ATOMIC SPECTROSCOPY, PERIODIC ORBITS AND GENERIC TWO-PARAMETER BIFURCATIONS

K. R. MEYER, J. B. DELOS, AND J.-M. MAO

ABSTRACT. Measurements of atomic spectra display recurrences associated with classical periodic orbits of the electron. As the energy is changed, bifurcations of these periodic orbits are visible. Calculations show that many of these bifurcations have the generic structures listed by Meyer [1970], but symmetries of the system force some bifurcations to have nongeneric structures. By imposing an external electric field, some symmetries can be broken. These physical systems force us to address new mathematical questions: what are the generic structures of bifurcations of periodic orbits of two-parameter area-preserving maps? We give a partial answer to this question, and we show how the results are visible in calculations.

1. Physics

It is possible to measure in the laboratory the periods T_k or the actions S_k of classical periodic orbits of an atomic electron. This is a deep and complicated statement. Electrons obey laws of quantum mechanics, not classical mechanics, so we know that it is impossible to measure both the position and the velocity of an electron, and we do not imagine that any one electron actually moves in time along a definite path. Instead, the electron's behavior is described by the Schroedinger wave equation.

There is, however, a close relationship between the propagation of Schrödinger waves and the motion of a stream of particles along classical paths. First, the centroid of a well-localized wave packet moves in time according to classical equations of motion. A packet can be made to follow closely a classical periodic orbit; then the time required for the packet to return to its original location is close to the period of the classical orbit. Second, the change of phase of a Schroedinger wave as it propagates from one point to another is approximately equal to the action $\int \mathbf{p} \cdot d\mathbf{q}$ integrated along a classical path between these points. Such changes of phase produce interference effects which are observable in laboratory experiments.

By computer calculation of classical orbits of electrons, it is possible to construct quantum wave functions, and we can use these wave functions to interpret and even to predict the results of measurements of the absorption spectra of atoms (Du and Delos [1988]). In this paper, we will not give any details about how this is done. We will just pretend that electrons are classical particles that obey Newton's laws. We will say that our friends (Holle et al., [1988]) found a way to place an atom in a magnetic field, and to kick an electron out of the atom such that they knew precisely how much kinetic energy the electron was given, but they could not tell in what direction it was kicked. They measured the time required for the electron to return to the atom (or the classical action around its orbit).

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A sample measurement is shown in Figure 1. The large peaks mean that, after repeating the measurement many times, they often found electrons returning after acquiring approximately 1.5, 3.0 or 4.5 units of action, but they did not ever find electrons returning with (for example) 0.7 units of action. We call this set of observations the recurrence spectrum for the given kinetic energy.

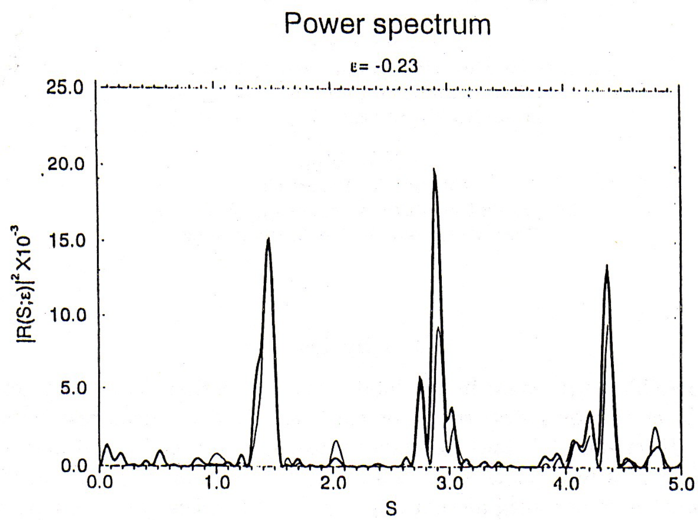

FIGURE 1. Heavy line: a measured recurrence spectrum for a hydrogen atom in a magnetic field. The horizontal coordinate represents classical action, and the vertical axis is called the recurrence strength; it is proportional to the number of electrons that return to the atom on orbits of given action. (It is actually measured by evaluating the Fourier transform of the absorption spectrum.) Light line: corresponding theoretical recurrence spectrum.

They then repeated the measurements with different initial kinetic energies given to the electron. The results are shown in Figure 2 – Main et al. [1994]. Again each peak corresponds to one or more recurrences – classical orbits which at the given energy return to the atom after acquiring a certain quantity of action. The most striking feature of this figure is the splitting and proliferation of peaks as the energy increases. These are bifurcations – as we vary the energy continuously, we pass through points at which a returning orbit splits, producing additional recurrences.

Mathematical analysis shows that bifurcations of periodic orbits fall into certain characteristic patterns. Bifurcation theory is a very old subject, having roots in the work of Poincaré, but many long-neglected questions remain unanswered. A special aspect of the bifurcations visible here arises because atomic electrons obey Hamiltonian equations of motion, so their orbits conserve energy, and ensembles preserve volume in phase space and area in Poincaré planes. Bifurcations that occur in such systems have special structures that do not necessarily occur in more general, dissipative systems. Many macroscopic systems also obey Hamiltonian equations of motion to some degree of approximation, but nevertheless, it appears that these experiments are the first that *force* us to confront questions about the structure of bifurcations of periodic orbits in Hamiltonian systems.

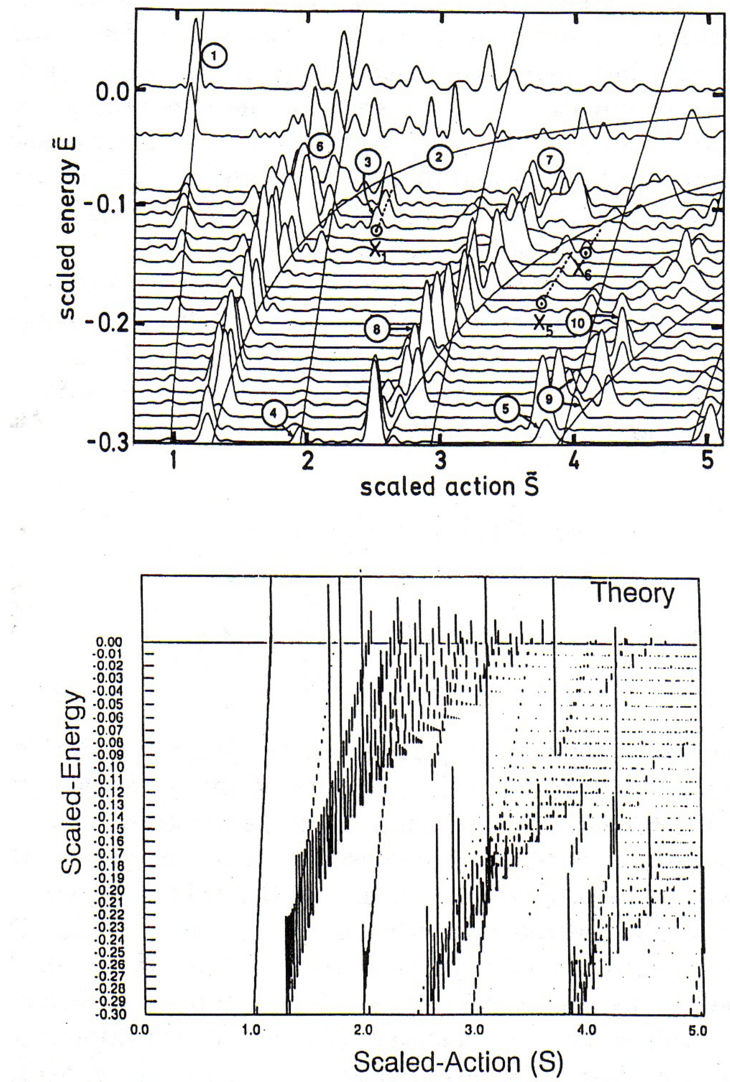

FIGURE 2. (a) About 25 recurrence spectra measured at various values of electron energy are drawn in a single graph. The horizontal axis is again classical action, while the vertical axis is electron energy, the parameter e in Hamiltonian H_1. (The electric field parameter f equals zero in this experiment.) (b) A corresponding family of theoretical recurrence spectra is shown as a needle graph. In both figures we see bifurcation and proliferation of recurrences with increasing e. This is correlated with the change from orderly to chaotic classical motion of the electron. The structures in this experiment are explained in detail by Main et al. [1994]. Peak 3 is produced in a saddle-node bifurcation, peaks 4 and 5 are associated with a 4-island chain bifurcation, the mountain range 6 is related to orbits that are produced in an orderly sequence of pitchforks and period-doublings, and peaks 9 and 10 arise from period-triplings.

With properly-chosen coordinates, the Hamiltonian for an atomic electron in fixed parallel electric and magnetic fields is

$$\begin{aligned} H_1 &= T(p_q, p_r) + V(q, r) \\ &= \frac{1}{2}(p_q^2 + p_r^2) - 4e(q^2 + r^2) \\ &\quad - 2q^2 r^2 (q^2 + r^2) + 2(q^6 + r^6) \\ &\quad - 16fqr(q^2 + r^2) \end{aligned}$$

What is essential about this? (a) There are two degrees of freedom. (b) The kinetic energy is purely quadratic in the momenta, so the system has "time-reversal invariance". (c) The potential energy contains two parameters, e and f. (In atomic physics, the parameter e combines the conserved total energy and the magnetic field strength, while f is proportional to the electric field strength. Also, in this physical application, H_1 has the fixed value $H_1(p_q, p_r, q, r) = 2$.) (d) The potential energy is invariant under inversion $(q, r) \to (-q, -r)$. (e) If $f = 0$, the potential energy is invariant under reflections $(q, r) \to (-q, r) \to (q, -r)$. Small but nonzero values of f break this reflection symmetry. (Additional reflection symmetries are also present.) (f) The periodic orbits that are detected in the experiment are the ones that pass through the origin (q=0, r=0) going in any direction.

Let us now pose general questions. (1) Given an arbitrary, smooth Hamiltonian function $H(p_q, p_r, q, r; e, f)$ defined in a phase-space (p_q, p_r, q, r) with smooth dependence on one or more parameters e, f, given that it possesses periodic orbits (PO's), how do these orbits bifurcate as the parameters are varied? What can be said about the geometrical structure of the newly created PO's? This question, fundamental to a physicist, may not be sufficiently well-posed to have any definite mathematical answer. However, a closely related question has been answered. (2) Such Hamiltonian differential equations induce two-dimensional area-preserving maps (Poincaré surfaces of section). What are the generic structures of bifurcations of PO's of smooth two-dimensional one-parameter area-preserving maps? This question was answered by Meyer [1970]; it was shown that there are five and only five generic types of bifurcation. (3) What structures are generic under symmetries, such as those mentioned above? This question was answered in Rimmer [1982], also see Mao and Delos [1992], deAguiar et al. [1987]. (4) What are the generic structures of two-dimensional two-parameter area-preserving maps?

To illustrate the importance of this question, let us consider a specific example. For $f = 0$, the Hamiltonian H_1 has a periodic orbit having $r = 0, p_r = 0$; if we vary the parameter e, then at a certain point that orbit undergoes an "antipitchfork" bifurcation: it changes from stable to unstable, and simultaneously two other unstable PO's merge with it and are destroyed. This antipitchfork bifurcation is a nongeneric structure – it exists because of the symmetries of the system. It is common for an unstable PO to collide with a stable PO (at which point they annihilate each other), but it is not common for two distinct unstable PO's to collide simultaneously with a stable PO. Now if f is changed to a nonzero value, the reflection symmetry of $V(q, r)$ is broken and the stable PO moves off the $r = 0$ line. What happens when it bifurcates? Does it still change from stable to unstable? Is the antipitchfork structure still present? This change of f corresponds to imposing an electric field on the atom. A

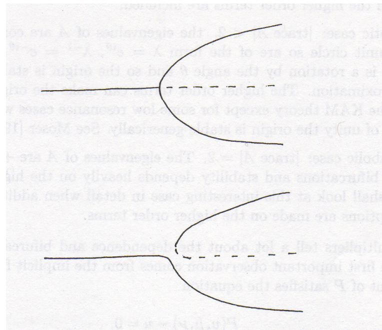

FIGURE 3. A representation of a pitchfork bifurcation (stable goes unstable and two new stable orbits of the same period are created), and a representation of a "broken pitchfork" (the stable orbit moves aside to make way for a saddle-node bifurcation).

change in the structure of this bifurcation might have observable physical consequences for the system. What are they?

Full answers to all of these questions are not now available. We can begin below with a partial answer to question (4) above. We will show that pitchfork, antipitchfork, and period-doubling bifurcations break in certain characteristic ways when the symmetry is broken (Figure 3).

To emphasize that the result is very general, and does not depend in any way on the special physics of Hamiltonian H_1, we change the notation. The Poincaré plane is denoted (x, y) and we begin with an area-preserving mapping of the plane that depends on two parameters (μ, ν).

2. Mathematics

Notation. Let P be a smooth, area preserving mapping of a region $\mathbf{O}$ in the plane, $\mathbf{R}^2$, into the plane which depends on two parameters. Let $u = (x, y)$ be coordinates in the plane and let the two parameters be denoted by μ and ν. We are interested in the nature and bifurcation of fixed points and periodic points of P as the parameters are varied. The region $\mathbf{O}$ should contain an open neighborhood of the fixed point in question. We denote the two components of P by (X, Y) and so $P : (x, y) \to (X, Y)$. Sometimes we will show the dependence on the parameters by writing $X(x, y, \mu, \nu)$ etc. Iterates of P will be denoted by $P^k = P \circ P \circ \cdots \circ P = (X^k, Y^k)$. There are several places where $\pm$ are needed, so α and β will be ± 1.

That P is area preserving means that the Jacobian matrix $DP(u) = \partial(X, Y)/\partial(x, y)$ has determinant identically equal to one. Let P have a fixed point at u_0, $P(u_0) = u_0$ and let $A = DP(u_0)$. A is a 2×2 matrix with determinant $+1$ and characteristic equation $\lambda^2 - (\text{trace } A)\lambda + 1$. Its eigenvalues are called the *(characteristic) multipliers* of the fixed point and since $\det A = 1$ they are reciprocals, thus the multipliers will be denoted by λ, λ^{-1}.

The linearization or first approximation of P at the fixed point is the map $u \to Au$. Based on the linear approximation there are three basic cases:

(1) Hyperbolic case: $|\text{trace } A| > 2$. The eigenvalues of A are real and satisfy $0 < \lambda < 1 < \lambda^{-1}$ or $\lambda^{-1} < -1 < \lambda < 0$. The fixed point is unstable by the linear approximation and by classical results the fixed point is still unstable when the higher order terms are included.

(2) Elliptic case: $|\text{trace } A| < 2$. the eigenvalues of A are complex and lie on the unit circle so are of the form $\lambda = e^{i\theta}$, $\lambda^{-1} = e^{-i\theta}$. The linearized map is a rotation by the angle θ and so the origin is stable for the linear approximation. The higher order terms can make the origin unstable, but by the KAM theory except for some low resonance cases where λ is a small root of unity the origin is stable generically. See Moser [1962, 1968].

(3) Parabolic case: $|\text{trace } A| = 2$. The eigenvalues of A are $+1, +1$ or $-1, -1$. The bifurcations and stability depends heavily on the higher order terms. We shall look at this interesting case in detail when additional generic assumptions are made on the higher order terms.

The multipliers tell a lot about the dependence and bifurcation of the fixed points. The first important observation comes from the implicit function theorem. A fixed point of P satisfies the equation

$$P(u, \mu, \nu) - u = 0. \tag{2.1}$$

Assume that $u = u_0$ is a fixed point for P for some value of the parameters, say $\mu = \mu_0$, $\nu = \nu_0$, thus (u_0, μ_0, ν_0) satisfies equation (2.1). The Jacobian of (2.1) at u_0 is $DP(u_0, \mu_0, \nu_0) - I = A - 1$ and so if $+1$ is not a multiplier the hypotheses of the implicit function theorem hold and there is a smooth function $\eta(\mu, \nu)$ defined for μ, ν near μ_0, ν_0 which satisfies $P(\eta(\mu, \nu), \mu, \nu) = \eta(\mu, \nu)$. Moreover, $(\eta(\mu, \nu)$ is the only solution near u_0. Thus the fixed point can be continued as an isolated fixed point for values of the parameters near μ_0, ν_0. The eigenvalues vary continuously with the parameters also. Thus a hyperbolic (respectively elliptic) continues as a hyperbolic (respectively elliptic) fixed point, but parabolic fixed points can and in general do change type.

The fixed point is called *elementary* if its multipliers are not $+1$. In this case we can change coordinates and parameters by $u' = u - \eta(\mu, \nu)$, $\mu' = \mu - \mu_0$, $\nu' = \nu - \nu_0$ so that in the primed variables the fixed point of P is at the origin for all small values of the parameters. We shall assume that this change has been made and drop the primes on the variables.

The above argument shows that a fixed point can bifurcate only when its multipliers are $+1$. However, there may be periodic points which bifurcate from the fixed point. The above argument shows that the fixed point is isolated as a periodic point of period k if $DP^k(0) = A^k$ does not have eigenvalues $+1$. This can happen only if the multipliers are roots of unity.

If there are no parameters then generically all the fixed points are either hyperbolic or elliptic and the multipliers of the elliptic points are not roots of unity. If there is one parameter then fixed points with multipliers ± 1 or other roots of unity occur generically for isolated values of the parameter. The bifurcations which can occur in generic one parameter families are described in Meyer [1970], but see the pictures in Abraham and Marsden [1978].

This paper will begin the classification of the generic bifurcation when the mapping P depends on two parameters. In this case there are curves in parameter space where P

has fixed points with multipliers that are a specific root of unity. Only the parabolic case is considered here when the multipliers are ± 1. The case when the multipliers are $+1$ is discussed in the next section and when they are -1 in the subsequent section. The bifurcations for higher roots of unit will be the topic of a later paper.

Creation – Multipliers = +1. Poincaré (1899) associated to the map P a generating function G with the property that fixed points of P are critical points of G and vice versa. Specifically, let $P = (X, Y)$ be defined in a disk about the origin in the plane and consider the differential form

$$\Omega = (Y - y)d(X + x) - (X - x)d(Y + y). \tag{2.2}$$

Since P is an area preserving $d(XdY - xdy) = dX \wedge dY - dx \wedge dy = 0$ and similarly $d(YdX - ydx) = dY \wedge dX - dy \wedge dx = 0$. These identities and

$$\Omega = (YdX - ydx) - (XdY - xdy) + d(xY - xX)$$

imply that $d\Omega = 0$, i.e. Ω is closed. Since we are working on a disk Poincaré's lemma asserts that a closed form is exact so there is a function G such that $dG = \Omega$.

The basic facts about this generating function are given in the following lemma and the proof can be found in Meyer [1970]. Also see the original discussion in Poincaré [1899] and another discussion in Weinstein [1972].

Lemma 2.1. *Assume that for $\mu = \nu = 0$ the map P has a fixed point at the origin whose multipliers are not equal to -1. Then the generating function G defined by (2.2) is a function of x, y for x, y, μ, ν small. It has the following properties:*

1. *A critical point of G (i.e. where $G_x = G_y = 0$) is a fixed point of P and conversely.*
2. *A nondegenerate maximum or minimum of G corresponds to an elliptic fixed point of P and conversely.*
3. *A nondegenerate saddle point of G corresponds to an hyperbolic fixed point of P and conversely.*

To obtain a rough picture of the map draw the level lines of G – but remember this is only a first approximation of the full picture.

From catastrophe theory if there are no parameters then generically G has only nondegenerate critical points and so generically P has only elliptic of hyperbolic fixed points. If there is one parameter then G can have a fold critical points i.e. G might be of the form

$$G = \pm y^2/2 + x^3/6 - \mu x. \tag{2.3}$$

This gives rise to the elliptic-hyperbolic (sometimes called saddle-node) bifurcation discussed in Meyer [1970] and subsequent papers. Two parameters gives rise to the cusp catastrophe with generating function

$$G = \pm y^2/2 + x^4/12 - \mu x^2/2 + (2/3)\nu x = \alpha y^2/2 + x^4/12 - \mu x^2/2 + (2/3)\nu x. \tag{2.4}$$

See Poston and Stewart [1978] for a readable introduction to catastrophe theory and additional references.

Remark: *By Thom's theorem on the classification of elementary catastrophes there are coordinates such that a cusp catastrophe is of the above polynomial form, but these coordinates*

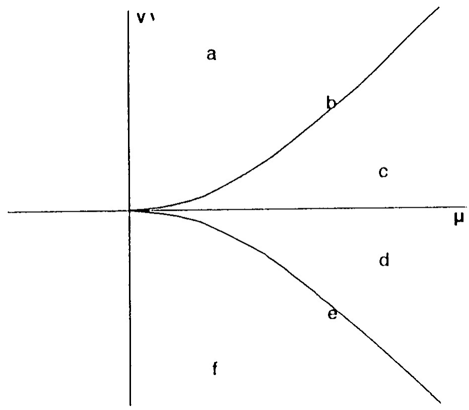

FIGURE 4. Regions in the parameter plane for the cusp bifurcation.

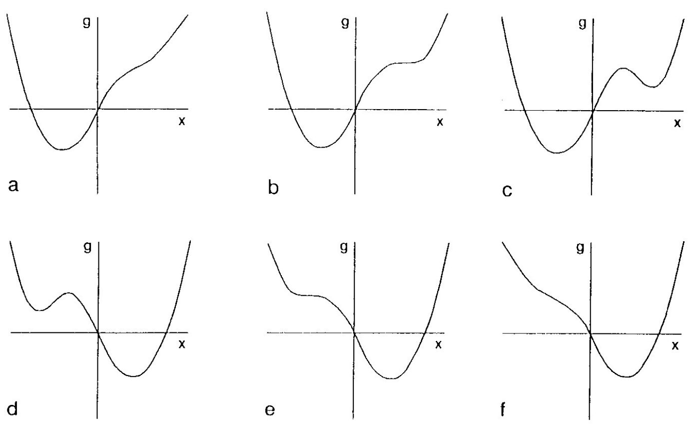

FIGURE 5. Graphs of g vs x for various values of parameters.

are not symplectic coordinates! Therefore, we will not derive the map from G, but simply study its critical points.

The critical points of G are solutions of

$$G_y = y = 0, \qquad G_x = x^3/3 - \mu x + 2\nu/3 = 0 \tag{2.5}$$

The singular locus where G has a degenerate critical point is found by solving $G_x = 0$ and $G_{xx} = x^2 - \mu = 0$. This locus is the cusp $\mu^3 = \nu^2$. Figure 4 labels various regions in the parameter plane. Regions b and e are on the singular locus. Figure 5 shows the graphs of $g(x) = G(x, 0, \mu, \nu)$ as a function of x for the various regions in the parameter plane.

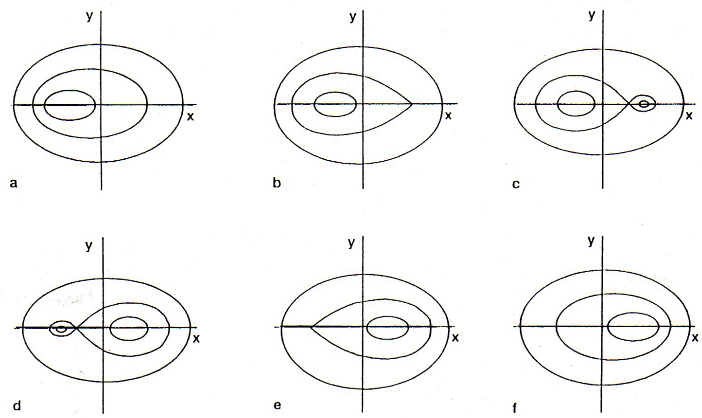

FIGURE 6. The cusp bifurcation, $\alpha = +1$.

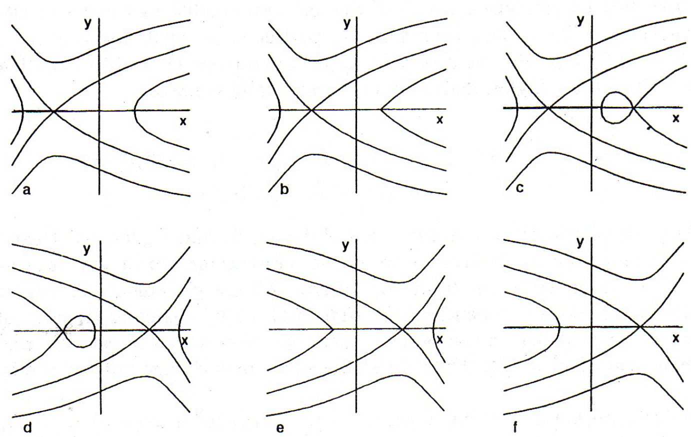

FIGURE 7. The cusp bifurcation, $\alpha = -1$.

If $\alpha = +1$ then a non-degenerate minimum x_0 of $g(x)$ gives rise to a non-degenerate minimum of G at $(x_0, 0)$ and hence to an elliptic fixed point of the map P. If $\alpha = +1$ then a non-degenerate maximum x_0 of $g(x)$ gives rise to a non-degenerate saddle point of G at $(x_0, 0)$ and hence to a hyperbolic fixed point of the map P. See Figure 6.

When $\alpha = -1$ it is the other way around. Namely, if $\alpha = -1$ then a non-degenerate minimum x_0 of $g(x)$ gives raise to a non-degenerate saddle of G at $(x_0, 0)$ and hence to an hyperbolic fixed point of the map P and a non-degenerate maximum x_0 of $g(x)$ gives rise to a non-degenerate maximum of G at at $(x_0, 0)$ and hence to an elliptic fixed point of the map P. See Figure 4

Figures 4-7 summarizes the new bifurcations which occur with two parameters when the fixed point has multiplier $+1$.

Period Doubling - Multipliers $= -1$ The discussion of period doubling for area preserving maps given below is a substantial improvement to the original discussion in Meyer [1970]. In this section we will proceed formally and not worry about the convergence of the normal form. One only has to fuss with the implicit function theorem to show that the formal periodic points are true periodic points. In fact by Artin's implicit function theorem a formal analysis suffices in the analytic case — see Artin [1968].

Assume when $\mu = \nu = 0$ that P has a fixed point at the origin with multipliers -1. Then the Jacobian matrix of P at the origin is symplectically similar to one of the following

$$\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix} \qquad \begin{pmatrix} -1 & \pm 1 \\ 0 & -1 \end{pmatrix}, \tag{2.6}$$

see Meyer and Hall [1992]. The first matrix is so degenerate that it takes three parameters to unfold it — see Arnold [1972]. That is, generically the first matrix in (2.6) may appear in a three parameter family not in a two parameter family. Since we are considering only the two parameter case we need only consider the second matrix.

Lemma 2.2. *Assume P has a fixed point at the origin with multipliers -1 and that $DP(0)$ is $\begin{pmatrix} -1 & \alpha \\ 0 & -1 \end{pmatrix}$ then the normal form for P is*

$$P(u) = -\Phi(u) \tag{2.7}$$

where Φ is the time 1-map of a Hamiltonian system with Hamiltonian G where G is of the form

$$\begin{aligned} G(u) = G(x,y) &= \alpha y^2/2 + K(x) \\ &= \alpha y^2/2 + ax^2/2 + bx^4/4 + cx^6/6 + \cdots . \end{aligned} \tag{2.8}$$

Here as above $\alpha = \pm 1, a, b, c$ etc. are constants (which depend on the parameters μ and ν of course.) The formal series K is even.

Proof. See Meyer and Hall [1992] pages 197-198. □

We shall proceed with a formal analysis, i.e. assume the system is in normal form. It should be clear that our conclusions are based on only a finite number of terms in the normal form and so the system need only be in normal form up to a certain degree. A liberal dose of the implicit function theorem will show that the formal analysis suffices, see for example the arguments in Meyer [1970] or in Hale and Chow [1982].

Lemma 2.3. *P has $u_0 = (x_0, y_0)$ as a periodic point of period 2 if $y_0 = 0$ and x_0 is a critical point of K ($K_x(x_0) = 0$). Moreover, $u_0 = (x_0, y_0)$ is an elliptic point of P if and only if u_0 is a non-degenerate maximum or minimum of G and u_0 is a hyperbolic point of P if and only if u_0 is a non-degenerate saddle point of G.*

Proof. Since K is even, if $u_0 = (x_0, 0)$ is a critical point of G then so is $-u_0 = (-x_0, 0)$. Thus, the Hamiltonian flow defined by G leaves $\pm u_0$ fixed, $\Phi(\pm u_0) = \pm u_0$. So $P(\pm u_o) = \mp u_0$ and u_0 is a periodic point of period 2.

Conversely, let u_0 be a 2-periodic point of P. Since K is even the time one map satisfies $\Phi(-u) = -\Phi(u)$, so $\phi^2(u_0) = u_0$. This means that u_0 is on a periodic orbit of period 2 of the flow defined by G. Since the flow is a small perturbation of the flow defined by the Hamiltonian $\alpha y^2/2$ all non-critical point periodic orbits have very long periods. Thus u_0 is a critical point.

If $\pm u_0$ is a non-degenerate maximum or minimum of G then u_0 is an elliptic critical point of the flow defined by G and $A = JDG(\pm u_0)$ has pure imaginary eigenvalues. Thus the eigenvalues of $\exp(A)$ are on the unit circle as are those of $\exp(2A)$. But $\exp(2A) = DP^2(\pm u_0)$, so the fixed point is elliptic. A similar argument shows that a non-degenerate saddle point of G corresponds to a hyperbolic periodic point of P. The converse follows by the same line of reasoning. □

Thus all we need to do is study the generic unfolding of critical points of functions like G and really just K. We will call G the *generating function.*

In Meyer [1970] the condition for a periodic doubling bifurcation was complicated by the fact that the map was not put into a normal form. Then there was one parameter, μ and $a(\mu)$, $b(\mu)$, $c(\mu)$, etc. depended on the parameter. For the one parameter case the generic assumptions are $\alpha = \pm 1$, $a(0) = 0$, $a'(0) \neq 0$ and $b(0) \neq 0$.

Here is how to interpret these conditions: (1) $\alpha = \pm 1$ means that when the map has multiplier -1 generically the higher degenerate first matrix in (2.6) can be avoided; (2) $a(0) = 0$ means that the map has the multiplier -1 when $\mu = 0$; (3) $a'(0) \neq 0$ means that the Jacobian of P passes through the second matric in (2.6) with non-zero speed and the multipliers are $\pm\sqrt{(-a\alpha\mu)} + \cdots$; (4) $b(0) \neq 0$ means the first term that cannot be made to vanish by a normalization transformation does not vanish.

With two parameters $\mu,$, ν one of the last two conditions can be violated for some specific value of the parameters. In particular we shall continue to assume $\alpha = \pm 1$, $a(0,0) = 0$. But we may have $a_\mu(0,0) = 0$ (case 1) or b(0,0)=0 (case 2). In both these cases higher dirivatives are generically nonzero.

$$\mathit{Case}\ 1: \quad \alpha = \pm 1, \quad a(0,0) = 0, \quad a_\mu(0,0) = 0, \quad a_{\mu\mu} \neq 0$$

$$a_\nu \neq 0, \quad b(0,0) \neq 0$$

The full normal form contains terms of degree six and higher, but these terms will not change the qualitative nature of the bifurcation. So we will truncate the series after the fourth order term. By Lemma 2.3 the placement and type of the periodic points do not depend on the sign of G, so by changing the sign of G if necessary the coefficient b can be made positive. Now scale the variable x so that the coefficient of x^4 is $1/4$. The values of α and a may change but not the form of G.

By assumption a is of the form $a(\mu,\nu) = d(\mu,\nu)\mu^2 + 2e(\mu,\nu)\mu\nu + f(\mu,\nu)\nu$ where $d(0,0) \neq 0$ and $f(0,0) \neq 0$. Completing the square gives

$$a(\mu,\nu) = d\{\mu + [e/d]\nu\}^2 + \{f - [e^2/d]\nu)\}\nu.$$

Change parameters by $\mu' = \sqrt{|d|}\{\mu + [e/d]\nu\}^2$ and $\nu' = -\{f - [e^2/d]\nu\}\nu$. With these parameters $a(\mu',\nu') = \beta\mu'@ - \nu'$ where $\beta = \pm 1$. Make this change of parameters and drop the primes.

The prototype generating function in this case is

$$G = \alpha y^2/2 + K(x), \qquad K(x) = -(\nu - \beta\mu^2)x^2/2 + x^4/4. \tag{2.9}$$

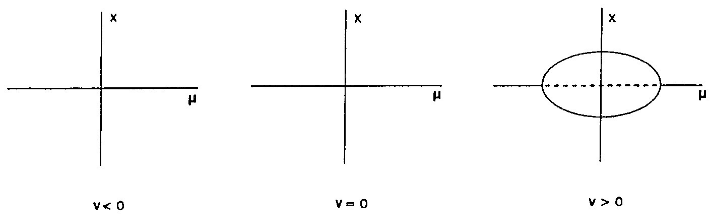

FIGURE 8. Period doubling in case 1 when $\beta > 0$.

The critical points are at the origin and at $(x, 0)$ where x satisfies

$$\nu - \beta\mu^2 = x^2 \tag{2.10}$$

This equation has two solutions (one periodic orbit of period 2) when $\nu - \beta\mu^2$ is positive, namely at

$$x = \pm\sqrt{(\nu - \beta\mu^2}, \tag{2.11}$$

and these are nondegenerate minima of K.

Since $G = \alpha y^2/2 + K(x)$ when $\alpha = +1$ a minimum of K gives rise to minimum of G and so to an elliptic point of P and a maximum of K gives rise to a saddle point of G and so to a hyperbolic point of P. When $\alpha = -1$ a minimum of K gives rise to a saddle point of G and so to a hyperbolic point of P and a maximum of K gives rise to a maximum of G and so to an elliptic point of P.

Lemma 2.4. *When $\alpha = +1$, P has an elliptic periodic point of period 2 which bifurcates from the origin when $\nu - \beta\mu^2$ is positive. When $\alpha = 11$, P has a hyperbolic periodic point of period 2 which bifurcates from the origin when $\nu - \beta\mu^2$ is positive.*

The exact nature of the bifurcation will be illustrated in the following sequence of figures. We can rewrite (2.10) as

$$\nu = \beta\mu^2 + x^2 \tag{2.12}$$

and look at the equation as the equation of a conic section in the μ, x plane. In the case $\beta = +1$ then (2.12) is the equation of a circle for $\nu > 0$. In the case $\beta = -1$ then (2.12) is two lines through the origin when $\nu = 0$ and the equation of a hyperbola when ν is nonzero. Think of the nature of the bifurcations which occur as μ varies for fixed ν. This is illustrated in the sequence of figures in Figures 8 and 9. These figures seek to illustrate the full four dimensional phase-parameter space (x, y, μ, ν). Since $y = 0$ always it will be ignored and the sequence of x, μ planes are given for different values of ν.

$x = 0$ is always a fixed point and it is hyperbolic when $\alpha(\nu - \beta\mu^2)$ is positive and elliptic when it is negative. Thus when $\beta\nu < 0$ the origin is of the same type for all μ. But when $\beta\nu > 0$ the origin changes its stability type at $\mu = \pm\sqrt{\beta\nu}$. In the Figures solid lines and

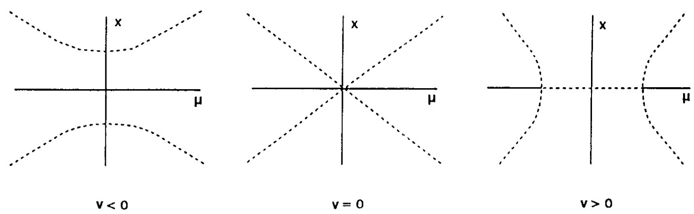

FIGURE 9. Period doubling in case 1 when $\beta < 0$.

dashed lines represent periodic points of different stability type. A bifurcation occurs when the origin changes stability type.

Figure 8 illustrates $\beta = +1$ and Figure 9 illustrates $\beta = -1$. The origin is of one stability type for all μ when $\beta\nu < 0$. When $\beta\nu > 0$ the origin has the opposite stability type for $-\sqrt{\beta\nu} < \mu < \sqrt{\beta\nu}$. The periodic point bifurcates from the origin at $\pm\sqrt{\beta\nu}$ as illustrated.

To summarize this case, if in the normal form (3), $a_\mu(\mu,\nu) = 0$ for $\mu = \nu = 0$, then for $\nu < 0$, as μ increases we find an ordinary period-doubling bifurcation which then reverses itself. If $\beta = +1$ a stable period-1 orbit goes unstable and a new stable orbit of twice the period bifurcates out of it; the new orbit moves away, then comes back to the now-unstable period-1 orbit, collides with it, and disappears, leaving the original orbit stable again. (This phenomenon was seen in a (non-Hamiltonian) electrical network by Hilborn [1990], who dubbed it "period-bubbling".) If $\beta = -1$, as μ increases, an unstable orbit of period two approaches a stable period-1 orbit, collides with it and disappears, leaving the period-1 orbit unstable; then later the unstable period-2 orbit reappears, at which point the period-1 orbit goes stable. For either sign of β, the words "stable" and "unstable" can be interchanged in the above description.

$$\textit{Case 2:}\quad \alpha = \pm 1,\ \ a(0,0) = b(0,0) = 0\ \ c(0,0) \neq 0,$$
$$a_\mu(0,0)b_\nu(0,0) - a_\nu(0,0)b_\mu(0,0) \neq 0.$$

Again truncate K in Lemma 3 2.3 at the sixth order since higher order terms will not affect the qualitative features of the bifurcations and let the coefficient $c(\mu,\nu)$ be constant for simplicity. These assumptions simply make the analysis easier. Scale by $x \to |c|^{-1/6}x$ so that the coefficient x^6 in K is $\beta = \pm 1$.

Without loss of generality we can assume that $a \equiv \mu$ and $b \equiv \beta\nu$ since the Jacobian condition $a_\mu(0,0)b_\nu(0,0) - a_\nu(0,0)b_\mu(0,0) \neq 0$ implies that $\mu' = a(\mu,\nu)$, $\nu' = \beta b(\mu,\nu)$ is a valid change of parameters. Having made the change of parameters $(\mu,\nu) \to (\mu',\nu')$ we drop the primes.

Thus in this case the generating function will be

$$G = \alpha y^2/2 + \beta K(x), \quad K(x) = \beta\mu x^2/2 + \nu x^4/4 + x^6/6. \tag{2.13}$$

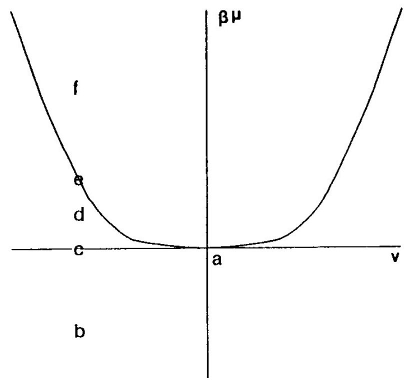

FIGURE 10. Parameter space for period doubling, case 2. $\mathcal{R} = \{0,0,0,0\}$ when $\mu = \nu = 0$ (Region a). $\mathcal{R} = \{x_1, -x_1\}, x_1 > 0$ when $\beta\mu < 0$. (Region b). $\mathcal{R} = \{x_1, 0, -x_1, 0\}, x_1 > 0$ when $\mu = 0$ and $\nu < 0$ (Region (c). $\mathcal{R} = \{x_1, x_2, -x_1, -x_2\} x_1 > x_2 > 0$ when $0 < 4\beta\mu < \nu^2$ (Region d). $\mathcal{R} = \{x_1, x_1, -x_1, -x_1\}, x_1 > 0$ when $4\beta\mu = \nu^2$ (Region e). $\mathcal{R}$ is empty otherwise (Region f).

The critical points of G are at $y = 0$ and x_0 where x_0 is a critical point of K. The critical points of K are at $x = 0$ and at solutions of

$$x^4 + \nu x^2 + \beta\mu = 0. \tag{2.14}$$

Equation (2.9) is a quadratic in x^2 so easy to solve. Roots are symmetric about the origin since (2.9) is even. Let the set of roots be $\mathcal{R}$. The following summaries are real solutions of (2.9) (the regions refer to regions in parameter space shown in Figure (10):

Since $G = \alpha y^2/2 + \beta K(x)$ when α and β are the same sign a minimum of K gives rise to minimum or maximum of G and so to an elliptic point of P and a maximum of K gives rise to saddle point of G and so to a hyperbolic fixed point of P. When α and β are of opposite sign a minimum of K gives rise to a saddle point of G and so a hyperbolic point of P a maximum of K gives rise to minimum or maximum of G and so to an elliptic point of P.

Figure 11 shows the graph of K in the various regions, and Figures 12 and 13 show the fixed points of P in the various regions.

Summarizing case 2, if $\nu < 0$ and $\alpha\beta < 0$, then as $\beta\mu$ increases through zero, we begin with a stable periodic 1 orbit with an unstable period 2 orbit nearby. The period 1 orbit goes unstable, sending out a stable period 2 orbit, which moves toward the unstable period 2 orbit; they collide and annihilate each other, leaving only the original period 1 orbit, which is now unstable. For $\alpha\beta < 0$, interchange "stable" and "unstable" in this description.

3. COMPUTATIONS

In order to illustrate the splitting of a pitchfork into a saddle-center bifurcation with a separate orbit close by, we generated Poincaré surfaces of section for the Hamiltonian

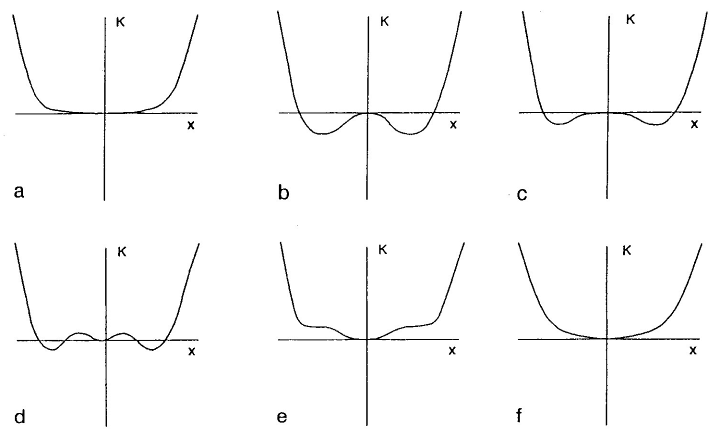

FIGURE 11. Period doubling case 2, K vs x.

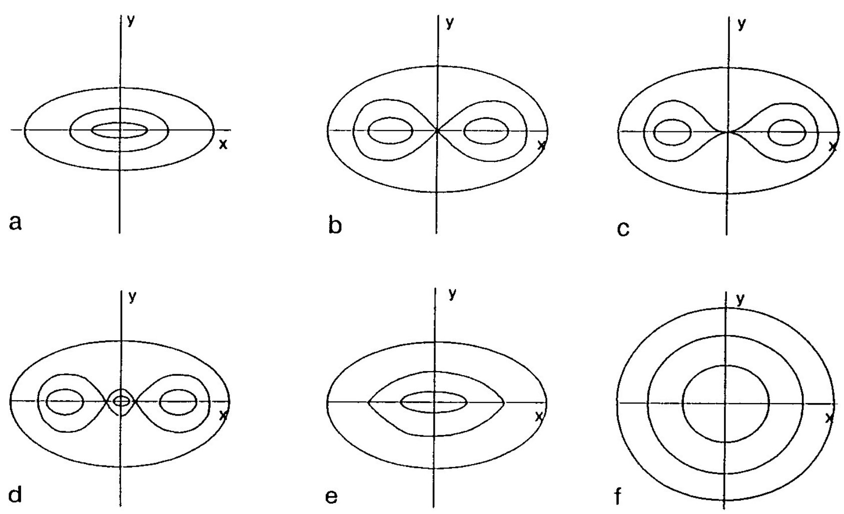

FIGURE 12. Period doubling case 2, $\alpha\beta > 0$.

H_1 near $e = -0.13$ with f small. As stated above, if $f = 0$ the potential energy has reflection symmetry, and a pitchfork bifurcation appears. For small but nonzero f, this symmetry is broken, so we might expect the nongeneric pitchfork bifurcation to be broken. The calculations told us that we have more to learn.

For $f = 0$,the SOS is shown in Figure 14. We see a stable PO in the center with two unstable PO's symmetrically placed about it. Calculations show that as e increases, these two u PO's move toward the stable PO in the center, collide with it, and disappear, leaving

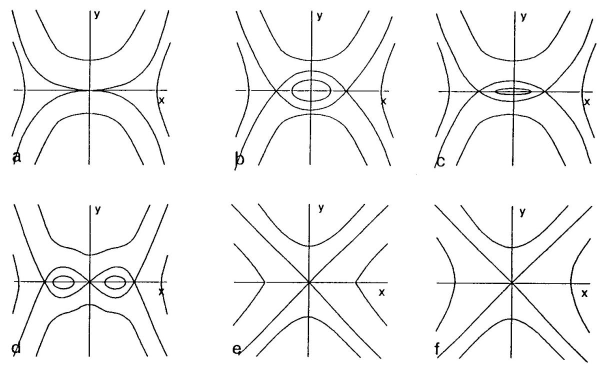

FIGURE 13. Period doubling case 2, $\alpha\beta < 0$.

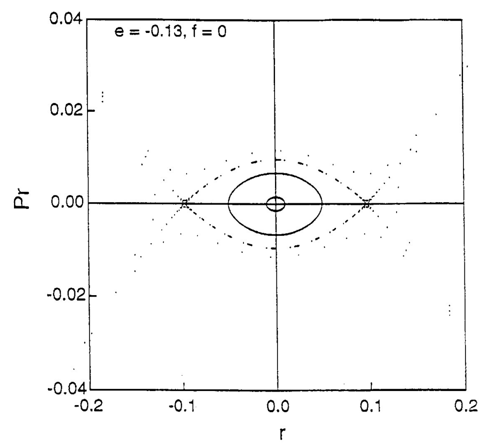

FIGURE 14. Calculated Poincaré surface of section near an "antipitchfork" bifurcation. As e increases, the two x-points will move toward the o-point, collide with it and leave a single x-point in the center.

the central orbit unstable. This is the standard "antipitchfork" bifurcation. Now we set $f = 0.001$. In (q, r) space the PO did indeed shift off the line $r = 0$. However the SOS retained its reflection symmetry about the p_r axis, and the antipitchfork structure was perfectly preserved for nonzero f (Figure 15).

We might have anticipated this. In this case, the reflection symmetry ($r \to -r$) of the SOS is induced by the inversion symmetry of the potential energy, not the reflection symmetry. The parameter f breaks that reflection symmetry but not the inversion symmetry, so it preserves the pitchfork structure.

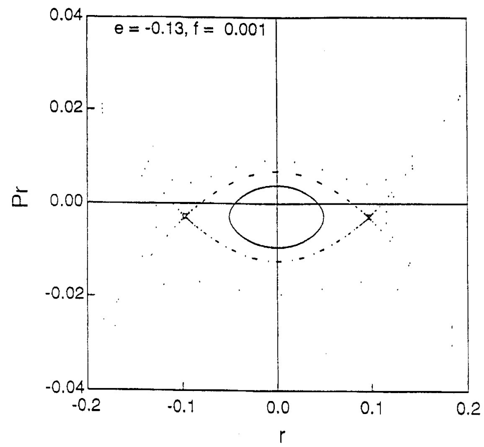

FIGURE 15. SOS for the Hamiltonian H_1 with small but nonzero f. The pitchfork structure is preserved.

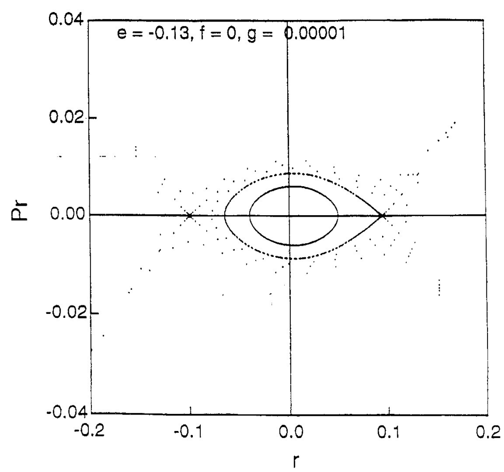

FIGURE 16. SOS for the Hamiltonian H_2. The pitchfork is broken into one of the standard forms of a cusp bifurcation.

We decided to break all the symmetries by adding to the Hamiltonian another term,

$$H_2 = H_1 + 16g(q + r/2)^5.$$

(Such a term does not arise in atomic systems, but it illustrates the theory.) A numerically-determined SOS at $e = -0.13, f = 0, g = 1 \times 10^{-5}$ is shown in Figure 16. It corresponds precisely to that predicted in Figure 4c.

A similar broken-pitchfork bifurcation was also studied by Prado and de Aguiar [1994], again by breaking symmetries in a two dimensional Hamiltonian. Another case was calculated by Schweizer et al. [1993]. They studied the bifurcations of the "parallel orbit" of an atomic electron in parallel electronic and magnetic fields. This is known to have an orderly sequence of pitchfork and period-doubling bifurcations. If the electric field is turned at small angle to the magnetic field, cylindrical symmetry is broken, the system becomes 3-dinensional, and the bifurcations have broken-pitchfork structure.

These calculations raise a fifth question, that should be added to the list in Section 1. (5) Can we list the types of two-parameter bifurcations that will be generic in the presence of symmetries? Specifically, we want a systematic way to go from symmetries of the Hamiltonian to symmetries of the normal form to symmetries of the SOS to symmetries of the bifurcations.

4. Conclusion

Experimental measurements of atomic absorption spectra display bifurcations of periodic orbits. These bifurcations often have the generic structures that are predicted by mathematical analysis. Some special, nongeneric bifurcations also occur because of the symmetries of the Hamiltonian. As symmetries are broken, nongeneric bifurcations turn into generic bifurcations in certain typical (generic) ways. Interpretation and prediction of these measurements will be aided by further development of the mathematical theory of bifurcations.

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Figure 2a was kindly provided to us by J. Main and G. Wiebusch, and Figure 2b by J. Shaw.

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Department of Mathematical Sciences, University of Cincinnati, Cincinnati, Ohio 45221

Permanent address: Physics Department, College of William and Mary, Williamsburg VA 23185, Current address: Institute for Theoretical Atomic and Molecular Physics, Harvard-Smithsonian Center for Astrophysics, 60 Garden Street, Cambridge, MA 02138

Mathematics Department, Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong