algebraic multiplicity equal to or greater than 2; (2) *a flip singularity*, when there is a multiplier equal to -1; (3) *a Neimark–Sacker singularity*, when there is a conjugate pair of complex multipliers with modulus 1.

Under some genericity conditions, each of these singularities implies a certain bifurcation scenario. These conditions always include some *spectral conditions* on the critical multipliers, i.e., multiplicity restrictions and the absence of other critical multipliers. Furthermore, there are *nondegeneracy conditions* that can be formulated in terms of the system at the critical parameter values, and *transversality conditions* that are determined by the system's dependence on the parameter (see [17]). We shall list all relevant genericity conditions in the following sections.

Generically, the first critical case (fold) corresponds to a point on the periodic solution family where the curve turns quadratically with respect to the free parameter. This phenomenon is called a *limit point* (*fold*) *bifurcation*: Two periodic solutions collide and disappear when the parameter passes the critical value. The second case (flip) indicates generically a *period-doubling* of the periodic solution; i.e., there are nearby periodic solutions of approximately double period. It is also called the *flip bifurcation*. Finally, the third case (Neimark–Sacker) corresponds generically to a bifurcation of an *invariant torus*, on which the flow contains periodic or quasi-periodic motions. This phenomenon is often called the *Neimark–Sacker bifurcation*. There is some ambiguity in calling a bifurcation by the same name as the corresponding singularity. However, this is a common practice in the applied literature.

The aim of this paper is to formulate the computation and continuation of the three generic periodic solution bifurcation curves as *minimally extended BVPs* to which standard numerical approximation methods as well as convergence theory apply. *Fully extended BVPs* for continuing periodic solution bifurcations have been implemented in AUTO [6] (see also [7], [15]). The latter approach doubles the number of function components in the case of the period-doubling and fold bifurcations, and triples it in the case of the torus bifurcation. Fully extended BVPs also yield a more complicated Jacobian sparsity structure (after discretization) than that corresponding to the underlying periodic BVP. There are efficient solution techniques for such sparse linear systems; see, for example, [10]. However, these are not very easy to implement and they are specific for each bifurcation. By contrast, the minimal BVPs

presented in this paper for the period-doubling and fold bifurcations have the same number of function components as the periodic solution problem. In the torus case the number of BVP function components is only doubled, but the resulting system is overdetermined. The most important numerical advantage is that only one type of sparse system needs to be solved, namely the one corresponding to the underlying periodic BVP. Conceptually, the approach used in this paper is similar to the *bordering technique* for equilibrium bifurcations [5], [12], [13], [17].

The paper is organized as follows. Section 2 is devoted to the computation of one-parameter families of periodic solutions to (1.1). Classical results on the regularity of BVPs defining families of periodic solutions are proved here for completeness. Sections 3 and 4 present the main results of the paper. Here we construct functionals that vanish at bifurcation points of periodic solutions and we prove that they are well-defined and regular. As is usual, only some of the nondegeneracy conditions that appear in bifurcation analysis are necessary for regularity. Section 5 deals with various computational issues, including efficient computation of the defining systems and their derivatives. A numerical example is given in section 6.

2. Computation and continuation of periodic solutions. Numerical continuation is a technique to compute solution curves to an underdetermined system of equations. Details can be found, for example, in [1], [3], [12], and [16]. It is a basic ingredient of the numerical bifurcation algorithms implemented in AUTO [6] and CONTENT [18]. In this case only one parameter is free, so for practical purposes the parameter vector reduces to a scalar. In this paper we restrict our discussion to issues that are specific to the case of periodic orbits.

To compute a periodic solution of period T of (1.1), one first fixes the period by rescaling time. Then (1.1) becomes

$$x'(t) = Tf(x(t), \alpha), \tag{2.1}$$

and we look for solutions of period 1, that is,

$$x(0) = x(1). \tag{2.2}$$

The period T is one of the unknowns of the problem. In a continuation context, we assume that a solution $(x_{k-1}(\cdot), T_{k-1}, \alpha_{k-1})$ is known, and we want to find $(x_k(\cdot), T_k, \alpha_k)$, which we denote by $(x(\cdot), T, \alpha)$. Equations (2.1) and (2.2) together do not fix the solution completely, since any solution can be translated freely in time; that is, if $x(t)$ is a solution, then so is $x(t+\sigma)$ for any σ. To fix the solution it is necessary to add a "phase condition." In AUTO [6] and CONTENT [18] the integral constraint

$$\int_0^1 x^*(\tau) x'_{k-1}(\tau)\, d\tau = 0 \tag{2.3}$$

is used to fix the phase. (We use "*" to denote transpose.)

The periodic solution is now determined by (2.1), (2.2), (2.3), which together form a BVP with an integral constraint.

In our continuation context, the periodic orbit $x(t)$ and the scalars T and α vary along the solution family. In the setting of Keller's pseudoarclength continuation method [16] the continuation equation is

$$\int_0^1 (x(\tau) - x_{k-1}(\tau))^* \dot{x}_{k-1}(\tau)\, d\tau \; + (T - T_{k-1})\dot{T}_{k-1} + (\alpha - \alpha_{k-1})\dot{\alpha}_{k-1} = \Delta s, \tag{2.4}$$

where the derivatives are taken with respect to arclength in the function space, and should not be confused with the time derivatives in, for example, (2.3).

A widely used method to discretize the above BVP is the method of orthogonal collocation with piecewise polynomials. It is used in COLSYS [2], as well as in AUTO and CONTENT. The method is known for its high accuracy [4], and it is particularly suitable for difficult problems, due to its known optimal mesh adaptation techniques [21]. The numerical continuation of the discretized equations leads to structured, sparse linear systems [9]. To describe these systems it is convenient to formulate the BVP in terms of operators on function spaces.

Denote by $\mathcal{C}^k([a,b],\mathbf{R}^n)$ the space of k times continuously differentiable functions defined on $[a,b]$ and with values in $\mathbf{R}^n$. Let D be the differentiation operator acting from $\mathcal{C}^1([a,b],\mathbf{R}^n)$ to $\mathcal{C}^0([a,b],\mathbf{R}^n)$. Any $n\times n$ matrix $M(t)$ smoothly depending on $t\in[a,b]$ defines an operator from $\mathcal{C}^1([a,b],\mathbf{R}^n)$ into itself by the matrix multiplication $(M\psi)(t)=M(t)\psi(t)$. The Dirac evaluation operator at the point t is denoted δ_t.

For a given $\phi\in\mathcal{C}^0([0,1],\mathbf{R}^n)$ we denote by Int_ϕ the linear functional from $\mathcal{C}^0([0,1],\mathbf{R}^n)$ into $\mathbf{R}$ defined by

$$\mathrm{Int}_\phi(v)=\langle\phi,v\rangle=\int_0^1\phi^*(\tau)v(\tau)\,d\tau.$$

Suppose we want to compute a periodic solution of (1.1); i.e., we want to solve the system (2.1), (2.2), (2.3), and (2.4) for $(x(t),T,\alpha)$ by a Newton-like method. The Fréchet derivative operator corresponding to this problem has the form

$$\begin{pmatrix} D-Tf_x(x(t),\alpha) & -f(x(t),\alpha) & -Tf_\alpha(x(t),\alpha)\\ \delta_0-\delta_1 & 0 & 0\\ \mathrm{Int}_{x'_{k-1}(\cdot)} & 0 & 0\\ \mathrm{Int}_{\dot{x}_{k-1}(\cdot)} & \dot{T}_{k-1} & \dot{\alpha}_{k-1}\end{pmatrix}. \tag{2.5}$$

The discrete version of these linear operators is a square matrix that has a large matrix corresponding to $D-Tf_x(x(t),\alpha)$ in the upper left corner, bordered on the right by two extra columns and at the bottom by $n+2$ extra rows. The big matrix in the upper left corner is a block band matrix. Systems of this form are solved in AUTO by a specially adapted elimination algorithm that computes the multipliers as a by-product [9].

Consider the fundamental variational equation

$$X'-Tf_x(x(t),\alpha)X=0 \tag{2.6}$$

and the adjoint equation

$$X'+Tf_x^*(x(t),\alpha)X=0. \tag{2.7}$$

Denote by $\Phi(t)$ the fundamental matrix solution of (2.6), for which $\Phi(0)=I$, where $I=I_{n\times n}$ is the n-dimensional identity matrix. Then $\Phi(1)$ is the monodromy matrix of the periodic solution. The eigenvalues of $\Phi(1)$ are the Floquet multipliers, and there is always at least one multiplier that is equal to 1. A corresponding eigenvector is $x'(0)$. For a *regular periodic solution* the multiplier 1 has geometric multiplicity 1. Similarly, denote by $\Psi(t)$ the fundamental matrix solution to (2.7) for which $\Psi(0)=I$. One has $\Psi(t)=[(\Phi(t))^{-1}]^*$.

If $v(t)$ is a vector solution to (2.6) with initial values $v(0) = v_0$ and $w(t)$ is a vector solution to (2.7) with initial values $w(0) = w_0$, then the inner product satisfies $w^*(t)v(t) = w_0^* v_0$; i.e., it is independent of time t.

The left and right eigenvectors of the monodromy matrix $\Phi(1)$ for a geometrically simple eigenvalue 1 will be denoted p_0, q_0, respectively. It is easily seen that p_0 (respectively, q_0) is also the right (respectively, left) eigenvector of $\Psi(1)$ for the eigenvalue 1. Furthermore, q_0 is a scalar multiple of $x'(0)$.

We now state some basic facts about the linear operator (2.5) when linearized about a regular periodic solution $(x(t), T, \alpha)$.

PROPOSITION 1. *If $(x(t), T, \alpha)$ is a regular periodic solution of (2.1), then the operator*

$$\begin{bmatrix} D - Tf_x(x(t), \alpha) \\ \delta_1 - \delta_0 \end{bmatrix} \; : \; \mathcal{C}^1([0,1], \mathbf{R}^n) \to \mathcal{C}^0([0,1], \mathbf{R}^n) \times \mathbf{R}^n \tag{2.8}$$

has a one-dimensional kernel spanned by Φq_0. Its range has codimension 1; if $\zeta \in \mathcal{C}^0([0,1], \mathbf{R}^n)$, $r \in \mathbf{R}^n$, then $(\zeta, r)^*$ is in the range if and only if $\langle \Psi p_0, \zeta \rangle = p_0^* r$. In particular, if $r = 0$, then $(\zeta, 0)^*$ is in the range if and only if $\langle \Psi p_0, \zeta \rangle = 0$.

Proof. First, let $v(t)$ be in the kernel of (2.8). Then v must have the form $v(t) = \Phi(t)v_0$ for a vector v_0. Since $0 = (\delta_1 - \delta_0)v = v(1) - v(0) = (\Phi(1) - I)v_0$, we infer that v_0 must be a right eigenvector of $\Phi(1)$ for the eigenvalue 1.

Next, let $\zeta \in \mathcal{C}^0([0,1], \mathbf{R}^n)$, $r \in \mathbf{R}^n$, be given. If $(\zeta, r)^*$ is in the range of (2.8), then there must exist a $v \in \mathcal{C}^1([0,1], \mathbf{R}^n)$ for which

$$v'(t) - Tf_x(x(t), \alpha)v(t) = \zeta(t).$$

The general solution of this linear differential equation is

$$v(t) = \Phi(t) \left[v_0 + \int_0^t \Psi^*(\tau)\zeta(\tau) \, d\tau \right],$$

where $v_0 = v(0)$ is an initial vector. Also, we must have $v(1) - v(0) = r$, that is,

$$(\Phi(1) - I)v_0 + \Phi(1) \int_0^1 \Psi^*(\tau)\zeta(\tau) \, d\tau = r.$$

Such a vector v_0 can be found if and only if

$$p_0^* \left(\Phi(1) \int_0^1 \Psi^*(\tau)\zeta(\tau) \, d\tau \; - r \right) = 0,$$

that is, if

$$p_0^* \int_0^1 \Psi^*(\tau)\zeta(\tau) \, d\tau \; - p_0^* r = 0,$$

from which the second result follows. ∎

COROLLARY 1. *If $(x(t), T, \alpha)$ is a regular periodic solution of (2.1), then the operator*

$$\begin{bmatrix} D - Tf_x(x(t), \alpha) \\ \delta_1 - \delta_0 \\ \mathrm{Int}_\phi \end{bmatrix} \; : \; \mathcal{C}^1([0,1], \mathbf{R}^n) \; \to \; \mathcal{C}^0([0,1], \mathbf{R}^n) \times \mathbf{R}^n \times \mathbf{R} \tag{2.9}$$

is one-to-one if and only if $\langle \phi, \Phi q_0 \rangle \neq 0$.

PROPOSITION 2. *If* $(x(t), T, \alpha)$ *is a regular periodic solution of* (2.1)*, then the operator*

$$\begin{bmatrix} D + Tf_x^*(x(t),\alpha) \\ \delta_1 - \delta_0 \end{bmatrix} \; : \; \mathcal{C}^1([0,1],\mathbf{R}^n) \; \rightarrow \; \mathcal{C}^0([0,1],\mathbf{R}^n) \times \mathbf{R}^n$$

has a one-dimensional kernel spanned by Ψp_0*. Its range has codimension* 1*; if* $\zeta \in \mathcal{C}^0([0,1],\mathbf{R}^n)$*,* $r \in \mathbf{R}^n$*, then* $(\zeta, r)^*$ *is in the range if and only if* $\langle \Phi q_0, \zeta \rangle = q_0^* r$*. In particular, if* $r = 0$*, then* $(\zeta, 0)^*$ *is in the range if and only if* $\langle \Phi q_0, \zeta \rangle = 0$.

Proof. The proof is similar to the proof of Proposition 1. □

COROLLARY 2. *If* $(x(t), T, \alpha)$ *is a regular periodic solution of* (2.1)*, then the operator*

$$\begin{bmatrix} D + Tf_x^*(x(t),\alpha) \\ \delta_1 - \delta_0 \\ \mathrm{Int}_\psi \end{bmatrix} \; : \; \mathcal{C}^1([0,1],\mathbf{R}^n) \; \rightarrow \; \mathcal{C}^0([0,1],\mathbf{R}^n) \times \mathbf{R}^n \times \mathbf{R} \tag{2.10}$$

is one-to-one if and only if $\langle \psi, \Psi p_0 \rangle \neq 0$.

PROPOSITION 3. *Let* $(x(t), T, \alpha)$ *be a regular periodic solution of* (2.1)*, and let* $\phi_0, \psi_0 \in \mathcal{C}^0([0,1],\mathbf{R}^n)$ *be such that* $\langle \phi_0, \Phi q_0 \rangle \neq 0$*,* $\langle \psi_0, \Psi p_0 \rangle \neq 0$*. Then the operator*

$$\begin{bmatrix} D - Tf_x(x(t),\alpha) & \psi_0 \\ \delta_1 - \delta_0 & 0 \\ \mathrm{Int}_{\phi_0} & 0 \end{bmatrix} \; : \; \mathcal{C}^1([0,1],\mathbf{R}^n) \times \mathbf{R} \; \rightarrow \; \mathcal{C}^0([0,1],\mathbf{R}^n) \times \mathbf{R}^n \times \mathbf{R}$$

is one-to-one and onto.

Proof. To prove that the operator is one-to-one, suppose that

$$\begin{bmatrix} D - Tf_x(x(t),\alpha) & \psi_0 \\ \delta_1 - \delta_0 & 0 \\ \mathrm{Int}_{\phi_0} & 0 \end{bmatrix} \begin{pmatrix} v \\ G \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

for $v \in \mathcal{C}^1([0,1],\mathbf{R}^n), G \in \mathbf{R}$. In particular, it follows that

$$\begin{bmatrix} D - Tf_x(x(t),\alpha) \\ \delta_0 - \delta_1 \end{bmatrix} v = \begin{pmatrix} -G\psi_0 \\ 0 \end{pmatrix}.$$

Since $\langle \psi_0, \Psi p_0 \rangle \neq 0$, it follows from the last statement in Proposition 1 that $G = 0$. By Corollary 1 and the assumption that $\langle \phi_0, \Phi q_0 \rangle \neq 0$, it follows that $v = 0$ as well.

To prove that the operator is onto we consider the equation

$$\begin{bmatrix} D - Tf_x(x(t),\alpha) & \psi_0 \\ \delta_1 - \delta_0 & 0 \\ \mathrm{Int}_{\phi_0} & 0 \end{bmatrix} \begin{pmatrix} v \\ G \end{pmatrix} = \begin{pmatrix} \zeta \\ r \\ s \end{pmatrix}, \tag{2.11}$$

where $\zeta \in \mathcal{C}^0([0,1],\mathbf{R}^n), r \in \mathbf{R}^n, s \in \mathbf{R}$. In particular, the first two equations can be written

$$\begin{bmatrix} D - Tf_x(x(t),\alpha) \\ \delta_1 - \delta_0 \end{bmatrix} v = \begin{pmatrix} \zeta - G\psi_0 \\ r \end{pmatrix}. \tag{2.12}$$

By Proposition 1 this equation is solvable for v, say, $v = v_p$, if

$$\langle \Psi p_0, \zeta - G\psi_0 \rangle = p_0^* r,$$

that is, if we choose

$$G = G_p \equiv \frac{\langle \Psi p_0, \zeta \rangle - p_0^* r}{\langle \Psi p_0, \psi_0 \rangle},$$

where, by assumption, the denominator does not vanish. Now

$$v(t) = v_p(t) + c\Phi(t)q_0$$

is also a solution of (2.12) for any constant c. The third equation in (2.11) can now be written as

$$\int_0^1 \phi_0^*(\tau)[v_p(\tau) + c\Phi(\tau)q_0]d\tau = s.$$

By the assumption that $\langle \phi_0, \Phi q_0 \rangle \neq 0$ it follows that the third equation is satisfied if we take

$$c = \frac{s - \int_0^1 \phi_0^*(\tau)v_p(\tau)d\tau}{\int_0^1 \phi_0^*(\tau)\Phi(\tau)q_0 \; d\tau} \; . \qquad \square$$

PROPOSITION 4. *Let $(x(t), T, \alpha)$ be a regular periodic solution of (2.1), and let $\phi_0, \psi_0 \in \mathcal{C}^0([0,1], \mathbf{R}^n)$ be such that $\langle \phi_0, \Phi q_0 \rangle \neq 0$, $\langle \psi_0, \Psi p_0 \rangle \neq 0$. Then the operator*

$$\begin{bmatrix} D + Tf_x^*(x(t), \alpha) & \phi_0 \\ \delta_1 - \delta_0 & 0 \\ \mathrm{Int}_{\psi_0} & 0 \end{bmatrix} \; : \; \mathcal{C}^1([0,1], \mathbf{R}^n) \times \mathbf{R} \; \rightarrow \; \mathcal{C}^0([0,1], \mathbf{R}^n) \times \mathbf{R}^n \times \mathbf{R}$$

is one-to-one and onto.

Proof. The proof is similar to the proof of Proposition 3. $\square$

3. Test functionals for bifurcations of periodic solutions. For the fold and Hopf singularities of equilibria, several test functions, and corresponding minimally extended defining systems, are discussed in [12] and incorporated in CONTENT [11]. To obtain similar systems for the case of periodic orbits, we define *simple singularities* of periodic solutions, specifically the limit point, the period-doubling bifurcation, and the torus bifurcation, and we then construct functionals that vanish at these singularities.

3.1. A test functional for the fold bifurcation. Let $(x(t), T, \alpha)$ define a periodic solution of (1.1); i.e., it satisfies (2.1), (2.2), and (2.3). We say that the solution has a *simple fold singularity* if the monodromy matrix $\Phi(1)$ has an eigenvalue $+1$ with algebraic multiplicity 2 and geometric multiplicity 1, while there are no other critical multipliers.[1]

Let p_0 and q_0 denote the corresponding left and right eigenvectors, which satisfy

$$(\Phi(1) - I)q_0 = 0, \qquad (\Psi(1) - I)p_0 = 0,$$

$$(\Phi(1) - I)^* p_0 = 0, \qquad (\Psi(1) - I)^* q_0 = 0,$$

with

$$p_0^* p_0 = q_0^* q_0 = 1.$$

[1] A geometrically double eigenvalue $+1$ corresponds to a higher degeneracy. Recall that by definition a *regular* periodic solution has a geometrically simple multiplier $+1$.

At a simple fold, where the multiplier 1 has algebraic multiplicity 2, we also have generalized eigenvectors p_1 and q_1 satisfying

$$(\Phi(1) - I)q_1 = q_0, \qquad (\Psi(1) - I)p_1 = p_0,$$

where q_1 and p_1 can be chosen so that

$$q_1^* q_0 \;=\; p_1^* p_0 \;=\; 0.$$

Note that in the multiplicity-2 case we also have $p_0^* q_0 = p_1^*(\Psi(1) - I)^* q_0 = 0$.

PROPOSITION 5. *If $(x(t), T, \alpha)$ is a regular periodic solution of (2.1), then the operator*

$$\begin{bmatrix} D - Tf_x(x(t),\alpha) & -f(x(t),\alpha) \\ \delta_1 - \delta_0 & 0 \\ \mathrm{Int}_{f(x(\cdot),\alpha)} & 0 \end{bmatrix} \tag{3.1}$$

from $\mathcal{C}^1([0,1],\mathbf{R}^n) \times \mathbf{R}$ into $\mathcal{C}^0([0,1],\mathbf{R}^n) \times \mathbf{R}^n \times \mathbf{R}$ is one-to-one if the multiplier 1 has algebraic multiplicity 1. If the multiplier 1 has algebraic multiplicity 2, i.e., at a simple fold, then the operator has a one-dimensional kernel, spanned by the vector

$$\begin{pmatrix} v \\ 1 \end{pmatrix} \in \mathcal{C}^1([0,1],\mathbf{R}^n) \times \mathbf{R}, \tag{3.2}$$

where $v(t) = \frac{c_0}{T}\Phi(t)(c_2 q_0 - (q_1 - t q_0))$, where c_2 is determined by the condition that

$$q_0^* \int_0^1 \Phi^*(\tau)\Phi(\tau)[c_2 q_0 - (q_1 - \tau q_0)]\; d\tau = 0,$$

and where c_0 is determined by the condition that $x'(0) = c_0 q_0$.

Proof. Consider the homogeneous equations

$$\begin{bmatrix} D - Tf_x(x(t),\alpha) & -f(x(t),\alpha) \\ \delta_1 - \delta_0 & 0 \\ \mathrm{Int}_{f(x(\cdot),\alpha)} & 0 \end{bmatrix} \begin{pmatrix} v \\ S \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}. \tag{3.3}$$

From the first equation in (3.3) we have

$$\begin{aligned} v(t) \;&=\; \Phi(t)\left[v_0 + S\int_0^t \Psi^*(\tau) f(x(\tau),\alpha)\; d\tau\right] \;=\; \Phi(t)\left[v_0 + \tfrac{S}{T}\int_0^t \Psi^*(\tau) x'(\tau)\; d\tau\right] \\ &=\; \Phi(t)\left[v_0 + \tfrac{S}{T}\int_0^t \Psi^*(\tau)\Phi(\tau)\; d\tau\; x'(0)\right] \;=\; \Phi(t)\left[v_0 + \tfrac{St}{T} x'(0)\right], \end{aligned}$$

where we used the facts that $\Psi^*(\tau)\Phi(\tau) = I$ and $x'(t) = \Phi(t)x'(0)$. Above, $v_0 = v(0)$ is an initial vector. By the second equation in (3.3) we have

$$0 = v(1) - v(0) = (\Phi(1) - I)v_0 + \frac{S}{T}x'(0),$$

that is,

$$(\Phi(1) - I)v_0 = -\frac{S}{T}x'(0).$$

Now $(\Phi(1) - I)x'(0) = 0$, so that $x'(0) = c_0 q_0$, for some $c_0 \in \mathbf{R}$, $c_0 \neq 0$. Thus we must solve

$$(\Phi(1) - I)v_0 = -c_0 \frac{S}{T} q_0, \tag{3.4}$$

where q_0 spans the kernel of $\Phi(1) - I$.

If the multiplier 1 has algebraic multiplicity 1, then we must have $S = 0$, $v_0 = c_1 q_0$, and hence $v(t) = c_1 \Phi(t) q_0$. By the third equation in (3.3)

$$0 = \int_0^1 f^*(x(\tau), \alpha) v(\tau)\ d\tau = \frac{1}{T} \int_0^1 x'^*(\tau) v(\tau)\ d\tau = \frac{1}{T} \int_0^1 \left[\Phi(\tau) x'(0)\right]^* c_1 \Phi(\tau) q_0\ d\tau$$

or

$$c_0 c_1\ q_0^* \left(\int_0^1 \Phi^*(\tau)\Phi(\tau)\ d\tau \right)\ q_0 = 0,$$

from which it follows that $c_1 = 0$. Thus $v(t) \equiv 0$. It follows that the operator (3.1) is one-to-one.

At a simple fold the multiplier 1 has algebraic multiplicity 2. In this case (3.4) is also solvable if S is nonzero, namely

$$v_0 = -c_0 \frac{S}{T} q_1 + c_2 q_0,$$

where $c_2 \in \mathbf{R}$ is arbitrary. The third equation in (3.3) then implies

$$\begin{aligned}
0 &= \int_0^1 x'^*(\tau) v(\tau)\ d\tau \\
&= \int_0^1 x'^*(\tau) \Phi(\tau) [v_0 + \tfrac{S\tau}{T} x'(0)]\ d\tau \\
&= \int_0^1 x'^*(\tau) \Phi(\tau) [-c_0 \tfrac{S}{T} q_1 + c_2 q_0 + \tfrac{S\tau}{T} c_0 q_0]\ d\tau \\
&= \int_0^1 [\Phi(\tau) x'(0)]^* \Phi(\tau) [-c_0 \tfrac{S}{T} q_1 + c_2 q_0 + \tfrac{S\tau}{T} c_0 q_0]\ d\tau \\
&= c_0 q_0^* \int_0^1 \Phi^*(\tau)\Phi(\tau) [-c_0 \tfrac{S}{T} q_1 + c_2 q_0 + \tfrac{S\tau}{T} c_0 q_0]\ d\tau,
\end{aligned}$$

from which it follows that

$$c_2 = \frac{c_0 S q_0^* \int_0^1 \Phi^*(\tau)\Phi(\tau)[q_1 - \tau q_0]\ d\tau}{T\ q_0^* \int_0^1 \Phi^*(\tau)\Phi(\tau)\ d\tau\ q_0}. \qquad \square$$

PROPOSITION 6. *Let $(x(t), T, \alpha)$ be a regular periodic solution of (2.1) and consider the operator*

$$M_1 = \begin{bmatrix} D - T f_x(x(t), \alpha) & -f(x(t), \alpha) \\ \delta_1 - \delta_0 & 0 \\ \mathrm{Int}_{f(x(\cdot), \alpha)} & 0 \end{bmatrix} \tag{3.5}$$

from $\mathcal{C}^1([0,1], \mathbf{R}^n) \times \mathbf{R}$ into $\mathcal{C}^0([0,1], \mathbf{R}^n) \times \mathbf{R}^n \times \mathbf{R}$. If the multiplier 1 has algebraic multiplicity 1, then M_1 is onto. If it has algebraic multiplicity 2, i.e., at a simple fold,

then the range of M_1 has codimension 1 *and the vector*

$$\begin{pmatrix} \Psi p_0 \\ -p_0 \\ 0 \end{pmatrix} \in \mathcal{C}^0([0,1],\mathbf{R}^n) \times \mathbf{R}^n \times \mathbf{R} \tag{3.6}$$

is complementary to the range space.

Proof. Consider a vector $(\xi,\eta,\omega)^*$ in $\mathcal{C}^0([0,1],\mathbf{R}^n) \times \mathbf{R}^n \times \mathbf{R}$. This vector is in the range of M_1 if and only if there exist $(v,S)^*$ in $\mathcal{C}^1([0,1],\mathbf{R}^n) \times \mathbf{R}$ such that

$$M_1 \begin{pmatrix} v \\ S \end{pmatrix} = \begin{pmatrix} \xi \\ \eta \\ \omega \end{pmatrix}. \tag{3.7}$$

The first equation in (3.7) implies that

$$v(t) = \Phi(t) \left[v(0) + \int_0^t \Psi^*(\tau)(\xi(\tau) + Sf(x(\tau),\alpha))\, d\tau \right].$$

The second equation in (3.7) then implies

$$\eta = v(1) - v(0) = (\Phi(1) - I)v(0) + \Phi(1) \int_0^1 \Psi^*(\tau)(\xi(\tau) + Sf(x(\tau),\alpha))\, d\tau.$$

Now

$$\int_0^1 \Psi^*(\tau) f(x(\tau),\alpha) d\tau = \frac{1}{T} \int_0^1 \Psi^*(\tau) x'(\tau)\, d\tau = \frac{1}{T} \int_0^1 \Psi^*(\tau) c_0 \Phi(\tau) q_0\, d\tau = \frac{c_0}{T} q_0.$$

So

$$\eta = (\Phi(1) - I)v(0) + \frac{Sc_0}{T} q_0 + \Phi(1) \int_0^1 \Psi^*(\tau)\xi(\tau)\, d\tau. \tag{3.8}$$

If 1 is an algebraically simple eigenvalue of $\Phi(1)$, then q_0 is not in the range of $(\Phi(1) - I)$. For given ξ and η, (3.8) can be solved for $v(0)$ and S. Moreover, the solution is unique up to the addition of a scalar multiple of q_0 to $v(0)$. Since

$$\int_0^1 (x'(\tau))^* \Phi(\tau) q_0\, d\tau = c_0 \int_0^1 (\Phi(\tau) q_0)^* \Phi(\tau) q_0\, d\tau \neq 0,$$

the scalar is determined uniquely by the third equation in (3.7).

If 1 is an algebraically double eigenvalue of $\Phi(1)$, i.e., at a fold point, then (3.8) is solvable if and only if

$$p_0^* \eta = p_0^* \int_0^1 \Psi^*(\tau)\xi(\tau)\, d\tau.$$

If so, the third equation in (3.7) again determines the solution uniquely. ∎

PROPOSITION 7. *If $(x(t),T,\alpha)$ is a regular periodic solution of* (2.1)*, then the operator*

$$\begin{bmatrix} D + Tf_x^*(x(t),\alpha) & -f(x(t),\alpha) \\ \delta_1 - \delta_0 & 0 \\ \mathrm{Int}_{f(x(\cdot),\alpha)} & 0 \end{bmatrix} \tag{3.9}$$

from $\mathcal{C}^1([0,1],\mathbf{R}^n)\times\mathbf{R}\to\mathcal{C}^0([0,1],\mathbf{R}^n)\times\mathbf{R}^n\times\mathbf{R}$ *is one-to-one if the multiplier* 1 *has algebraic multiplicity* 1. *If the multiplier* 1 *has algebraic multiplicity* 2, *i.e., at a simple fold, then the operator has a one-dimensional kernel, spanned by* $(\Psi^* p_0, 0)^* \in \mathcal{C}^1([0,1],\mathbf{R}^n)\times\mathbf{R}$.

Proof. Consider the homogeneous equations

$$\begin{bmatrix} D+Tf_x^*(x(t),\alpha) & -f(x(t),\alpha) \\ \delta_1-\delta_0 & 0 \\ \mathrm{Int}_{f(x(\cdot),\alpha)} & 0 \end{bmatrix}\begin{pmatrix} w \\ R \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}. \tag{3.10}$$

From the first equation in (3.10) we have

$$w(t) = \Psi(t)\left[w_0 + \frac{R}{T}\int_0^t \Phi^*(\tau)x'(\tau)\,d\tau\right],$$

where $w_0 = w(0)$ is an initial vector. The second equation in (3.10) implies

$$0 = w(1) - w(0) = (\Psi(1)-I)w_0 + \frac{R}{T}\Psi(1)\int_0^1 \Phi^*(\tau)x'(\tau)\,d\tau$$

or

$$(\Psi(1)-I)w_0 = -\frac{R}{T}\Psi(1)\int_0^1 \Phi^*(\tau)\Phi(\tau)\,d\tau\;x'(0).$$

Given R, this equation is solvable for w_0 if

$$-Rq_0^*\Psi(1)\int_0^1 \Phi^*(\tau)\Phi(\tau)\,d\tau\;x'(0) = 0,$$

that is, recalling that $x'(0) = c_0 q_0$, $c_0 \neq 0$, and $q_0^*\Psi(1) = q_0^*$ if

$$c_0 R q_0^*\int_0^1 \Phi^*(\tau)\Phi(\tau)\,d\tau\;q_0 = 0.$$

It follows that $R = 0$, independently of the algebraic multiplicity of the eigenvalue 1. Thus $w(t) = \Psi(t)w_0$, where $(\Psi(1)-I)w_0 = 0$, so that $w_0 = c_3 p_0$ for some $c_3 \in \mathbf{R}$.

From the third equation in (3.10) it follows that

$$\begin{aligned} 0 &= \int_0^1 w^*(\tau)x'(\tau)\,d\tau = \int_0^1 [c_3\Psi(\tau)p_0]^*\Phi(\tau)x'(0)\,d\tau \\ &= c_0\;c_3\;p_0^*\int_0^1 \Psi^*(\tau)\Phi(\tau)\,d\tau\;q_0 = c_0\;c_3\;p_0^* q_0. \end{aligned}$$

If the multiplier 1 has algebraic multiplicity 1, then $p_0^* q_0 \neq 0$. In this case $c_3 = 0$ and hence $w(t) \equiv 0$; that is, the operator (3.9) is one-to-one.

If the multiplier 1 has algebraic multiplicity 2, then $p_0^* q_0 = 0$, and we can choose $c_3 \neq 0$. In this case $w_0 \neq 0$; hence $w(t) \not\equiv 0$. It follows that the operator (3.9) has a one-dimensional kernel. ∎

PROPOSITION 8. *If* $(x(t), T, \alpha)$ *is a regular periodic solution of* (2.1), *then the operator*

$$M_2 = \begin{bmatrix} D+Tf_x^*(x(t),\alpha) & -f(x(t),\alpha) \\ \delta_1-\delta_0 & 0 \\ \mathrm{Int}_{f(x(\cdot),\alpha)} & 0 \end{bmatrix} \tag{3.11}$$

from $\mathcal{C}^1([0,1],\mathbf{R}^n)\times\mathbf{R}\to\mathcal{C}^0([0,1],\mathbf{R}^n)\times\mathbf{R}^n\times\mathbf{R}$ *is onto if the multiplier* 1 *has algebraic multiplicity* 1. *If the multiplier* 1 *has algebraic multiplicity* 2, *i.e., at a simple fold, then the range has codimension* 1, *and the vector* $(0,0,1)^*\in\mathcal{C}^0([0,1],\mathbf{R}^n)\times\mathbf{R}^n\times\mathbf{R}$ *is complementary to the range space.*

Proof. Consider a vector $(\xi,\eta,\omega)^*$ in $\mathcal{C}^0([0,1],\mathbf{R}^n)\times\mathbf{R}^n\times\mathbf{R}$. This vector is in the range of M_2 if and only if there exist $(w,R)^*$ in $\mathcal{C}^1([0,1],\mathbf{R}^n)\times\mathbf{R}$ such that

$$M_2\begin{pmatrix} w \\ R \end{pmatrix}=\begin{pmatrix} \xi \\ \eta \\ \omega \end{pmatrix}. \tag{3.12}$$

The first equation in (3.12) implies that

$$w(t)=\Psi(t)\left[w(0)+\int_0^t\Phi^*(\tau)(\xi(\tau)+Rc_0\Phi(\tau)q_0)\;d\tau\right].$$

The second equation in (3.12) then implies

$$\eta=w(1)-w(0)=(\Psi(1)-I)w(0)+\Psi(1)\int_0^1\Phi^*(\tau)(\xi(\tau)+Rc_0\Phi(\tau)q_0)d\tau.$$

We thus obtain the equation

$$(\Psi(1)-I)w(0)=\eta-Rc_0\Psi(1)\int_0^1\Phi^*(\tau)\Phi(\tau)q_0\;d\tau-\Psi(1)\int_0^1\Phi^*(\tau)\xi(\tau)\;d\tau.$$

This equation is solvable for $w(0)$ if and only if

$$q_0^*\eta=Rc_0q_0^*\int_0^1\Phi^*(\tau)\Phi(\tau)q_0\;d\tau+q_0^*\int_0^1\Phi^*(\tau)\xi(\tau)d\tau.$$

The latter equation is solvable uniquely for R, so the previous one is solvable for $w(0)$ and defines it up to the addition of a scalar multiple of p_0.

Now suppose that $(w,R)^*$ solve the first two equations in (3.12), where $w(0)=w_0+rp_0$ and r is arbitrary. The third equation in (3.12) then requires

$$c_0q_0^*(w_0+rp_0)=\omega+\text{two integral terms which are linear in }\xi(t)\text{ and }R.$$

If the eigenvalue 1 of $\Phi(1)$ has algebraic multiplicity 1, then this equation has a unique solution in r and thus M_2 is one-to-one and onto. If the eigenvalue has algebraic multiplicity 2, then the range of M_2 has codimension at most 1. If we set $\xi(t)\equiv 0$, $\eta=0$, $\omega=1$, then necessarily $R=0$, $\omega=0$ as well, and thus the third equation in (3.12) cannot be solved. So the range of M_2 has codimension 1, and $(0,0,1)^*$ is a vector complementary to the range. ∎

PROPOSITION 9. *Let* $(x(t),T,\alpha)$ *be a regular periodic solution of* (2.1) *that has a simple fold singularity; i.e.,* $\Phi(1)$ *has eigenvalue* 1 *with algebraic multiplicity* 2. *Then there exist* $v_{01},w_{01},\;v_{11},w_{11}\in\mathcal{C}^0([0,1],\mathbf{R}^n)$, $w_{02},v_{12}\in\mathbf{R}^n$, $w_{03},v_{02},v_{13},w_{12}\in\mathbf{R}$ *such that*

$$N_1=\begin{bmatrix} D-Tf_x(x(t),\alpha) & -f(x(t),\alpha) & w_{01} \\ \delta_1-\delta_0 & 0 & w_{02} \\ \mathrm{Int}_{f(x(\cdot),\alpha)} & 0 & w_{03} \\ \mathrm{Int}_{v_{01}} & v_{02} & 0 \end{bmatrix}$$

and

$$N_2 = \begin{bmatrix} D + Tf_x^*(x(t),\alpha) & -f(x(\cdot),\alpha) & v_{11} \\ \delta_1 - \delta_0 & 0 & v_{12} \\ \mathrm{Int}_{f(x(\cdot),\alpha)} & 0 & v_{13} \\ \mathrm{Int}_{w_{11}} & w_{12} & 0 \end{bmatrix}$$

from $\mathcal{C}^1([0,1],\mathbf{R}^n)\times\mathbf{R}^n\times\mathbf{R}$ *to* $\mathcal{C}^0([0,1],\mathbf{R}^n)\times\mathbf{R}^n\times\mathbf{R}\times\mathbf{R}$ *are one-to-one and onto.*

For any such choice of the bordering elements we define $v, w \in \mathcal{C}^1([0,1],\mathbf{R}^n)$ *and* $S, G, H, R \in \mathbf{R}$ *by the equations*

$$N_1 \begin{pmatrix} v \\ S \\ G \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \tag{3.13}$$

and

$$N_2 \begin{pmatrix} w \\ R \\ H \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ -1 \end{pmatrix}. \tag{3.14}$$

Then in a neighborhood of $(x(t),T,\alpha)$, $G = 0$ *if and only if* $H = 0$. *Moreover, this happens if and only if the regular periodic solution has a simple fold singularity.*

Proof. We choose

$$\begin{pmatrix} v_{01}(t) \\ v_{02} \end{pmatrix} = \begin{pmatrix} v(t) \\ 1 \end{pmatrix},$$

where v is given in the statement of Proposition 5. Further we set

$$\begin{pmatrix} w_{01}(t) \\ w_{02} \\ w_{03} \end{pmatrix} = \begin{pmatrix} \Psi^*(t)p_0 \\ 0 \\ 0 \end{pmatrix}.$$

By Propositions 5 and 6, N_1 is one-to-one and onto. We further set

$$\begin{pmatrix} w_{11}(t) \\ w_{12} \end{pmatrix} = \begin{pmatrix} \Psi^*(t)p_0 \\ 0 \end{pmatrix},$$

$$\begin{pmatrix} v_{11}(t) \\ v_{12} \\ v_{13} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}.$$

By Propositions 7 and 8, N_2 is one-to-one and onto. The last statement in the proposition is proved by standard arguments. ∎

3.2. A test functional for the period-doubling bifurcation. By definition, at a *simple flip singularity* there is an algebraically simple Floquet multiplier equal to -1 and no other multipliers with unit modulus, except for an algebraically simple multiplier $+1$. The left and right eigenvectors of the monodromy matrix $\Phi(1)$ for the eigenvalue -1 will be denoted by p_2 and q_2, respectively. They are also the right and left eigenvector, respectively, of $\Psi(1)$ for the eigenvalue -1.

PROPOSITION 10. *If $(x(t), T, \alpha)$ corresponds to a simple flip singularity, then the operator*

$$\begin{bmatrix} D - Tf_x(x(t),\alpha) \\ \delta_0 + \delta_1 \end{bmatrix} \; : \; \mathcal{C}^1([0,1],\mathbf{R}^n) \to \mathcal{C}^0([0,1],\mathbf{R}^n) \times \mathbf{R}^n$$

has a one-dimensional kernel spanned by Φq_2. Its range has codimension 1; if $\zeta \in \mathcal{C}^0([0,1],\mathbf{R}^n)$, $r \in \mathbf{R}^n$, then $(\zeta, r)^*$ is in the range if and only if $\langle \Psi p_2, \zeta\rangle = -p_2^* r$. In particular, if $r = 0$, then $(\zeta, 0)^*$ is in the range if and only if $\langle \Psi p_2, \zeta\rangle = 0$.

Proof. The proof is similar to the proof of Proposition 1. □

COROLLARY 3. *If $(x(t), T, \alpha)$ corresponds to a simple flip singularity, then the operator*

$$\begin{bmatrix} D - Tf_x(x(t),\alpha) \\ \delta_0 + \delta_1 \\ \mathrm{Int}_\phi \end{bmatrix} \; : \; \mathcal{C}^1([0,1],\mathbf{R}^n) \; \to \; \mathcal{C}^0([0,1],\mathbf{R}^n) \times \mathbf{R}^n \times \mathbf{R} \tag{3.15}$$

is one-to-one if and only if $\langle \phi, \Phi q_2\rangle \neq 0$.

PROPOSITION 11. *If $(x(t), T, \alpha)$ corresponds to a simple flip singularity, then the operator*

$$\begin{bmatrix} D + Tf_x^*(x(t),\alpha) \\ \delta_0 + \delta_1 \end{bmatrix} \; : \; \mathcal{C}^1([0,1],\mathbf{R}^n) \; \to \; \mathcal{C}^0([0,1],\mathbf{R}^n) \times \mathbf{R}^n$$

has a one-dimensional kernel spanned by Ψp_2. Its range has codimension 1; if $\zeta \in \mathcal{C}^0([0,1],\mathbf{R}^n)$, $r \in \mathbf{R}^n$, then $(\zeta, r)^*$ is in the range if and only if $\langle \Phi q_2, \zeta\rangle = -q_2^* r$. In particular, if $r = 0$, then $(\zeta, 0)^*$ is in the range if and only if $\langle \Phi q_2, \zeta\rangle = 0$.

Proof. The proof is similar to the proof of Proposition 2. □

COROLLARY 4. *If $(x(t), T, \alpha)$ corresponds to a simple flip singularity, then the operator*

$$\begin{bmatrix} D + Tf_x^*(x(t),\alpha) \\ \delta_0 + \delta_1 \\ \mathrm{Int}_\psi \end{bmatrix} \; : \; \mathcal{C}^1([0,1],\mathbf{R}^n) \; \to \; \mathcal{C}^0([0,1],\mathbf{R}^n) \times \mathbf{R}^n \times \mathbf{R} \tag{3.16}$$

is one-to-one if and only if $\langle \psi, \Psi p_2\rangle \neq 0$.

PROPOSITION 12. *Let $(x(t), T, \alpha)$ correspond to a simple flip singularity, and let $\phi_0, \psi_0 \in \mathcal{C}^0([0,1],\mathbf{R}^n)$ be such that $\langle \phi_0, \Phi q_2\rangle \neq 0$, $\langle \psi_0, \Psi p_2\rangle \neq 0$. Then the operator*

$$\begin{bmatrix} D - Tf_x(x(t),\alpha) & \psi_0 \\ \delta_0 + \delta_1 & 0 \\ \mathrm{Int}_{\phi_0} & 0 \end{bmatrix} \; : \; \mathcal{C}^1([0,1],\mathbf{R}^n) \times \mathbf{R} \; \to \; \mathcal{C}^0([0,1],\mathbf{R}^n) \times \mathbf{R}^n \times \mathbf{R}$$

is one-to-one and onto.

Proof. The proof is similar to the proof of Proposition 3. □

PROPOSITION 13. *Let $(x(t), T, \alpha)$ correspond to a simple flip singularity, and let $\phi_0, \psi_0 \in \mathcal{C}^0([0,1],\mathbf{R}^n)$ be such that $\langle \phi_0, \Phi q_2\rangle \neq 0$, $\langle \psi_0, \Psi p_2\rangle \neq 0$. Then the operator*

$$\begin{bmatrix} D + Tf_x^*(x(t),\alpha) & \phi_0 \\ \delta_0 + \delta_1 & 0 \\ \mathrm{Int}_{\psi_0} & 0 \end{bmatrix} \; : \; \mathcal{C}^1([0,1],\mathbf{R}^n) \times \mathbf{R} \; \to \; \mathcal{C}^0([0,1],\mathbf{R}^n) \times \mathbf{R}^n \times \mathbf{R}$$

is one-to-one and onto.

Proof. The proof is similar to the proof of Proposition 4. ∎

PROPOSITION 14. *Let $(x(t), T, \alpha)$ be a periodic solution close to a simple flip singularity, and let $\phi_0, \psi_0 \in \mathcal{C}^0([0,1], \mathbf{R}^n)$ be such that $\langle \phi_0, \Phi q_2 \rangle \neq 0$, $\langle \psi_0, \Psi p_2 \rangle \neq 0$, so that the operators M_3 and M_4 (defined below) from $\mathcal{C}^1([0,1], \mathbf{R}^n) \times \mathbf{R}$ into $\mathcal{C}^0([0,1], \mathbf{R}^n) \times \mathbf{R}^n \times \mathbf{R}$ are both one-to-one and onto. Let $v, w \in \mathcal{C}^1([0,1], \mathbf{R}^n)$, G, $H \in \mathbf{R}$ be defined by the equations*

$$M_3 \begin{pmatrix} v \\ G \end{pmatrix} \equiv \begin{bmatrix} D - Tf_x(x(t), \alpha) & \psi_0 \\ \delta_0 + \delta_1 & 0 \\ \mathrm{Int}_{\phi_0} & 0 \end{bmatrix} \begin{pmatrix} v \\ G \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \tag{3.17}$$

$$M_4 \begin{pmatrix} w \\ H \end{pmatrix} \equiv \begin{bmatrix} D + Tf_x^*(x(t), \alpha) & \phi_0 \\ \delta_0 + \delta_1 & 0 \\ \mathrm{Int}_{\psi_0} & 0 \end{bmatrix} \begin{pmatrix} w \\ H \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ -1 \end{pmatrix}. \tag{3.18}$$

Then $G = H$. Furthermore, $G = 0$ if and only if the periodic solution corresponds to a simple flip singularity. If so, then $v(0)$ is the right eigenvector of the monodromy matrix for the eigenvalue -1.

Proof. Multiplying the first equation in (3.17) on the left with $w^*(t)$, integrating over the interval $[0,1]$, and using the last equation in (3.18) we obtain

$$\int_0^1 w^* v'(\tau)\, d\tau - T \int_0^1 w^*(\tau) f_x(x(\tau), \alpha) v(\tau)\, d\tau - G = 0.$$

Integrating the first term by parts, using the second equations in (3.17) and (3.18), we obtain

$$-\int_0^1 v^*(\tau) w'(\tau)\, d\tau - T \int_0^1 v^*(\tau) f_x^*(x(\tau), \alpha) w(\tau)\, d\tau - G = 0.$$

Using the first equation in (3.18) we get

$$-\langle v, (-H\phi_0) \rangle - G = 0.$$

Using the third equation in (3.17) we obtain $G = H$. The other statements in the proposition are now obvious. ∎

3.3. A test functional for the torus bifurcation. We say that a periodic solution has a *simple Neimark–Sacker singularity* if the monodromy matrix $\Phi(1)$ has a conjugate pair of simple complex multipliers with modulus 1 (i.e., $e^{\pm i\theta}$, $0 < \theta < \pi$) and no other multipliers with unit modulus, except an algebraically simple eigenvalue $+1$. Furthermore, let $p_1, p_2 \in \mathbf{R}^n$ (respectively, $q_1, q_2 \in \mathbf{R}^n$) be such that $p_1 + ip_2$ (respectively, $q_1 + iq_2$) is a left (respectively, right) complex eigenvector of the monodromy matrix $\Phi(1)$. Thus

$$\begin{aligned} (p_1 + ip_2)^H \Phi(1) &= e^{i\theta}(p_1 + ip_2)^H, \\ \Phi(1)(q_1 + iq_2) &= e^{i\theta}(q_1 + iq_2), \\ \Psi(1)(p_1 + ip_2) &= e^{i\theta}(p_1 + ip_2), \\ (q_1 + iq_2)^H \Psi(1) &= e^{i\theta}(q_1 + iq_2)^H, \end{aligned}$$

where $(p_1 + ip_2)^H = p_1^* - ip_2^*$, $(q_1 + iq_2)^H = q_1^* - iq_2^*$.

In this section it is convenient to extend the definition of $x(t), \Phi(t)$, and $\Psi(t)$ to the interval $[0,2]$ by periodicity with period 1 and to redefine

$$\mathrm{Int}_\phi(v) = \langle \phi, v \rangle = \int_0^2 \phi^*(\tau) v(\tau)\ d\tau.$$

We start with the following result.

PROPOSITION 15. *Let $(x(t), T, \alpha)$ define a periodic solution; i.e., it satisfies* (2.1), (2.2), *and* (2.3). *Let $(x(t), T, \alpha)$ correspond to a simple Neimark–Sacker singularity with multipliers $e^{\pm i\theta}$, $0 < \theta < \pi$. Let $\kappa = \cos\theta$ and consider the operator*

$$\left[\begin{array}{c} D - Tf_x(x(t),\alpha) \\ \delta_0 - 2\kappa\delta_1 + \delta_2 \end{array} \right] \ :\ \mathcal{C}^1([0,2],\mathbf{R}^n) \ \rightarrow\ \mathcal{C}^0([0,2],\mathbf{R}^n) \times \mathbf{R}^n. \tag{3.19}$$

Then we have the following:

(i) *The operator* (3.19) *has a two-dimensional kernel spanned by $\Phi(t)q_1$ and $\Phi(t)q_2$.*

(ii) *The operator* (3.19) *has a range with* codim 2. *The vectors*

$$\left(\begin{array}{c} \Psi p_1 \\ 0 \end{array} \right), \left(\begin{array}{c} \Psi p_2 \\ 0 \end{array} \right) \in \mathcal{C}^0([0,2],\mathbf{R}^n) \times \mathbf{R}^n$$

span a two-dimensional subspace that is complementary to the range of (3.19).

Proof. Let v be in the kernel of (3.19). Then v must have the form $v(t) = \Phi(t)v_0$ with $v_0 \in \mathbf{R}^n$. We further have

$$0 = (\delta_0 - 2\kappa\delta_1 + \delta_2)v = v(0) - 2\kappa v(1) + v(2) = (\Phi(1) - e^{i\theta}I)(\Phi(1) - e^{-i\theta}I)v_0.$$

We infer that it is necessary and sufficient that v_0 is in the span of q_1, q_2.

As a first step in the proof of (ii) we consider $\zeta \in \mathcal{C}^0([0,2],\mathbf{R}^n)$, $r \in \mathbf{R}^n$, and we give a necessary and sufficient condition in order that $(\zeta, r)^*$ be in the range of (3.19). First, there must exist a $v \in \mathcal{C}^1([0,2],\mathbf{R}^n)$ for which

$$v'(t) - Tf_x(x(t),\alpha)v(t) = \zeta(t).$$

The general solution of this linear differential equation is

$$v(t) = \Phi(t)\left[v_0 + \int_0^t \Psi^*(\tau)\zeta(\tau)\ d\tau \right],$$

where $v_0 = v(0)$ is an initial vector. Also, we must have $v(0) - 2\kappa v(1) + v(2) = r$, that is,

$$(\Phi(1) - e^{i\theta}I)(\Phi(1) - e^{-i\theta}I)v_0 - 2\kappa\Phi(1)\int_0^1 \Psi^*(\tau)\zeta(\tau)\ d\tau + \Phi(1)^2\int_0^2 \Psi^*(\tau)\zeta(\tau)d\tau = r.$$

This is an equation for v_0 which is solvable if and only if

$$-2\kappa p^H\Phi(1)\int_0^1 \Psi^*(\tau)\zeta(\tau)\ d\tau + p^H\Phi(1)^2\int_0^2 \Psi^*(\tau)\zeta(\tau)\ d\tau = p^H r$$

or, equivalently,

$$-2\kappa e^{i\theta}\int_0^1 p^H\Psi^*(\tau)\zeta(\tau)\ d\tau + e^{2i\theta}\int_0^2 p^H\Psi^*(\tau)\zeta(\tau)\ d\tau = p^H r.$$

If we define the linear functional L by setting

$$L(\zeta) = -2\kappa e^{i\theta} \int_0^1 p^H \Psi^*(\tau)\zeta(\tau)\ d\tau + e^{2i\theta} \int_0^2 p^H \Psi^*(\tau)\zeta(\tau)\ d\tau, \tag{3.20}$$

then we infer that $(\zeta, r)^*$ is in the range of (3.19) if and only if $L(\zeta) = p^H r$.

As a second step in the proof of (ii) we compute $L(\Psi p_1)$ and $L(\Psi p_2)$. We have

$$L(\Psi p_1) = -2\cos\theta e^{i\theta} \int_0^1 p^H \Psi^*(\tau)\Psi(\tau)p_1\ d\tau + e^{2i\theta} \int_0^2 p^H \Psi^*(\tau)\Psi(\tau)p_1\ d\tau$$

$$= e^{i\theta}(-2\cos\theta + \cos\theta + i\sin\theta) \int_0^1 p^H \Psi^*(\tau)\Psi(\tau)p_1\ d\tau + e^{2i\theta} \int_0^1 p^H \Psi^*(1+\tau)\Psi(1+\tau)p_1\ d\tau.$$

Now we note that

$$\Psi(1+\tau)p_1 = \Psi(\tau)\Psi(1)p_1 = \Psi(\tau)(\cos\theta p_1 - \sin\theta p_2)$$

and

$$p^H \Psi^*(1+\tau) = [\Psi(\tau)\Psi(1)p]^H = [e^{i\theta}\Psi(\tau)p]^H = e^{-i\theta} p^H \Psi^*(\tau).$$

Hence

$$L(\Psi p_1) = i\sin\theta e^{i\theta} \int_0^1 p^H \Psi^*(\tau)\Psi(\tau)p\ d\tau = (-\sin\theta + i\cos\theta)\sin\theta \int_0^1 \|\Psi(\tau)p\|^2\ d\tau.$$

By a similar argument we find that

$$L(\Psi p_2) = (\cos\theta + i\sin\theta)\sin\theta \int_0^1 \|\Psi(\tau)p\|^2 d\tau.$$

As a third step in the proof of (ii) we show that the range of (3.19) has codimension 2 by proving that every $(\xi, r)^*$ can be written in a unique way as

$$\begin{pmatrix} \xi \\ r \end{pmatrix} = \begin{pmatrix} \xi_0 \\ r_0 \end{pmatrix} + \alpha \begin{pmatrix} 0 \\ p_1 \end{pmatrix} + \beta \begin{pmatrix} 0 \\ p_2 \end{pmatrix}, \tag{3.21}$$

with $(\xi_0, r_0)^*$ in the range of (3.19) and $\alpha, \beta \in \mathbf{R}$.

Obviously $\xi_0 = \xi$, and r_0 has to satisfy the conditions

$$p^H r_0 = L(\xi), \quad r_0 = r - \alpha p_1 - \beta p_2.$$

These conditions imply

$$\begin{pmatrix} p_1^* p_1 & p_1^* p_2 \\ p_2^* p_1 & p_2^* p_2 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} p_1^* r - \mathrm{Re}\ [L(\xi)] \\ p_2^* r + \mathrm{Im}\ [L(\xi)] \end{pmatrix}.$$

This nonsingular linear system defines α, β in a unique way. Next, r_0 is defined by the requirement $r_0 = r - \alpha p_1 - \beta p_2$, and with this choice we have $p^H r_0 = L(\xi)$.

As the fourth and last step to prove (ii) we will show that

$$\begin{pmatrix} \Psi p_1 \\ 0 \end{pmatrix}, \begin{pmatrix} \Psi p_2 \\ 0 \end{pmatrix},$$

and we will also span a two-dimensional space complementary to the range of (3.19). To this end we decompose

$$\begin{pmatrix} \Psi p_1 \\ 0 \end{pmatrix} = \begin{pmatrix} \Psi p_1 \\ r_1 \end{pmatrix} + \alpha_1 \begin{pmatrix} 0 \\ p_1 \end{pmatrix} + \beta_1 \begin{pmatrix} 0 \\ p_2 \end{pmatrix},$$

$$\begin{pmatrix} \Psi p_2 \\ 0 \end{pmatrix} = \begin{pmatrix} \Psi p_2 \\ r_2 \end{pmatrix} + \alpha_2 \begin{pmatrix} 0 \\ p_1 \end{pmatrix} + \beta_2 \begin{pmatrix} 0 \\ p_2 \end{pmatrix}$$

in the decomposition of (3.21). Then $\alpha_1, \beta_1, \alpha_2, \beta_2$ are defined by the matrix equation

$$\begin{pmatrix} p_1^* p_1 & p_1^* p_2 \\ p_2^* p_1 & p_2^* p_2 \end{pmatrix} \begin{pmatrix} \alpha_1 & \alpha_2 \\ \beta_1 & \beta_2 \end{pmatrix} = \begin{pmatrix} -\text{Re } [L(\Psi p_1)] & -\text{Re } [L(\Psi p_2)] \\ \text{Im } [L(\Psi p_1)] & \text{Im } [L(\Psi p_2)] \end{pmatrix}.$$

The proof of (ii) is complete if we show that

$$\begin{pmatrix} \alpha_1 & \alpha_2 \\ \beta_1 & \beta_2 \end{pmatrix}$$

is a nonsingular matrix or, equivalently, that

$$\begin{pmatrix} -\text{Re } [L(\Psi p_1)] & -\text{Re } [L(\Psi p_2)] \\ \text{Im } [L(\Psi p_1)] & \text{Im } [L(\Psi p_2)] \end{pmatrix}$$

is nonsingular. By the second step this matrix is equal to

$$\begin{pmatrix} \sin\theta & -\cos\theta \\ \cos\theta & \sin\theta \end{pmatrix} \sin\theta \int_0^1 \|\Psi(\tau)p\|^2 d\tau. \tag{3.22}$$

Since $\sin\theta \neq 0$ in (3.22) the proof is complete. ∎

PROPOSITION 16. *Let $(x(t), T, \alpha)$ define a periodic solution; that is, it satisfies* (2.1), (2.2), *and* (2.3). *Let $(x(t), T, \alpha)$ correspond to a simple Neimark–Sacker singularity with multipliers $e^{\pm i\theta}$, $0 < \theta < \pi$. Set $\kappa = \cos\theta$ and consider the operator*

$$\begin{bmatrix} D + Tf_x^*(x(t), \alpha) \\ \delta_0 - 2\kappa\delta_1 + \delta_2 \end{bmatrix} : \mathcal{C}^1([0,2], \mathbf{R}^n) \to \mathcal{C}^0([0,2], \mathbf{R}^n) \times \mathbf{R}^n. \tag{3.23}$$

Then we have the following:

(i) *The operator* (3.23) *has a two-dimensional kernel spanned by $\Psi(t)p_1$ and $\Psi(t)p_2$.*

(ii) *The operator* (3.23) *has a range of codimension* 2. *The vectors*

$$\begin{pmatrix} \Phi q_1 \\ 0 \end{pmatrix}, \begin{pmatrix} \Phi q_2 \\ 0 \end{pmatrix} \in \mathcal{C}^0([0,2], \mathbf{R}^n) \times \mathbf{R}^n$$

span a two-dimensional subspace that is complementary to the range of (3.23).

Proof. The proof is similar to the proof of the preceding proposition. ∎

COROLLARY 5. *Let $(x(t), T, \alpha)$ correspond to a simple Neimark–Sacker singularity of a periodic solution. If $\kappa = \cos\theta$, then the operators*

$$\begin{bmatrix} D - Tf_x(x(t), \alpha) & \Psi p_1 & \Psi p_2 \\ \delta_0 - 2\kappa\delta_1 + \delta_2 & 0 & 0 \\ \text{Int}_{\Phi(\cdot)q_1} & 0 & 0 \\ \text{Int}_{\Phi(\cdot)q_2} & 0 & 0 \end{bmatrix} : \mathcal{C}^1([0,2], \mathbf{R}^n) \times \mathbf{R}^2 \to \mathcal{C}^0([0,2], \mathbf{R}^n) \times \mathbf{R}^n \times \mathbf{R}^2$$

and

$$\begin{bmatrix} D+Tf_x^*(x(t),\alpha) & \Phi q_1 & \Phi q_2 \\ \delta_0 - 2\kappa\delta_1 + \delta_2 & 0 & 0 \\ \mathrm{Int}_{\Psi(\cdot)p_1} & 0 & 0 \\ \mathrm{Int}_{\Psi(\cdot)p_2} & 0 & 0 \end{bmatrix} : \mathcal{C}^1([0,2],\mathbf{R}^n)\times\mathbf{R}^2 \to \mathcal{C}^0([0,2],\mathbf{R}^n)\times\mathbf{R}^n\times\mathbf{R}^2$$

are both one-to-one and onto.

Proof. The proof is standard. □

PROPOSITION 17. *Let $(x(t),T,\alpha)$ be close to a simple Neimark–Sacker singularity of periodic solutions and κ close to the value $\cos\theta$ at the singular point. Furthermore, let (ψ_0,ψ_1) span a space sufficiently close to the span of $(\Psi p_1,\Psi p_2)$, and let (ϕ_0,ϕ_1) span a space sufficiently close to $(\Phi q_1,\Phi q_2)$, so that the operators*

$$M_5 = \begin{bmatrix} D-Tf_x(x(t),\alpha) & \psi_0 & \psi_1 \\ \delta_0 - 2\kappa\delta_1 + \delta_2 & 0 & 0 \\ \mathrm{Int}_{\phi_0} & 0 & 0 \\ \mathrm{Int}_{\phi_1} & 0 & 0 \end{bmatrix} : \mathcal{C}^1([0,2],\mathbf{R}^n)\times\mathbf{R}^2 \to \mathcal{C}^0([0,2],\mathbf{R}^n)\times\mathbf{R}^n\times\mathbf{R}^2$$

and

$$M_6 = \begin{bmatrix} D+Tf_x^*(x(t),\alpha) & \phi_0 & \phi_1 \\ \delta_0 - 2\kappa\delta_1 + \delta_2 & 0 & 0 \\ \mathrm{Int}_{\psi_0} & 0 & 0 \\ \mathrm{Int}_{\psi_1} & 0 & 0 \end{bmatrix} : \mathcal{C}^1([0,2],\mathbf{R}^n)\times\mathbf{R}^2 \to \mathcal{C}^0([0,2],\mathbf{R}^n)\times\mathbf{R}^n\times\mathbf{R}^2$$

are both one-to-one and onto. Let $v_1,v_2,w_1,w_2 \in \mathcal{C}^1([0,2],\mathbf{R}^n), G,H \in \mathbf{R}^{2\times 2}$ be defined by the equations

$$M_5 \begin{pmatrix} v_1 & v_2 \\ G_{11} & G_{12} \\ G_{21} & G_{22} \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \\ 1 & 0 \\ 0 & 1 \end{pmatrix}, \tag{3.24}$$

$$M_6 \begin{pmatrix} w_1 & w_2 \\ H_{11} & H_{21} \\ H_{12} & H_{22} \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \\ -1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{3.25}$$

If $(x(t),T,\alpha)$ is a periodic solution, then $G=0$ if and only if $H=0$. Moreover, this happens if and only if $(x(t),T,\alpha)$ corresponds to a simple Neimark–Sacker singularity of periodic solutions with the multipliers $e^{\pm i\theta}$, where $\kappa=\cos(\theta)$.

Proof. The proof is standard. □

4. Regularity of the defining systems. In this section we prove that, under natural nondegeneracy and transversality conditions, the test functionals constructed in the previous section are regular (with respect to the arclength parameter along the periodic solution family). This implies regularity of defining systems consisting of the periodic BVP (2.1), (2.2), (2.3), and the condition for the corresponding functional to vanish, for the two-parameter continuation of the bifurcation.

4.1. Regularity at a fold bifurcation. To prove the regularity of the test functional G for the simple fold singularity in Proposition 9, we proceed as in the case of the fold singularity of equilibria [12], [3].

The computation of periodic orbits is based on the equation

$$F(X,\alpha)=0, \tag{4.1}$$

where $X\equiv(x(\cdot),T)\in\mathcal{C}^1([0,1],\mathbf{R})\times\mathbf{R}$, and $F(X)\in\mathcal{C}^0([0,1],\mathbf{R})\times\mathbf{R}^n\times\mathbf{R}$ is given by

$$F(X)\equiv\begin{pmatrix} x'(t)-Tf(x(t),\alpha) \\ x(1)-x(0) \\ \displaystyle\int_0^1 x^*(\tau)x'_{k-1}(\tau)\ d\tau \end{pmatrix}$$

(see (2.1), (2.2), and (2.3)). The Fréchet derivative $F_X(X,\alpha)$ of this operator (with x_{k-1} substituted by x upon differentiation) is M_1 as defined in (3.1). By Propositions 5 and 6, if the periodic orbit has a simple fold singularity, then F_X is singular. Moreover, the left and right singular vectors are then

$$\begin{pmatrix} \Psi p_0 \\ -p_0 \\ 0 \end{pmatrix}$$

and

$$\begin{pmatrix} v \\ 1 \end{pmatrix},$$

given in (3.2) and (3.6), respectively. By definition, a simple fold point is *nondegenerate* if

$$\begin{pmatrix} \Psi p_0 \\ -p_0 \\ 0 \end{pmatrix}^* F_{XX}\begin{pmatrix} v \\ 1 \end{pmatrix}\begin{pmatrix} v \\ 1 \end{pmatrix}\neq 0. \tag{4.2}$$

Let α be a scalar parameter in (1.1). A nondegenerate fold point is called *regular* if $[F_X\ \ F_\alpha]$ is onto at the singularity. This is the usual *transversality condition* for the limit point bifurcation, which can be equivalently expressed as

$$\begin{pmatrix} \Psi p_0 \\ -p_0 \\ 0 \end{pmatrix}^* F_\alpha\neq 0. \tag{4.3}$$

Let s denote arclength along the family of periodic orbits. We think of X and α as functions of s so that (4.1) is an identity in s. By (3.13) this also defines G as a function of s. Suppose that a fold singularity occurs at $s=s_0$. We will prove that $G_s(s_0)\neq 0$ near a regular fold point, i.e., a simple fold singularity where both (4.2) and (4.3) hold.

Taking derivatives of (3.13) with respect to s we find

$$N_1\begin{pmatrix} v_s \\ S_s \\ G_s \end{pmatrix}=\begin{pmatrix} (F_{XX}X_s+F_{X\alpha}\alpha_s)\begin{pmatrix} v \\ S \end{pmatrix} \\ 0 \end{pmatrix}. \tag{4.4}$$

In this expression

$$\begin{pmatrix} v \\ S \end{pmatrix}$$

is a right singular vector of F_X. Furthermore, at the fold singularity $\alpha_s = 0$. Since $F_X X_s + F_\alpha \alpha_s \equiv 0$ it follows that X_s is also a right singular vector of F_X. Now by (4.4) we have $G_s(s_0) \neq 0$ if and only if

$$F_{XX} \begin{pmatrix} v \\ 1 \end{pmatrix} \begin{pmatrix} v \\ 1 \end{pmatrix}$$

is not in the range of M_1; under our assumptions this is equivalent to (4.2).

4.2. Regularity at a period-doubling bifurcation. We have seen that locally, near a simple flip singularity, the system consisting of (2.1), (2.2), (2.3), and $G = 0$ (where G is given by (3.17)) defines the set of simple flips in $(x(\cdot), T, \alpha)$-space if the conditions $\langle \phi_0, \Phi q_2 \rangle \neq 0$, $\langle \psi_0, \Psi p_2 \rangle \neq 0$ hold. We will now prove that this is a regular system if an appropriate transversality condition for the period-doubling bifurcation holds.

Let s denote arclength along the family of periodic orbits so that $(x(s)(t), T(s), \alpha(s))$ is a solution of (2.1), (2.2), and (2.3) for all s near the bifurcation value s_0. The simplicity of the flip singularity implies that -1 is the algebraically simple eigenvalue of $\Phi(s_0)(1)$ so that it can be continued smoothly, together with its left and right eigenvectors, for nearby values of s. Specifically, we denote by $\lambda(s)$ an eigenvalue of $\Phi(s)(1)$, with left and right eigenvectors $p(s), q(s)$, that is,

$$\begin{array}{ll} \Phi(s)(1)q(s) = \lambda(s)q(s), & p^*(s)\Phi(s)(1) = \lambda(s)p^*(s), \\ \Psi(s)(1)p(s) = \lambda^{-1}(s)p(s), & q^*(s)\Psi(s)(1) = \lambda^{-1}(s)q^*(s), \\ p(s_0) = p_2, & q(s_0) = q_2, \\ \lambda(s_0) = -1. & \end{array} \tag{4.5}$$

The simplicity condition implies that

$$p^*(s)q(s) \neq 0$$

for all s sufficiently close to s_0. By standard arguments, (4.5) implies

$$p^*(s)q(s)\lambda_s(s) = p^*(s)\Phi_s(s)(1)q(s). \tag{4.6}$$

To get an explicit formula for $\Phi_s(s_0)(1)$ we start from the observation that

$$(D - T(s)f_x(x(s), \alpha(s)))\Phi = 0.$$

Taking derivatives, and using somewhat simplied notation, we obtain

$$(D - Tf_x)\Phi_s = (Tf_x)_s\Phi.$$

Multiplying on the right by an arbitrary vector $\xi \in \mathbf{R}^n$, we have

$$(D - Tf_x)\Phi_s\xi = (Tf_x)_s\Phi\xi.$$

This is a linear differential equation for $\Phi_s\xi$ with solution

$$\Phi_s(s)(t)\xi = \Phi(s)(t)\left[\zeta + \int_0^t \Psi^*(s)(\tau)(Tf_x)_s(s)(\tau)\Phi(s)(\tau)\xi \, d\tau\right]$$

for some $\zeta \in \mathbf{R}^n$. For $t = 0$ this reduces to

$$\Phi_s(s)(0)\xi = \Phi(s)(0)\zeta.$$

Since $\Phi(s)(0) = I$, $\Phi_s(s)(0) = 0$, this implies that $\zeta = 0$, so that

$$\Phi_s(s)(t)\xi = \Phi(s)(t) \int_0^t \Psi^*(s)(\tau)(Tf_x)_s(s)(\tau)\Phi(s)(\tau)\xi \; d\tau \tag{4.7}$$

for all $\xi \in \mathbf{R}^n$. From (4.6) we get

$$p^*(s)q(s)\lambda_s(s) = \lambda(s)p^*(s) \int_0^1 \Psi^*(\tau)(Tf_x)_s(s)(\tau)\Phi(s)(\tau)q(s) \; d\tau. \tag{4.8}$$

The natural transversality condition for the period-doubling bifurcation is $\lambda_s(s_0) \neq 0$. We now show that this is equivalent to $G_s(s_0) \neq 0$, thus establishing regularity.

PROPOSITION 18. *The conditions $\lambda_s(s_0) \neq 0$ and $G_s(s_0) \neq 0$ are equivalent near a simple flip singularity.*

Proof. The equations (3.17) are to be considered as identities in s; by taking derivatives we obtain

$$(D - Tf_x)v_s = (Tf_x)_s v - \psi_0 G_s, \tag{4.9}$$

$$(\delta_0 + \delta_1)v_s = 0, \tag{4.10}$$

$$\mathrm{Int}_{\phi_0} v_s = 0.$$

The solution of (3.17) at $s = s_0$ is given by $G(s_0) = 0$, $v(s_0)(t) = \Phi(s_0)(t)q_2$. Now, at $s = s_0$ (4.9) is a linear differential equation for $v_s(s_0)(t)$ with solution

$$v_s(s_0)(t) = \Phi(s_0)(t) \left[\zeta + \int_0^t \Psi^*(s_0)(\tau)((Tf_x)_s(s_0)(\tau)v(s_0)(\tau) - \psi_0 G_s(s_0)) \; d\tau \right]$$

for some vector $\zeta \in \mathbf{R}^n$. Using (4.10) we find

$$0 = (I + \Phi(s_0)(1))\zeta + \Phi(s_0)(1) \int_0^1 \Psi^*(s_0)(\tau)((Tf_x)_s(s_0)(\tau)\Phi(s_0)(\tau)q_2 - \psi_0 G_s(s_0)) \; d\tau.$$

This equation in ζ has a solution if and only if

$$p^*(s_0)\Phi(s_0)(1) \int_0^1 \Psi^*(s_0)(\tau)((Tf_x)_s(s_0)(\tau)\Phi(s_0)(\tau)q_2 - \psi_0 G_s(s_0)) \; d\tau = 0,$$

that is,

$$p_2^* \int_0^1 \Psi^*(s_0)(\tau)(Tf_x)_s(s_0)(\tau)\Phi(s_0)(\tau)q_2 \; d\tau = \langle \psi_0, \Psi p_2 \rangle G_s(s_0).$$

By (4.8) this implies

$$-(p_2^* q_2)\lambda_s(s_0) = \langle \psi_0, \Psi p_2 \rangle G_s(s_0).$$

Since $p_2^* q_2$ and $\langle \psi_0, \Psi p_2 \rangle$ are nonzero, this completes the proof. ∎

4.3. Regularity at a torus bifurcation. Again, let s denote arclength along the family of periodic orbits so that $(x(s)(t), T(s), \alpha(s))$ is a solution of (2.1), (2.2), and (2.3) for all s near the critical value s_0 corresponding to a simple Neimark–Sacker singularity. Thus $\Phi(s_0)(1)$ has algebraically simple eigenvalues $e^{\pm i\theta}$. Let $\lambda(s) = \lambda_1(s)+i\lambda_2(s)$, $p(s) = p_1(s)+ip_2(s)$, $q(s) = q_1(s)+iq_2(s)$ be the smooth continuations of the critical multiplier $e^{i\theta}$ and the corresponding left and right eigenvectors. The natural transversality condition for the torus bifurcation is the requirement that $\lambda(s)$ crosses the unit circle in the complex plane at nonzero velocity, i.e.,

$$\lambda_1(s_0)\lambda_{1s}(s_0) + \lambda_2(s_0)\lambda_{2s}(s_0) \neq 0. \tag{4.11}$$

PROPOSITION 19. *The system consisting of* (2.1), (2.2), (2.3), *and the conditions*

$$\begin{array}{rcl} G_{11} &=& 0,\\ G_{12} &=& 0,\\ G_{21} &=& 0,\\ G_{22} &=& 0, \end{array} \tag{4.12}$$

where the G_{ij} are defined in Proposition 17, *together form a regular defining system for periodic solutions having a simple Neimark–Sacker singularity if the natural transversality condition* (4.11) *is satisfied.*

Proof. To prove that the system (2.1), (2.2), (2.3), (4.12) is a regular defining system (i.e., has full linear rank), we consider the implicit solution $(x(s)(t), T(s), \alpha(s))$ of (2.1), (2.2), (2.3). So $G_{11}, G_{12}, G_{21}, G_{22}$ are functions of s, κ only, and we have to prove that

$$\begin{pmatrix} G_{11s} & G_{11\kappa} \\ G_{12s} & G_{12\kappa} \\ G_{21s} & G_{21\kappa} \\ G_{22s} & G_{22\kappa} \end{pmatrix}$$

has rank 2. Assume that $c_1, c_2 \in \mathbf{R}$ are such that

$$c_1 G_{ijs} + c_2 G_{ij\kappa} = 0, \quad (i, j = 1, 2). \tag{4.13}$$

We start by noting that $p^H(s)q(s) \neq 0$ in a neighborhood of $s = s_0$. By standard arguments

$$(p^H q)\lambda_s = p^H \Phi_s(1) q, \tag{4.14}$$

where for simplicity of notation we have suppressed the dependence on s. To get an expression for $\Phi_s(1)$ we start from the identity

$$(D - Tf_x)\Phi \equiv 0.$$

Taking derivatives with respect to s and multiplying with any vector $\zeta \in \mathbf{R}^n$ we find

$$(D - Tf_x)\Phi_s\zeta = (Tf_x)_s\Phi\zeta.$$

The solution of this linear differential equation in $\Phi_s\zeta$ is

$$\Phi_s\zeta(t) = \Phi(s)(t)\left[\xi + \int_0^t \Psi^*(s)(\tau)(Tf_x)_s(s)(\tau)\Phi(s)(\tau)\zeta \; d\tau\right],$$

where ξ is determined by the initial conditions. Since for $t = 0$ we have $\Phi(0) = I, \Phi_s(0) = 0$, it follows that $\xi = 0$. Choosing $\zeta = q$ we obtain from (4.14) that

$$(p^H q)\lambda_s = \lambda p^H \int_0^1 \Psi^*(s)(\tau)(Tf_x)_s(s)(\tau)\Phi(s)(\tau)q \; d\tau. \tag{4.15}$$

From (3.24) we infer that

$$M_5 \begin{bmatrix} v_{1s} & v_{2s} \\ G_{11s} & G_{12s} \\ G_{21s} & G_{22s} \end{bmatrix} = \begin{bmatrix} (Tf_x)_s v_1 & (Tf_x)_s v_2 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{bmatrix}, \tag{4.16}$$

$$M_5 \begin{bmatrix} v_{1\kappa} & v_{2\kappa} \\ G_{11\kappa} & G_{12\kappa} \\ G_{21\kappa} & G_{22\kappa} \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ 2v_1(1) & 2v_2(1) \\ 0 & 0 \\ 0 & 0 \end{bmatrix}. \tag{4.17}$$

Combining (4.13), (4.16), and (4.17) we obtain

$$M_5 \begin{bmatrix} c_1 v_{1s} + c_2 v_{1\kappa} & c_1 v_{2s} + c_2 v_{2\kappa} \\ 0 & 0 \\ 0 & 0 \end{bmatrix} = \begin{bmatrix} c_1(Tf_x)_s v_1 & c_1(Tf_x)_s v_2 \\ 2c_2 v_1(1) & 2c_2 v_2(1) \\ 0 & 0 \\ 0 & 0 \end{bmatrix}.$$

Hence

$$\begin{pmatrix} c_1(Tf_x)_s v_1 \\ 2c_2 v_1(1) \end{pmatrix}, \begin{pmatrix} c_1(Tf_x)_s v_2 \\ 2c_2 v_2(1) \end{pmatrix}$$

are both in the range of (3.19). As an essential step in the proof of Proposition 15 it was shown that this implies

$$c_1 L((Tf_x)_s v_1) = 2c_2 p^H v_1(1),$$

$$c_1 L((Tf_x)_s v_2) = 2c_2 p^H v_2(1),$$

where the linear operator L is defined in (3.20). Since v_1, v_2 are in the kernel of (3.19) we have

$$v_1(\tau) = \Phi(\tau)v_1(0), \quad v_2(\tau) = \Phi(\tau)v_2(0).$$

Combining the last four formulae we find

$$c_1 L((Tf_x)_s \Phi q) = 2c_2 p^H \Phi(1)q = 2c_2 e^{i\theta}(p^H q). \tag{4.18}$$

Now,

$$\begin{aligned} L((Tf_x)_s \Phi q) &= -2\kappa e^{i\theta} \int_0^1 p^H \Psi^*(\tau)(Tf_x)_s \Phi(\tau)q \; d\tau + e^{2i\theta} \int_0^2 p^H \Psi^*(\tau)(Tf_x)_s \Phi(\tau)q \; d\tau \\ &= e^{i\theta}(\cos\theta + i\sin\theta - 2\cos\theta) \int_0^1 p^H \Psi^*(\tau)(Tf_x)_s \Phi(\tau)q \; d\tau \\ &\quad + e^{2i\theta} \int_0^1 p^H \Psi^*(1+\tau)(Tf_x)_s \Phi(1+\tau)q \; d\tau. \end{aligned}$$

Also,

$$p^H\Psi^*(1+\tau) = (\Psi(1+\tau)p)^H = (\Psi(\tau)\Psi(1)p)^H = p^H\Phi^{-1}(1)\Psi^*(\tau) = e^{-i\theta}p^H\Psi^*(\tau)$$

and

$$\Phi(1+\tau)q = \Phi(\tau)\Phi(1)q = e^{i\theta}\Phi(\tau)q.$$

Hence

$$L((Tf_x)_s\Phi q) = e^{i\theta}2i\sin\theta\int_0^1 p^H\Psi^*(\tau)(Tf_x)_s\Phi(\tau)q\ d\tau.$$

By (4.15) this implies

$$L((Tf_x)_s\Phi q) = 2i\sin\theta(p^Hq)\lambda_s.$$

Using (4.18) we further obtain

$$2ic_1\sin\theta(p^Hq)\lambda_s = 2c_2e^{i\theta}(p^Hq).$$

Dividing by $2(p^Hq)$ we obtain

$$(-\sin\theta\lambda_{2s} + i\sin\theta\lambda_{1s})c_1 = (\cos\theta + i\sin\theta)c_2.$$

Taking real and imaginary parts of this complex equality we find

$$\begin{pmatrix} -\sin\theta\lambda_{2s} & -\cos\theta \\ \sin\theta\lambda_{1s} & -\sin\theta \end{pmatrix}\begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}.$$

The determinant of the 2×2 matrix in this expression is equal to

$$\sin\theta(\cos\theta\lambda_{1s} + \sin\theta\lambda_{2s}) = \sin\theta(\lambda_1\lambda_{1s} + \lambda_2\lambda_{2s}).$$

By (4.11) and $\sin\theta \neq 0$ this implies that $c_1 = c_2 = 0$, which completes the proof. □

5. Computational issues. In this section we discuss computational issues related to the implementation of our defining systems, namely the computation of the derivatives of the test functionals with respect to the unknowns of the system, $x(t), \alpha, T$, as well as the problem of adapting the defining systems along the bifurcation branch. We also explicitly show the BVPs that must be solved.

5.1. Fold bifurcation. Proposition 9 implies that locally, near a simple fold singularity of periodic solutions, the system consisting of (2.1), (2.2), (2.3), and

$$G = 0$$

defines the set of simple folds in $(x(\cdot), T, \alpha)$-space; here G is defined by (3.13). Under natural nondegeneracy and transversality conditions, the regularity of this system was proved in section 4.1.

We need the derivatives of G with respect to the unknowns of the system, i.e., with respect to $x(\cdot), \alpha, T$.

Denoting by z any component of α or T we infer from (3.13) that

$$N_1 \begin{pmatrix} v_z \\ S_z \\ G_z \end{pmatrix} = \begin{pmatrix} [Tf_x(x(t),\alpha]_z v + [f(x(t),\alpha)]_z S \\ 0 \\ -\mathrm{Int}_{[f(x(\cdot),\alpha)]_z} v \\ 0 \end{pmatrix}.$$

Numerically we solve a discretized version of this equation, say

$$N_1^d \begin{pmatrix} v_z \\ S_z \\ G_z \end{pmatrix} = \begin{pmatrix} ([Tf_x(x(t),\alpha]_z v + [f(x(t),\alpha)]_z S)_d \\ 0 \\ -(\mathrm{Int}_{[f(x(\cdot),\alpha)]_z} v)_d \\ 0 \end{pmatrix}, \tag{5.1}$$

where N_1^d is the discretized version of N_1, i.e., a large square matrix with a structure that can be efficiently factorized, for example, as in AUTO [9].

Note that a large number of linear systems having the same structured matrix N_1^d must be solved. Moreover, all right-hand sides are known before the factorization. Thus the solution can be done in a single factorization process, without storing the factors.

$(N_1^d)^T$ has a block structure that is very similar to N_1^d. If an efficient solution strategy for $(N_1^d)^T$ is also developed, then it is possible to avoid solving (5.1) for all relevant z. Instead, a single system with $(N_1^d)^T$ is to be solved. In transposed form it is given by

$$(w_1^*, w_2^*, w_3, w_4) N_1^d = (0, 0, 1). \tag{5.2}$$

Combining (5.1) and (5.2) we find

$$G_z = w_1^*([Tf_x(x(t),\alpha]_z v + [f(x(t),\alpha)]_z S)_d - w_3(\mathrm{Int}_{[f(x(\cdot),\alpha)]_z} v)_d.$$

Notice that (3.13) is equivalent to the system

$$\left\{ \begin{aligned} v'(t) - Tf_x(x(t),\alpha)v(t) - Sf(x(t),\alpha) + Gw_{01}(t) &= 0, \\ v(1) - v(0) + Gw_{02} &= 0, \\ \int_0^1 v^*(\tau) f(x(\tau),\alpha)\ d\tau + Gw_{03} &= 0, \\ \int_0^1 v^*(\tau) v_{01}(\tau)\ d\tau + Sv_{02} &= 1, \end{aligned} \right. \tag{5.3}$$

while (3.14) can be explicitly written as

$$\left\{ \begin{aligned} w'(t) + Tf_x^*(x(t),\alpha)w(t) - Rf(x(t),\alpha) + Hv_{11}(t) &= 0, \\ w(1) - w(0) + Hv_{12} &= 0, \\ \int_0^1 w^*(\tau) f(x(\tau),\alpha)\ d\tau + Hv_{13} &= 0, \\ \int_0^1 w^*(\tau) w_{11}(\tau)\ d\tau + Rw_{12} &= -1. \end{aligned} \right. \tag{5.4}$$

Discretizations of these systems, for example by orthogonal collocation, result in linearized Newton systems having the same sparsity as the linear systems arising from

(2.5). They can therefore be solved using the same numerical linear algebra algorithms.

In practice we need to adapt the auxiliary variables (i.e., $w_{01}, w_{02}, w_{03}, v_{01}, v_{02}, v_{11}, v_{12}, v_{13}$, w_{11}, and w_{12}) along a computed branch of fold bifurcations of periodic orbits. For the bordering rows in N_1 and N_2, the natural choice is to take the kernel vectors of M_1 and M_2, respectively, at a previously computed solution point. These kernel vectors are obtained as a by-product of solving (5.3) and (5.4). For the column bordering of N_1 we need a vector that is not in the range of M_1. By Proposition 6, a possible choice is

$$\begin{pmatrix} w_{01} \\ w_{02} \\ w_{03} \end{pmatrix} = \begin{pmatrix} \Psi p_0 \\ 0 \\ 0 \end{pmatrix},$$

which by Proposition 7 can be derived from the solution of (5.4). Finally, a bordering column for N_2 is given in Proposition 8:

$$\begin{pmatrix} v_{11} \\ v_{12} \\ v_{13} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}.$$

Therefore, problems (5.3) and (5.4) actually take the following simplified forms:

$$\begin{cases} v'(t) - Tf_x(x(t),\alpha)v(t) - Sf(x(t),\alpha) + Gw_{01}(t) &= 0, \\ v(1) - v(0) &= 0, \\ \displaystyle\int_0^1 v^*(\tau) f(x(\tau),\alpha)\ d\tau &= 0, \\ \displaystyle\int_0^1 v^*(\tau) v_{01}(\tau)\ d\tau + S &= 1 \end{cases}$$

and

$$\begin{cases} w'(t) + Tf_x^*(x(t),\alpha)w(t) - Rf(x(t),\alpha) &= 0, \\ w(1) - w(0) &= 0, \\ \displaystyle\int_0^1 w^*(\tau) f(x(\tau),\alpha)\ d\tau + H &= 0, \\ \displaystyle\int_0^1 w^*(\tau) w_{11}(\tau)\ d\tau &= -1. \end{cases}$$

5.2. Period-doubling. By Proposition 14, simple flips are determined by (2.1), (2.2), (2.3), and the condition $G = 0$, where G is given by (3.17), assuming the conditions $\langle \phi_0, \Phi q_2 \rangle \neq 0$, $\langle \psi_0, \Psi p_2 \rangle \neq 0$ hold. To solve such systems numerically, we need the derivatives of G with respect to the unknowns of the system, i.e., with respect to $x(t), \alpha, T$. These can be approximated by finite differences, using (3.17). As in the fold case, they can be obtained exactly by solving an "adjoint problem" to (3.17). In this case the adjoint problem is (3.18).

PROPOSITION 20. *Let z denote a component of the problem parameter vector α, or let z denote the period T, on both of which the quantity G in* (3.17) *depends. Let v and w be obtained from* (3.17) *and* (3.18)*, respectively. Then the derivative of G with respect to z can be written as*

$$G_z = -\int_0^1 w^*(\tau)[Tf_x(x(\tau),\alpha)]_z v(\tau)\ d\tau,$$

while the linear part of the variation of G with respect to $x \mapsto x + \delta x$ is given by

$$\delta G = -\int_0^1 w^*(\tau) T f_{xx}(x(\tau),\alpha)) v(\tau)(\delta x)(\tau)\ d\tau.$$

Proof. By differentiating (3.17) we obtain

$$M_1 \begin{pmatrix} v_z \\ G_z \end{pmatrix} = \begin{pmatrix} [T f_x(x(t),\alpha)]_z v \\ 0 \\ 0 \end{pmatrix}. \tag{5.5}$$

Multiplying the first equation in (5.5) from the left with w^*, integrating over the interval $[0,1]$, and using the third equation in (3.18) we get

$$\begin{aligned} &\int_0^1 w^*(\tau) v_z'(\tau)\ d\tau - \int_0^1 w^*(\tau) T f_x(x(\tau),\alpha) v_z(\tau)\ d\tau - G_z \\ &= \int_0^1 w^*(\tau)[T f_x(x(\tau),\alpha)]_z v(\tau)\ d\tau. \end{aligned}$$

Integrating the first term in this expression by parts, and using the second equations in (3.18) and (5.5), we obtain

$$\begin{aligned} &-\int_0^1 v_z^*(\tau) w'(\tau)\ d\tau - \int_0^1 v_z^*(\tau) T f_x^*(x(\tau),\alpha) w(\tau)\ d\tau - G_z \\ &= \int_0^1 w^*(\tau)[T f_x(x(\tau),\alpha)]_z v(\tau)\ d\tau. \end{aligned}$$

Using the first equation in (3.18) we get

$$-\int_0^1 v_z^*(\tau)(-\phi_0(\tau) H)\ d\tau - G_z = \int_0^1 w^*(\tau)[T f_x(x(\tau),\alpha)]_z v(\tau)\ d\tau.$$

By the last equation in (5.5) the first part of the proposition follows.

The linear parts of the variations of G and v under variation of x satisfy

$$M_1 \begin{pmatrix} \delta v \\ \delta G \end{pmatrix} = \begin{pmatrix} T f_{xx}(x(t),\alpha) v\ \delta x \\ 0 \\ 0 \end{pmatrix}.$$

Similar to the derivation above, this implies the second part of the proposition. ∎

Notice that (3.17) is equivalent to the system

$$\begin{cases} v'(t) - T f_x(x(t),\alpha) v(t) + G\psi_0(t) &= 0, \\ v(0) + v(1) &= 0, \\ \displaystyle\int_0^1 \phi_0^*(\tau) v(\tau)\ d\tau &= 1, \end{cases} \tag{5.6}$$

while (3.18) can be explicitly written as

$$\begin{cases} w'(t) + T f_x^*(x(t),\alpha) w(t) + H\phi_0(t) &= 0, \\ w(0) + w(1) &= 0, \\ \displaystyle\int_0^1 \psi_0^*(\tau) w(\tau)\ d\tau &= -1. \end{cases} \tag{5.7}$$

Discretizations of these systems, for example by orthogonal collocation, result in linearized Newton systems having the same sparsity as the linear systems arising from (2.5). They can therefore be solved using the same numerical linear algebra algorithms.

The natural choice for starting values of ϕ_0, ψ_0 is

$$\phi_0(t) = \Phi(t)q_2, \quad \psi_0(t) = \Psi(t)p_2.$$

In a continuation context, it is necessary to regularly update ϕ_0 and ψ_0. Specifically, v obtained from (3.17) can be used to update ϕ_0, and w obtained from (3.18) can be used to update ψ_0. Indeed, after convergence to a period-doubling bifurcation, v spans the kernel of

$$\begin{pmatrix} D - Tf_x(x(t),\alpha) \\ \delta_0 + \delta_1 \end{pmatrix},$$

and, similarly, w spans the kernel of

$$\begin{pmatrix} D + Tf_x^*(x(t),\alpha) \\ \delta_0 + \delta_1 \end{pmatrix}.$$

5.3. Torus bifurcation. We have proved in Proposition 17 that the matrix equation $G = 0$ can be used to continue numerically curves of periodic solutions having Neimark–Sacker singularities, in particular, torus bifurcation points. Some issues require further attention.

First of all, we mention that the BVP for G is defined on the interval $[0, 2]$ and that 3-*point boundary conditions* are involved (at $t = 0, 1$, and 2).

To solve the system (2.1), (2.2), (2.3), (4.12) efficiently by a Newton-like method, one needs the derivatives G_{ijz}, where z is T or a component of α. From (3.24) we infer that

$$M_5 \begin{pmatrix} v_{1z} & v_{2z} \\ G_{11z} & G_{12z} \\ G_{21z} & G_{22z} \end{pmatrix} = \begin{pmatrix} [Tf_x(x(t),\alpha]_z v_1 & [Tf_x(x(t),\alpha)]_z v_2 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}.$$

One also needs the derivatives with respect to κ; for this we find

$$M_5 \begin{pmatrix} v_{1\kappa} & v_{2\kappa} \\ G_{11\kappa} & G_{12\kappa} \\ G_{21\kappa} & G_{22\kappa} \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 2v_1(1) & 2v_2(1) \\ 0 & 0 \\ 0 & 0 \end{pmatrix}.$$

Numerically we solve the discretized versions of these equations, say

$$M_5^d \begin{pmatrix} v_{1z} & v_{2z} \\ G_{11z} & G_{12z} \\ G_{21z} & G_{22z} \end{pmatrix} = \begin{pmatrix} [Tf_x(x(t),\alpha]_z v_1 & [Tf_x(x(t),\alpha)]_z v_2 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}. \tag{5.8}$$

One also needs the derivatives with respect to κ; for this we find

$$M_5^d \begin{pmatrix} v_{1\kappa} & v_{2\kappa} \\ G_{11\kappa} & G_{12\kappa} \\ G_{21\kappa} & G_{22\kappa} \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 2v_1(1) & 2v_2(1) \\ 0 & 0 \\ 0 & 0 \end{pmatrix}, \tag{5.9}$$

where M_5^d is the discretized version of M_5, i.e., a large square matrix of the same structure as that factored efficiently in AUTO.

We again note that a large number of linear systems with the same structured matrix M_5^d has to be solved. All right-hand sides are known when the factorization is done. Thus the solution of all systems can be done during a single factorization process of M_5^d without storing the factors.

$(M_5^d)^*$ has a block structure that is very similar to that of M_5^d. If an efficient solution strategy for $(M_5^d)^*$ is also developed, then it is possible to avoid solving (5.8) for all relevant z and (5.9). Instead, a single system with $(M_5^d)^*$ is to be solved. In transposed form it is given by

$$\begin{pmatrix} w_1^{1*} & w_1^{2*} & G_{11} & G_{12} \\ w_2^{1*} & w_2^{2*} & G_{21} & G_{22} \end{pmatrix} M_5^d = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{5.10}$$

Combining (5.8) and (5.10) we find

$$\begin{pmatrix} G_{11z} & G_{12z} \\ G_{21z} & G_{22z} \end{pmatrix} = \begin{pmatrix} w_1^{1*}[Tf_x(x(t),\alpha)]_z v_1 & w_1^{1*}[Tf_x(x(t),\alpha)]_z v_2 \\ w_2^{1*}[Tf_x(x(t),\alpha)]_z v_1 & w_2^{1*}[Tf_x(x(t),\alpha)]_z v_2 \end{pmatrix}$$

if z is T or one of the components of x, α. For κ we find

$$\begin{pmatrix} G_{11\kappa} & G_{12\kappa} \\ G_{21\kappa} & G_{22\kappa} \end{pmatrix} = \begin{pmatrix} 2w_1^{2*}v_1(1) & 2w_1^{2*}v_2(1) \\ 2w_2^{2*}v_1(1) & 2w_2^{2*}v_2(1) \end{pmatrix}.$$

Next notice that (3.24) is equivalent to the system

$$\begin{cases} v_1' - Tf_x(x(t),\alpha)v_1 + G_{11}\psi_0 + G_{21}\psi_1 = 0, \\ v_2' - Tf_x(x(t),\alpha)v_2 + G_{12}\psi_0 + G_{22}\psi_1 = 0, \\ v_1(0) - 2\kappa v_1(1) + v_1(2) = 0, \\ v_2(0) - 2\kappa v_2(1) + v_2(2) = 0, \\ \int_0^2 \phi_0^*(\tau)v_1(\tau)\ d\tau = 1, \\ \int_0^2 \phi_1^*(\tau)v_2(\tau)\ d\tau = 0, \\ \int_0^2 \phi_0^*(\tau)v_1(\tau)\ d\tau = 0, \\ \int_0^2 \phi_1^*(\tau)v_2(\tau)\ d\tau = 1, \end{cases} \tag{5.11}$$

while (3.25) can be explicitly written as

$$
\left\{
\begin{array}{rcl}
w_1' + Tf_x^*(x(t),\alpha)w_1 + H_{11}\phi_0 + H_{21}\phi_1 &=& 0,\\
w_2' + Tf_x^*(x(t),\alpha)w_2 + H_{12}\phi_0 + H_{22}\phi_1 &=& 0,\\
w_1(0) - 2\kappa w_1(1) + w_1(2) &=& 0,\\
w_2(0) - 2\kappa w_2(1) + w_2(2) &=& 0,\\
\displaystyle\int_0^2 \psi_0^*(\tau)w_1(\tau)\ d\tau &=& -1,\\
\displaystyle\int_0^2 \psi_1^*(\tau)w_2(\tau)\ d\tau &=& 0,\\
\displaystyle\int_0^2 \psi_0^*(\tau)w_1(\tau)\ d\tau &=& 0,\\
\displaystyle\int_0^2 \psi_1^*(\tau)w_2(\tau)\ d\tau &=& -1.
\end{array}
\right. \tag{5.12}
$$

Discretizations of these systems, for example by orthogonal collocation, result in linearized Newton systems having the same sparsity as the linear systems arising from (2.5). They can therefore be solved using the same numerical linear algebra algorithms.

In a continuation context, the vector-functions $\phi_0, \phi_1, \psi_0, \psi_1$ should be updated. This can be done by solving both (5.11) and (5.12). Indeed, v_1, v_2 span the two-dimensional space in which ϕ_0, ϕ_1 should be chosen and w_1, w_2 similarly span the space in which ψ_0, ψ_1 should be chosen (some orthogonalization and scaling may be appropriate).

Finally, recall that we compute the Neimark–Sacker points by using essentially an overdetermined system. This necessitates some changes in the elimination strategy when solving the linear systems.

6. Numerical example. In this section we illustrate our new techniques on a test example, a simple feedback control system of Lur'e type:

$$
\left\{
\begin{array}{rcl}
\dot{x}_1 &=& x_2,\\
\dot{x}_2 &=& x_3,\\
\dot{x}_3 &=& -\alpha x_3 - \beta x_2 - x_1 + x_1^2,
\end{array}
\right. \tag{6.1}
$$

where α and β are positive parameters. It is well known (see, for example [17, section 5.4]) that the equilibrium $x_1 = x_2 = x_3 = 0$ of (6.1) has a supercritical Hopf bifurcation at

$$\alpha_0 = \frac{1}{\beta},$$

generating a stable periodic solution that exists for $\alpha < \alpha_0$. This periodic solution has a supercritical period-doubling bifurcation at $\alpha_1 \approx 0.630302$.

The discretized continuation problem (2.1), (2.2), and (2.3) for the periodic solution has been programmed in the MATLAB Continuation Toolbox [19]. The method of orthogonal collocation with piecewise polynomials is used, similar to the one implemented in AUTO. It is characterized by the number `NTST` of mesh points and the number `NCOL` of collocation points. At each computed point on the solution curve, a discrete version of (5.6) is set up and solved. This gives a value of the test function G to detect a flip singularity. A constant bordering function ψ_0 is used, while the

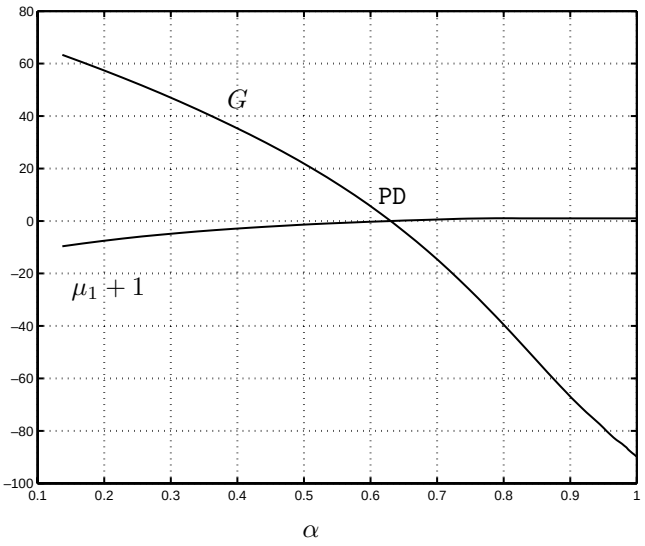

FIG. 1. *Test function* $G(\alpha)$ *and* $\mu_1(\alpha) + 1$ *for* $\beta = 1$.

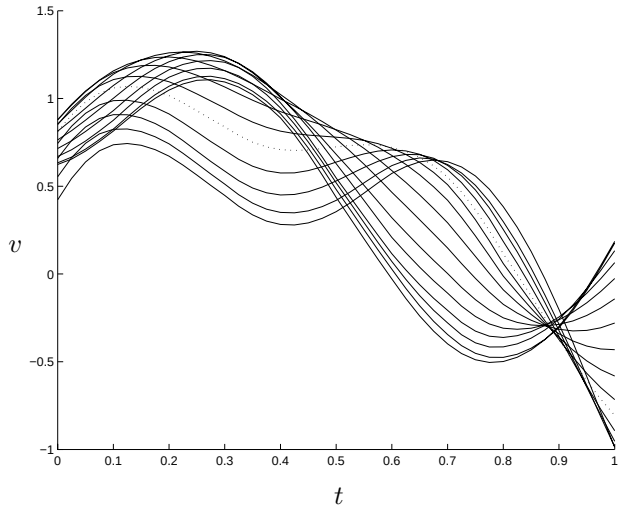

FIG. 2. *Solutions* $v(t)$ *at different* α*-values for* $\beta = 1$.

computed approximation to v is used to update the bordering function ϕ_0. Figures 1 and 2 are produced with `NTST=10` and `NCOL=4`.

Figure 1 shows the behavior of G as a function of α for $\beta = 1$. For this value of β, Hopf bifurcation occurs at $\alpha_0 = 1$. In the same figure, the function $\mu_1 + 1$ is plotted, where μ_1 is a nontrivial Floquet multiplier of the periodic solution for which $\mu_1(\alpha_1) = -1$. The multipliers are computed via a specially adapted elimination algorithm from AUTO. As can be seen, G vanishes together with $\mu_1 + 1$. Moreover, close examination of numerical data gives the above bifurcation value α_1 with seven correct decimal places.

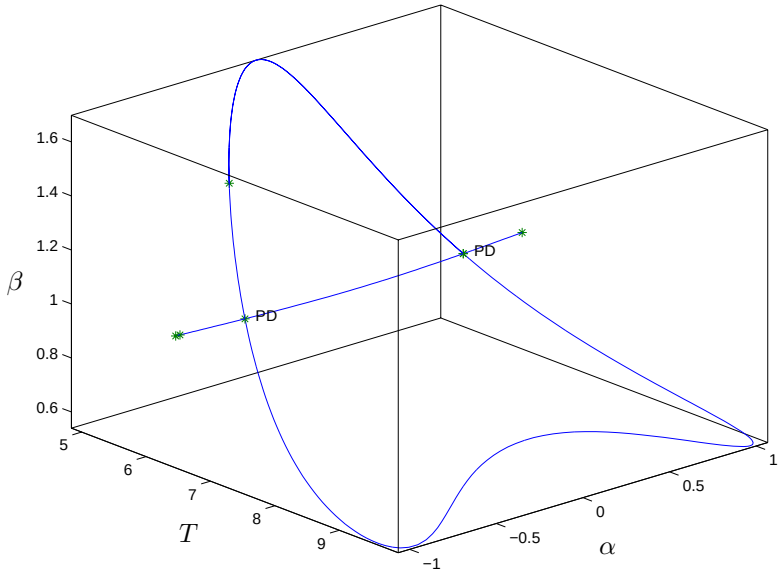

FIG. 3. *Cycle and period-doubling branches.*

Figure 2 shows a family of computed profiles $v(t)$ along the solution curve. The dashed solution corresponds to the bifurcation parameter value α_1. Finally, Figure 3 shows the two-parameter continuation of the period-doubling bifurcation curve, which corresponds to a close curve. The continuation is started at one of the PD points in the one-parameter path of periodic solutions discussed above.

We now briefly address the important issue of comparing our new method for continuing period-doubling bifurcations to the algorithm based on a fully extended system, i.e., (2.1), (2.2), and (2.3), augmented by

$$\begin{cases} v'(t) - T f_x(x(t), \alpha) v(t) &= 0, \\ v(0) + v(1) &= 0, \\ \displaystyle\int_0^1 \phi_0^*(\tau) v(\tau) \ d\tau &= 1, \end{cases}$$

as implemented in AUTO. The corresponding discretized system is nearly twice the size as the discretized minimally extended system composed of (2.1), (2.2), (2.3), and $G = 0$, where G is to be computed from (5.6). However, for the minimally extended system one has to solve the extra BVP (5.7) in order to calculate the Jacobian matrix of the discretized bordered system. For comparison, both methods were implemented in a similar fashion, using the standard sparse matrix solver in the Continuation Toolbox [19], and tested using different choices for the number of mesh points and the number of collocation points. Table 1 shows the execution times required by the two methods for computing the same number (300) of solution points along the period-doubling curve shown in Figure 3. Computations were done on a 350 Mhz PC.

Clearly the bordered system of this paper is faster, and its advantage widens as the number of mesh points and the number of collocation points increases. In the computations we used an adaptive step length, and the bordered system actually resulted in larger steps than the fully extended system. Details of the implementation and more extensive comparisons will be reported elsewhere.

TABLE 1

NTST	NCOL	Minimally extended system	Fully extended system
10	4	101,8 s	122,3 s
10	5	134,9 s	159,4 s
20	4	269,9 s	358,6 s
20	5	371,9 s	558,2 s
30	4	529,8 s	808,0 s
30	5	751,0 s	1260,3 s
40	4	886,0 s	1528,8 s
40	5	1376,8 s	2528,6 s

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