

Ghosts of Order on the Frontier of Chaos

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Then from the heart of the tempest Yahweh spoke and gave Job his answer. He said:

Brace yourself like a fighter; now it is my turn to ask questions and yours to inform me.

Where were you when I laid the earth's foundations?
Who decided the dimensions of it? Do you know?
Who laid its cornerstone when all the stars of morning were singing with joy?

Who pent up the sea when it leapt tumultuous out of the womb,
when I wrapped it in a robe of mist and made black clouds its swaddling bands?

Have you ever in your life given orders to the morning or sent the dawn to its post?

Have you journeyed all the way to the sources of the sea, or walked where the abyss is deepest?

Have you an inkling of the extent of the earth?
Which is the way to the home of the light and where does the darkness dwell?

The Jerusalem Bible

There are seven or eight categories of phenomena in the world that are worth talking about, and one of them is the weather. Any time you care to get in your car and drive across the country and over the mountains, come into our valley, cross Tinker Creek, drive up the road to the house, walk across the yard, knock on the door and ask to come in and talk about the weather, you'd be welcome.

Annie Dillard

Then we would write the beautiful letters of the alphabet, invented by smart foreigners long ago to fool time and distance.

Grace Paley

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Abstract

What kinds of motion can occur in classical mechanics? We address this question by looking at the structures traced out by trajectories in phase space; the most orderly, completely integrable systems are characterized by phase trajectories confined to low-dimensional, invariant tori. The KAM theory examines what happens to the tori when an integrable system is subjected to a small perturbation and finds that, for small enough perturbations, most of them survive.

The KAM theory is mute about the disrupted tori, but, for two-dimensional systems, Aubry and Mather discovered an astonishing picture: the broken tori are replaced by “cantori,” tattered, Cantor-set remnants of the original invariant curves. We seek to extend Aubry and Mather’s picture to higher dimensional systems and report two kinds of studies; both concern perturbations of a completely integrable, four-dimensional symplectic map. In the first study we compute some numerical approximations to Birkhoff periodic orbits; sequences of such orbits should approximate any higher dimensional analogs of the cantori. In the second study we prove converse KAM theorems; that is, we use a combination of analytic arguments and rigorous, machine-assisted computations to find perturbations so large that no KAM tori survive. We are able to show that the last few of our Birkhoff orbits exist in a regime where there are no tori.

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Chapter 1

Introduction

There is a maxim which is often quoted, that “The same causes will always produce the same effects.” ...

It follows from this, that if an event has occurred at a given time and place it is possible for an event exactly similar to occur at any other time and place.

There is another maxim which must not be confused with that quoted at the beginning of this article, which asserts “That like causes produce like effects.”

This is only true when small variations in the initial circumstances produce small variations in the final state of the system. In a great many physical phenomena this condition is satisfied; but there are other cases in which a small initial variation may produce a very great change in the final state of the system, as when the displacement of the “points” causes a railway train to run into another instead of keeping its proper course.

James Clerk Maxwell, 1877

Maxwell’s warning, that like causes need not produce like effects, can apply to even the simplest looking physical systems. Consider two equally massive stars bound in a binary system. Their orbits both lie in the same plane and, in a suitable coordinate system, their center of mass is at rest at the origin. If the orbits are nearly (but not quite) circular the system will look like the one pictured in figure (1.1). Now imagine adding a third body, a test mass so small that it does not disturb the motion of the stars. Place the test mass at the origin and give it a velocity v_0 normal to the plane

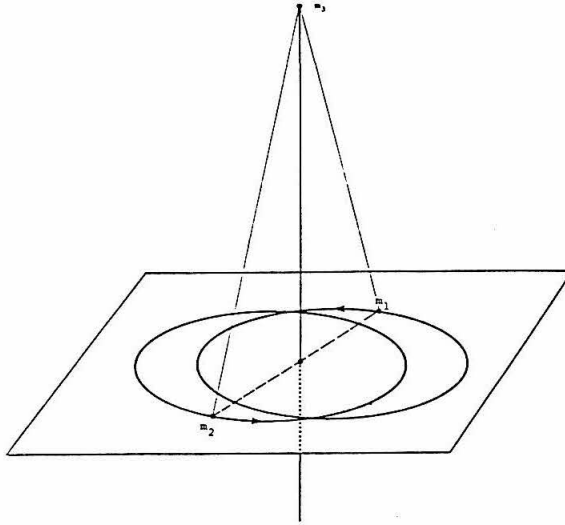


Figure 1.1: *A system of two equally massive stars, m_1 and m_2 , and a test mass, m_3 , which travels on a line through the center of mass. [Moser73]*

of the orbit. The test mass will bob up and down on the line through the origin and, if the initial velocity, v_0 , is near enough to the escape velocity, the subsequent motion of the test particle will display a fantastically sensitive dependence on the value of v_0 ; by suitable choice of v_0 one can arrange for test mass to begin in the orbital plane, spend $\approx s_1$ periods of the binary system above the plane, pass through to spend $\approx s_2$ periods below, then $\approx s_3$ above ... and so on, producing a sequence,

$$\cdots s_0, s_1, s_2 \cdots,$$

where each s_j is an integer counting the number of complete periods of the binary which pass between visits by the test mass. The s_j can be chosen completely independently, subject only to the restriction $s_j > C$ for a constant C .

This system is described by Moser in [Moser73]. He begins his study by drastically simplifying the problem; when $t = 0$ he notes the phase, θ_0 , of the binary orbit and the speed, v_0 , of the test mass, then asks for θ_1 and v_1 , the corresponding phase and speed at the instant when the test particle first returns to the orbital plane. Certainly

they depend only on θ_0 and v_0 , so he constructs some functions $\theta'(\theta, v)$ and $v'(\theta, v)$ such that

$$\theta_1 = \theta'(\theta_0, v_0) \quad \text{and} \quad v_1 = v'(\theta_0, v_0),$$

then uses them to find a sequence, $\dots(\theta_0, v_0), (\theta_1, v_1) \dots$, which captures the essential features of the dynamics. Moser shows that the wild behaviour described above occurs because the mapping,

$$(\theta, v) \rightarrow (\theta'(\theta, v), v'(\theta, v)), \tag{1.1}$$

behaves like the celebrated horseshoe example of Smale, [Smale65]. Smale constructed the horseshoe by a process of abstraction; he began by trying to understand the qualitative behaviour of a system of differential equations¹, but eventually pared away most of the original problem, leaving a simple, illuminating model of the dynamics. A detailed description of the horseshoe, along with a host of examples and criteria for recognizing horseshoe-like behaviour, appear in [Wig88]; for us it will be enough to recognize that complicated dynamics arise even in simple classical systems and that these dynamics can be explained in terms of structures in the phase space. For the rest of the thesis we will be concerned with a different relationship between structure and dynamics; we will examine how the highly structured phase space of an orderly classical system changes under perturbation.

1.1 Integrability and the KAM theorem

The most orderly of Hamiltonian systems are the *completely integrable* ones; these systems have so many constants of the motion, (N for an N -degree-of-freedom system,) that we can reformulate the problem in terms of action-angle variables² $(\boldsymbol{\theta}, \mathbf{J})$,

¹Smale gives a non-technical account of all this in one of the papers collected in [Smale80].

²We will use boldface symbols to denote n -dimensional objects, so that $\boldsymbol{\theta}$ is in \mathbf{T}^n , the n -dimensional torus, \mathbf{p} in \mathbf{R}^n . We will write θ_j for the angular coordinate of the j th image of some phase point, $(\boldsymbol{\theta}_0, \mathbf{p}_0)$, and x_j (which is in ordinary type) for the real number that is the j th

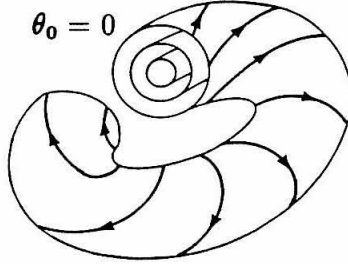


Figure 1.2: *The phase space of a completely integrable system.* [Arn78]

so that the Hamiltonian, $H(\mathbf{p}, \mathbf{q})$, becomes a function of the actions alone. Then Hamilton's equations are

$$\begin{aligned} \dot{J}_i &= -\frac{\partial H}{\partial \theta_i} = 0, \\ \dot{\theta}_i &= \frac{\partial H}{\partial J_i} \equiv \omega_i. \end{aligned} \quad (1.2)$$

Figure (1.2) illustrates the structure of the phase space for a completely integrable, 2 degree-of-freedom system. Conservation of energy restricts the motion to a three-dimensional energy surface, represented here as a solid torus. A phase trajectory winds around on a two-dimensional torus, covering it densely unless ω_1 and ω_2 are rationally dependent, that is, unless there are integers m_1 and m_2 such that

$$m_1 \omega_1 = m_2 \omega_2. \quad (1.3)$$

Tori for which (1.3) holds are called *resonant* and they are entirely covered by periodic phase trajectories.

Figure (1.2) also illustrates a construction we will use throughout the thesis, the Poincaré surface of section. This technique reduces the continuous Hamiltonian flow, (1.2), whose trajectories lie in a $(2n - 1)$ -dimensional energy surface, to a discrete-time map, T , which acts on a $(2n - 2)$ -dimensional surface. In figure (1.2), the surface component of some $\mathbf{x} \in \mathbf{R}^n$. Occasionally we will need to express, “the k th coordinate of the j th image of the phase point $(\boldsymbol{\theta}_0, \mathbf{p}_0)$.” That will be written $\theta_{j,k}$.

of section is given by $\theta_1 = 0$ and the map T carries a phase point, \boldsymbol{x} , to the next point where \boldsymbol{x}' 's trajectory intersects the surface. That is,

$$T(\boldsymbol{J}, \theta_1 = 0, \theta_2) = (\boldsymbol{J}, \theta_1 = 0, \theta_2 + 2\pi \frac{\omega_2}{\omega_1}).$$

The structures of integrability leave a clear signature on the surface of section; all the orbits of T are confined to circles, so that the orbit of a typical point hops around its circle, eventually filling it densely. Those circles that are cross sections of resonant tori are covered by periodic orbits; if a circle arises from a torus obeying a relation like (1.3), then the points on it are periodic with period m_2 and hop m_1 times around the circle before repeating.

This extremely regular structure has profound qualitative effects on the physics of the motion; integrable systems are far from satisfying the ergodic hypothesis of statistical mechanics. A phase trajectory, confined by conservation laws to an n -dimensional submanifold of the $(2n-1)$ -dimensional energy surface, does not even come close to exploring the whole of energetically accessible phase space and so predictions based on the microcanonical ensemble, which gives equal weight to all points with the same energy, will certainly be wrong. These remarks, along with the evident success of statistical mechanics, suggest that complete integrability must be rare, that most of the structure of integrability cannot survive perturbation. Indeed, Fermi believed that the slightest perturbation would completely disrupt integrability, [FPU55].

The fate of invariant tori is, however, much more complicated and wonderful; it is the subject of the most spectacular theorem in Hamiltonian dynamics.

Theorem (Kolmogorov-Arnold-Moser)

If an unperturbed (completely integrable) system is non-degenerate³, then for suffi-

³The non-degeneracy condition is that

$$\det \left| \frac{\partial \boldsymbol{\omega}}{\partial \boldsymbol{J}} \right| = \det \left| \frac{\partial^2 H_0}{\partial \boldsymbol{J}^2} \right| \neq 0,$$

ciently small conservative Hamiltonian perturbations, most non-resonant tori do not vanish, but are only slightly deformed, so that in the phase space of the perturbed system, too, there are invariant tori densely filled with phase curves winding around them conditionally-periodically, with a number of independent frequencies equal to the number of degrees of freedom. These invariant tori form a majority in the sense that the measure of the complement of their union is small when the perturbation is small.

That is, most tori survive small perturbations! The statement above is taken from textbook by Arnold, [Arn78]; His original proof appears in [Arn63]. Moser's book, [Moser73], offers a readable account, and [Bost86] gives a recent review.

1.2 The Taylor-Chirikov standard map

We conclude our introduction with a brief review of an exhaustively studied example, the Taylor-Chirikov standard map. It is a two-dimensional, area-preserving map acting on the set $S^1 \times \mathbf{R} = \{(x, p) | x \in [0, 1), p \in \mathbf{R}\}$.

$$\begin{aligned} p' &= p - \frac{k}{2\pi} \sin(2\pi x), \\ x' &= x + p' \bmod 1. \end{aligned} \tag{1.4}$$

Chirikov [Chkv79] describes this example as a periodically-kicked rotor, sampled at the frequency of the kicking; x is a normalized angle variable with p the corresponding angular momentum. Chirikov's rotor receives periodic, impulsive blows whose size and direction depend on the rotor's angular position at the moment the impulse is delivered. For $k = 0$, the system is completely integrable; p is a constant of the motion and the orbits are confined to one-dimensional curves.

Figure (1.3) shows the structure of the phase space for various values of the perturbation. Each panel shows the orbits of several points from the the set $\{(x, p) | x \in \underline{\hspace{2cm}}\}$ where $H_0(\mathbf{J})$ is the unperturbed Hamiltonian. It means that the $\omega_i(\mathbf{J})$ are independent as functions.

$[0, 1)$, $p \in [0, 1)$. Here we will give a qualitative discussion of these pictures, at the same time introducing ideas that we will study fully in later chapters. The series begins in the top panel with a small perturbation; many orbits still seem to lie on or between circles. The arcs in the corners of the picture, when associated by periodic boundary conditions, form ovals encircling the fixed point $z_0 \equiv (x = 0, p = 0)$. The ovals arise because z_0 is an *elliptic* fixed point; that is, the derivative of the map,

$$DT = \begin{bmatrix} \frac{\partial x'}{\partial x} & \frac{\partial x'}{\partial p} \\ \frac{\partial p'}{\partial x} & \frac{\partial p'}{\partial p} \end{bmatrix},$$

is such that the matrix DT_{z_0} has its eigenvalues on the unit circle. Consequently, points that start near z_0 stay nearby and their orbits form the arcs. If we were to restrict our attention to this *elliptic island* we would find that it has much the same structure as the whole phase space; the ovals would play the role of invariant circles and between them would lie yet smaller elliptic islands. If we magnified one of those islands ... the structure goes on forever. There is also another fixed point, at $z_1 \equiv (x = \frac{1}{2}, p = 0)$, but it is *hyperbolic*; the matrix DT_{z_1} has eigenvalues off the unit circle, so almost every orbit that begins near it eventually moves away with exponential speed. Besides the fixed points, there are always at least two periodic orbits for every rational rotation number $\frac{p}{q}$. Chapter 2 gives a longer and more technical discussion of periodic orbits and also discusses some special sets, the *cantori*, which are, in a sense, the ghosts of disrupted tori. The chapter begins with a review of the two-dimensional theory then shows some numerical work aimed at higher dimensional generalizations.

In the middle panel, many more elliptic islands are evident, as is a broad *stochastic layer*, a region that no longer contains any invariant tori; the orbits in such a region are quite complicated and chaotic, and are confined to a layer only because the phase space is two-dimensional and thus the invariant circles divide phase space into two disjoint pieces and so pairs of circles can trap even very chaotic orbits. In higher-

dimensional systems the tori have too low a dimension to isolate parts of the phase space; points not actually contained in tori are free to diffuse throughout the whole stochastic part of the phase space, though they do so only very slowly, in a process called *Arnold diffusion* [Arn64,Nekh71]. Although we will not have much more to say about Arnold diffusion, we will have cause to consider the topological consequences of higher dimension; in both the remaining chapters we will find that topology prevents us from proving results as strong as those available for two dimensional systems.

The final panel shows a perturbation large enough to guarantee very strong chaos; k is so large that Mather, [Ma84], has shown analytically that no invariant circles (of the type that wind all the way around the cylinder) remain. Numerical experiments by Greene suggest that no circles exist for $|k| > k_c \approx 0.971635406$. We leave this subject for the moment, but Chapter 3 is entirely devoted to converse KAM results, theorems that say, as Mather does, that for large enough perturbations, no tori exist at all. There we will review Mather's work, as well as the computer-assisted arguments of MacKay and Percival, then discuss higher-dimensional generalizations and show some new results.

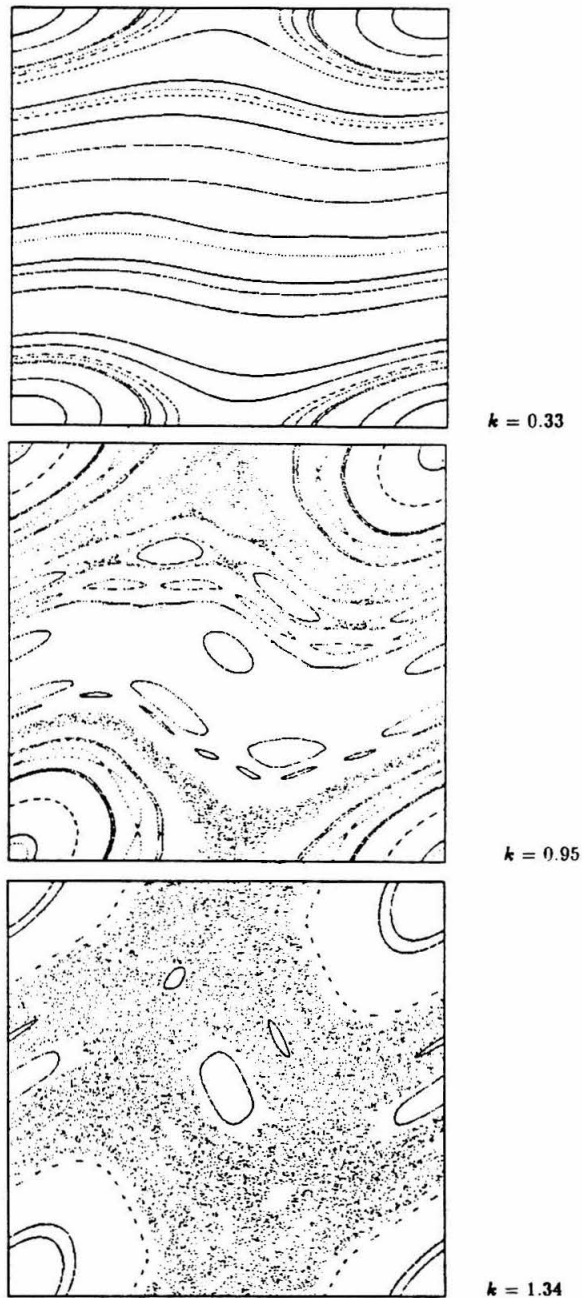


Figure 1.3: *Orbits of the standard map for several sizes of the perturbation k . Each panel shows 200 iterates from the orbits of 20 different initial conditions.*

Chapter 2

Ghosts of Order

In this chapter we ask, “What becomes of invariant tori?” We have seen that the phase space of completely integrable Hamiltonian systems is filled by such tori and that the KAM theory assures us that some of them persist even in the face of small perturbations. What becomes of the nonresonant tori for which KAM fails? In general, one can’t say. But for certain two-dimensional, area-preserving maps Mather [Ma82a] and, independently, Aubry [Aub83a], demonstrated the existence of some remarkable sets. They are reminiscent of invariant tori, but are not complete curves, rather, they look like graphs supported above a Cantor set. Orbits on these “cantori” are similar to rotation on an invariant torus; one may consider Mather’s sets the ghosts of destroyed invariant tori. Here we review the two-dimensional results, then present some numerical investigations¹ from an effort to find the higher-dimensional analogs of Mather’s sets. At the end of the chapter we discuss a topological obstacle that prevents simple generalization of the Aubry-Mather theory.

¹Kook and Meiss, [KM88], have reported similar studies; J. Meiss has been especially helpful in discussing this work.

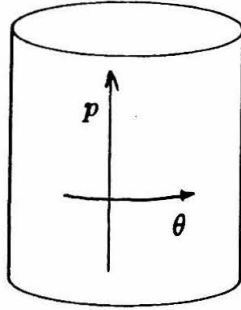


Figure 2.1: *The cylinder and its coordinate system.*

2.1 Basic Notions and Notations

In this section we give careful definitions of the maps we will study, the spaces they will act on, and the tools we will use to understand them. We will also review the two-dimensional theory, describing cantori and explaining how to approximate them by periodic orbits. In the course of the review we will introduce a variational principle that will be the foundation of all our work.

2.1.1 spaces and maps

We will study maps based on the Poincaré map of a near-integrable, action-angle system and so they will act on the *n-dimensional multi-annulus*, $\mathbf{A}^n = \mathbf{T}^n \times \mathbf{R}^n$, where \mathbf{T}^n is the *n-torus* and \mathbf{R}^n is *n-dimensional Euclidean space*. To avoid having to worry about factors of 2π , we will always normalize the angles, and so write points in \mathbf{A}^n as $(\boldsymbol{\theta}, \mathbf{p})$ where $\boldsymbol{\theta} = (\theta_1, \theta_2 \dots \theta_n)$ and the θ_i are periodic coordinates with period 1.

The one-dimensional annulus, $\mathbf{A} = \mathbf{T} \times \mathbf{R}$, is conveniently represented as a cylinder with coordinates as pictured in figure (2.1). Maps taking the cylinder to itself will be called T , or T_ϵ if they depend on parameters; maps acting on \mathbf{A}^n for $n > 1$ will be either f or f_ϵ . In all cases, our maps will be *symplectic*, that is, they will preserve

the standard symplectic form (see e.g. [Arn78,KB87]),

$$\Omega = \sum_{j=1}^n d\theta_j \wedge d\mathbf{p}_j. \quad (2.1)$$

For a map T on the cylinder, preservation of (2.1) means that T preserves area and orientation and so is equivalent to Liouville's theorem about the preservation of volume in phase space. For higher-dimensional systems, preservation of (2.1) also implies preservation of volume, but is stronger.

We will often need to work with a *lifting*, F_ϵ , of a symplectic map, f_ϵ , to the universal cover of \mathbf{A}^n . This is essentially a version of f_ϵ extended periodically so that it acts on the whole of $\mathbf{R}^n \times \mathbf{R}^n$. If $f_\epsilon : \mathbf{A}^n \rightarrow \mathbf{A}^n$, $f_\epsilon(\boldsymbol{\theta}, \mathbf{p}) = (\boldsymbol{\theta}'(\boldsymbol{\theta}, \mathbf{p}), \mathbf{p}'(\boldsymbol{\theta}, \mathbf{p}))$ then F_ϵ acts on $\mathbf{R}^n \times \mathbf{R}^n$, $F_\epsilon(\mathbf{x}, \mathbf{p}) = (\mathbf{x}'(\mathbf{x}, \mathbf{p}), \mathbf{p}'(\mathbf{x}, \mathbf{p}))$, and agrees with f_ϵ up to an integer translation. That is, if $f_\epsilon(\boldsymbol{\theta}_0, \mathbf{p}_0) = (\boldsymbol{\theta}_1, \mathbf{p}_1)$ and $F_\epsilon(\mathbf{x}_0 = \boldsymbol{\theta}_0, \mathbf{p}_0) = (\mathbf{x}_1, \mathbf{p}_1)$ then

$$\mathbf{x}_1 - \boldsymbol{\theta}_1 = \mathbf{m} \quad (2.2)$$

for some integer vector $\mathbf{m} \in \mathbf{Z}^n$. Further,

$$F_\epsilon(\mathbf{x}_0 + \mathbf{m}, \mathbf{p}_0) = F_\epsilon(\mathbf{x}_0, \mathbf{p}_0) + \mathbf{m}.$$

The choice of a lift, F_ϵ , which comes down to the choice of \mathbf{m} in (2.2) does not affect any qualitative features of the dynamics. For example, a lift of the standard map is

$$\begin{aligned} p' &= p - \frac{k}{2\pi} \sin(2\pi x), \\ x' &= x + p', \end{aligned}$$

which is just the same as (1.4) except that the position coordinate is no longer taken mod 1. We will always use the convention that $F_\epsilon : \mathbf{R}^n \times \mathbf{R}^n$ is a lift of $f_\epsilon : \mathbf{A}^n \rightarrow \mathbf{A}^n$.

2.1.2 a variational principle

The dynamics of an autonomous Hamiltonian system can be characterized with the principle of least action; to specify a segment of a phase trajectory, $\gamma(t) = (\mathbf{p}(t), \mathbf{q}(t))$,

one need only note the values of the position coordinates at the ends of the segment and require that γ be an extremal of the “reduced action” functional [Arn78],

$$S(\mathbf{q}_0, \mathbf{q}_1) = \int_{\mathbf{q}_0}^{\mathbf{q}_1} \mathbf{p} d\mathbf{q}. \quad (2.3)$$

In particular, one can get the momenta at the endpoints of the segment by taking derivatives of $S(\mathbf{q}_0, \mathbf{q}_1)$;

$$\mathbf{p}_1 = \frac{\partial S}{\partial \mathbf{q}_1} \quad \text{and} \quad \mathbf{p}_0 = -\frac{\partial S}{\partial \mathbf{q}_0}.$$

The analogous thing for a symplectic map $F_\epsilon : \mathbf{R}^n \rightarrow \mathbf{R}^n$ is an *action-generating function*, a function, $H_\epsilon : \mathbf{R}^n \times \mathbf{R}^n \rightarrow \mathbf{R}$, where $H_\epsilon = H_\epsilon(\mathbf{x}, \mathbf{x}')$ is such that if $F_\epsilon(\mathbf{x}_0, \mathbf{p}_0) = (\mathbf{x}_1, \mathbf{p}_1)$, then

$$\mathbf{p}_1 = \frac{\partial H_\epsilon}{\partial \mathbf{x}'} \quad \text{and} \quad \mathbf{p}_0 = -\frac{\partial H_\epsilon}{\partial \mathbf{x}} \quad (2.4)$$

The point of constructing a generating function is that it enables us to discuss dynamics entirely in terms of the position coordinates. In the next section we will demonstrate the usefulness of variational arguments by reviewing the theory of area-preserving twist maps of the cylinder. These maps get their name because of a geometric property of their action; a C^1 map T is *twist* if it carries every vertical line into a monotone curve; see figure (2.2). More analytically, if $T(\theta, p) = (\theta'(\theta, p), p'(\theta, p))$ is a symplectic map of the cylinder, then T is a uniform, differentiable, twist map if

$$\frac{\partial \theta'}{\partial p} \neq 0.$$

2.1.3 area-preserving twist maps

Here we will examine the kinds of orbits that can occur for an area-preserving twist map. Since we will be wanting to make variational arguments, we require that, in addition to being a twist map, T possess a generating function, $h(x, x')$. For

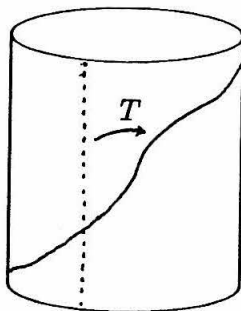


Figure 2.2: A twist map carries vertical lines to monotone curves.

convenience, we will work with a lift of T , call it \tilde{T} , and will use coordinates in $\mathbf{R} \times \mathbf{R}$ rather than on the cylinder. First we will use the generating function to construct some periodic orbits.

A periodic orbit is characterized by its period and by the number of times it winds around the cylinder before closing. Suppose we want an orbit that, in q steps, makes p turns. Such an orbit would appear on the universal cover as a sequence of points $\{\cdots(x_0, p_0), (x_1, p_1), \cdots(x_{q-1}, p_{q-1}), (x_p, q_p), \cdots\}$ with $x_{j+q} = x_j + p$. We could seek it by trying to find a sequence of position coordinates,

$$X = \{x_0, x_1, \dots, x_{q-1}, x_q; x_q = x_0 + p\}, \quad (2.5)$$

such that the function

$$L_{p,q}(X) = \sum_{j=0}^{q-1} h(x_j, x_{j+1}) \quad (2.6)$$

was minimized. We will call such a sequence a p - q *minimizing state*. If we could find one, then, automatically, we could compute the desired kind of periodic orbit. To see how, consider the condition that (2.6) be extremal:

$$\frac{\partial L_{p,q}}{\partial x_j} = \frac{\partial h}{\partial x}(x_j, x_{j+1}) + \frac{\partial h}{\partial x'}(x_{j-1}, x_j) = 0 \quad \text{for } j = 0, 1, \dots, q-1. \quad (2.7)$$

We will call these the *Euler-Lagrange equations*. Now, if X were the projection of some periodic orbit, we would be able to recover the missing momentum coordinates in two ways; we could use either

$$p_j = \frac{\partial h}{\partial x'}(x_{j-1}, x_j) \quad \text{or} \quad p_j = -\frac{\partial h}{\partial x}(x_j, x_{j+1}).$$

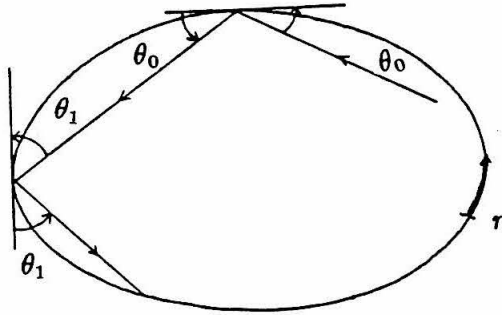


Figure 2.3: *The billiard ball dynamical system.* [Birk27]

The condition (2.7) is that these two be equal, so that if we can find a sequence like (2.5) we have found the desired periodic orbit. Arguments like this were first made by Birkhoff, who used them to construct periodic orbits for the map given by the motion of a point particle in a convex, rigid walled box. This system can be reduced to an area preserving twist map by considering the particle's collisions with the wall and using coordinates given by a length, r measured along the perimeter of the domain, and the variable $\sigma = -\cos(\theta)$ where θ is the angle the particle's path makes with the tangent to the wall, see figure (2.3). In this system the generating function is just the negative of the length of the path traced by the ball, and so the minimizing periodic orbit with $p = 2, q = 5$ is just the orbit that corresponds to the longest inscribed star. Besides the minimizing periodic orbit, there is another, a *minimax* orbit. To see how this orbit arises take one point of the minimizing orbit and slide it along the boundary, allowing the other points to shift so as to keep the total length of the star as large as possible. At first the length must decrease; we have assumed that the initial, undistorted star was the longest possible. Eventually, though, the length of the distorted star will have to stop decreasing and begin to increase because eventually the vertices will reach a configuration which is a cyclic permutation of the original star. The configuration for which the length again begins to increase must also be a stationary point of $L_{p,q}$; it satisfies the Euler-Lagrange equations and so it too corresponds to a genuine periodic orbit.

The action-minimizing periodic orbits, which are called *Birkhoff orbits*, are dis-

tinguished by the numbers p and q used in their construction. The rational number $\frac{p}{q}$, which is the orbit's average angular speed, is called the *rotation number* of the orbit. More generally, an orbit $(x_0, p_0), (x_1, p_1), \dots$ on the universal cover is said to have rotation number α if

$$\alpha = \lim_{n \rightarrow \infty} \frac{x_n - x_0}{n}. \quad (2.8)$$

This limit does not always exist. Most of the points in the stochastic regions of the standard map do not have well-defined rotation numbers, though all of the orbits lying on invariant circles do; orbits on non-resonant circles have irrational α .

Percival, who, in [Perc79], coined the term “cantorus,” proposed that one might be able to find orbits that had irrational rotation numbers, but did not lie on invariant tori. Mather looked for Percival's quasiperiodic orbits and, in [Ma82a], succeeded dramatically. He discovered whole, complicated sets of such orbits and revealed an unexpected, rich structure in the phase space. Serge Aubry, a condensed matter physicist who was investigating the ground states of certain one-dimensional models, independently discovered the same structures, see e.g., [Aub83a, Aub83b].

We can construct one of Mather's sets by taking a limit of Birkhoff periodic orbits. That is, we take a sequence of rational numbers $\{p_0/q_0, p_1/q_1 \dots\}$ that has an irrational ω as a limit, construct both the corresponding Birkhoff orbits, and see whether they accumulate on an interesting limit set. Katok, [Kat82], has shown that they do. If there is an invariant circle with rotation number ω , then the Birkhoff orbits accumulate on it. If there is no invariant circle, then the orbits accumulate on a cantorus,² a set that looks like an invariant circle with a countable set of holes cut out of it, see figure (2.4).

The cantori have many properties reminiscent of irrational invariant circles; orbits lying in the cantorus are dense and the motion on the cantorus, is, by a continuous change of coordinate, equivalent to rotation by the angle ω . Also, the cantorus has

²The limit set may also include some points in the gaps of the cantorus; to get the true cantorus one has to take a minimal (in the sense of ergodic theory) subset of the limit set.

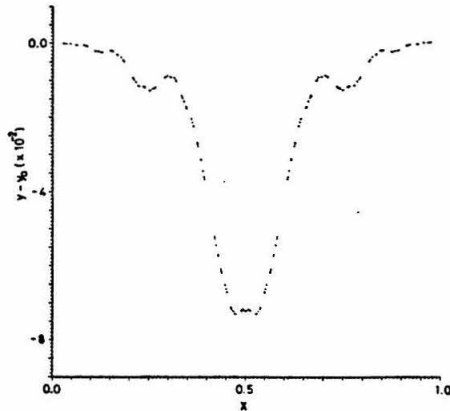


Figure 2.4: *A cantorus for the standard map. The vertical axis is measured in units of $y = p - \frac{k}{4\pi} \sin(2\pi x)$, where $k = 1.001635$ is the size of the perturbation and the rotation number is $\approx \frac{1}{\gamma^2}$ where $\gamma = \frac{1+\sqrt{5}}{2}$ is the golden mean. [MMP84]*

the same kind of smoothness³ as an invariant circle. If (θ_0, p_0) and (θ_1, p_1) are any two points from the cantorus then there is a constant L , independent of the θ s, such that

$$|p_0 - p_1| \leq L|\theta_0 - \theta_1|,$$

that is, the momenta are Lipschitz functions of the positions.

Katok's scheme for approximating the cantorus by a sequence of periodic orbits is different from the approach first used by Mather, but it is much better suited to numerical experiment; all computational investigations of cantori depend on approximation by periodic orbits e.g. [MMP84,MP87,Grn79].

2.2 Higher-dimensional analogs

In this section we formulate the numerical investigations reported in the rest of the chapter. Our studies are based on Katok and Bernstien's paper, [KB87] in which they study certain n -dimensional symplectic maps generated by a function $H_\epsilon(\mathbf{x}, \mathbf{x}')$ and prove the existence of action-minimizing periodic orbits. For these orbits, which are

³A theorem of Birkhoff states that the invariant circles are Lipschitz graphs.

defined by analogy with the Birkhoff orbits on the cylinder, the role of the rational rotation number $\frac{p}{q}$ is played by a *rotation vector*, $\frac{\mathbf{p}}{q}$ where q is the length of the orbit and $\mathbf{p} \in \mathbf{Z}^n$, $\mathbf{p} = (p_0, p_1, \dots, p_n)$ gives the number of times the orbit winds around each of the coordinate directions.⁴ As above, each rational vector has a corresponding type of p, q -minimizing state,

$$X = \mathbf{x}_0, \mathbf{x}_1, \dots, \mathbf{x}_{q-1}, \mathbf{x}_q; \mathbf{x}_q = \mathbf{x}_0 + \mathbf{p}$$

an action functional, $L_{p,q}$, some Euler-Lagrange equations,

$$L_{p,q}(X) = \sum_{j=0}^{q-1} H_\epsilon(\mathbf{x}_j, \mathbf{x}_{j+1}) \quad (2.9)$$

$$\frac{\partial L_{p,q}}{\partial \mathbf{x}_j} = \frac{\partial H_\epsilon}{\partial \mathbf{x}'}(\mathbf{x}_{j-1}, \mathbf{x}_j) + \frac{\partial H_\epsilon}{\partial \mathbf{x}}(\mathbf{x}_j, \mathbf{x}_{j+1}), \quad (2.10)$$

and at least one minimizing periodic orbit. Katok and Bernstien's maps are small perturbations of some completely integrable system whose unperturbed generating function, $H_0(\mathbf{x}, \mathbf{x}')$, satisfies $H_0(\mathbf{x}, \mathbf{x}') = h(\mathbf{x}' - \mathbf{x})$ where $h(\mathbf{u})$ is strictly convex, i.e., the Hessian matrix of h ,

$$\frac{\partial^2 h}{\partial \mathbf{u}^2} = \begin{bmatrix} \frac{\partial^2 h}{\partial u_0^2} & \frac{\partial^2 h}{\partial u_0 \partial u_1} & \dots & \frac{\partial^2 h}{\partial u_0 \partial u_{n-1}} \\ \frac{\partial^2 h}{\partial u_1 \partial u_0} & \frac{\partial^2 h}{\partial u_1^2} & \dots & \vdots \\ \vdots & & \ddots & \\ \frac{\partial^2 h}{\partial u_{n-1} \partial u_0} & \dots & & \frac{\partial^2 h}{\partial u_{n-1}^2} \end{bmatrix}, \quad (2.11)$$

is positive definite. This condition is a higher dimensional analog of the twist condition, but is not the only possible generalization; Herman, in [Herm88], gives another. In the next section we will present some explicit 4-d symplectic maps and their generating functions and in section 2.2.2 we show some pictures of minimizing periodic orbits and discuss how their shapes and stability depend on the size of the perturbation.

⁴For a two-dimensional Birkhoff periodic orbit, the rotation numbers $\frac{p}{q}$ and $\frac{2p}{2q}$ both yield the same minimizing periodic orbit. The corresponding statement need not be true in higher dimension; the rotation vectors $\frac{\mathbf{p}}{q}$ and $\frac{2\mathbf{p}}{2q}$ need not correspond to the same orbit. See section 2.3.

The real question here is “Are there cantori in 4-d symplectic maps?” On the analytic side, the answer seems to be “maybe.” Katok and Bernstien are able to show that if a sequence of rational rotation vectors $\{\frac{\mathbf{p}_0}{q_0}, \frac{\mathbf{p}_1}{q_1}, \dots\}$, $\mathbf{p}_i \in \mathbf{Z}^n, q \in \mathbf{Z}$, converges to some irrational rotation vector, $\boldsymbol{\omega} = (\omega_1, \omega_2, \dots, \omega_n)$, then the corresponding sequence of Birkhoff orbits also has a limit. Unfortunately their results on the properties of the limiting set are not as strong as those available for twist maps. They cannot say what the limiting set looks like or much about the motion on it. They are able to establish that the momenta should be Hölder continuous functions of the positions, but with index $\alpha = \frac{1}{2}$, that is, if $(\boldsymbol{\theta}_0, \mathbf{p}_0)$ and $(\boldsymbol{\theta}_1, \mathbf{p}_1)$ are points from this limit set, then, except perhaps for a single isolated point,

$$\|\mathbf{p}_0 - \mathbf{p}_1\| \leq C \|\boldsymbol{\theta}_0 - \boldsymbol{\theta}_1\|^{\frac{1}{2}}, \quad (2.12)$$

for some constant C , independent of the $\boldsymbol{\theta}_i$. We present some ambiguous numerical investigations aimed at verifying or improving this smoothness estimate, but are unable to report any definite results.

Finally, in section 2.3 we discuss a pathology foreseen by Hedlund. Hedlund’s examples complicate any discussion of the behaviour of very long orbits and are an obstacle to both analytic and numerical investigation of higher-dimensional cantori. These examples arise in the study of geodesics on tori, a problem related to ours by the principle of least action. The pathology appears for very strongly curved metrics; the corresponding regime for our problem is the realm of very strongly perturbed, far-from-integrable motion. Since we will study only small perturbations of integrable systems, we may hope to avoid Hedlund’s pathology; in section 2.3, we report some qualitative investigations indicating that, for our systems, it does not occur.

2.2.1 the maps and orbits

We follow [KB87] and study maps that are generated by functions of the form

$$H_\epsilon(\mathbf{x}, \mathbf{x}') = h(\mathbf{x}' - \mathbf{x}) - V_\epsilon(\mathbf{x}, \mathbf{x}'), \quad (2.13)$$

where $h(\mathbf{x}' - \mathbf{x}) : \mathbf{R}^n \rightarrow \mathbf{R}$, the unperturbed part of the generating function, satisfies (2.11) and the perturbation $V_\epsilon(\mathbf{x}, \mathbf{x}') : \mathbf{R}^n \times \mathbf{R}^n \rightarrow \mathbf{R}$, is a small, C^2 function satisfying $V_\epsilon(\mathbf{x} + \mathbf{m}, \mathbf{x}' + \mathbf{m}) = V_\epsilon(\mathbf{x}, \mathbf{x}') \forall \mathbf{m} \in \mathbf{Z}^n$. We will study 4-d symplectic maps generated by (2.13) with

$$h(\mathbf{x}, \mathbf{x}') = \frac{1}{2} \|\mathbf{x}' - \mathbf{x}\|^2, \quad V_\epsilon(\mathbf{x}, \mathbf{x}') = \epsilon V(\mathbf{x}).$$

Where

$$V(\mathbf{x}) = \begin{cases} \text{one of} \\ V_{trig}(\mathbf{x}) = -\frac{1}{M_{trig}} \left\{ \frac{1}{2}(\sin 2\pi x_0 + \sin 2\pi x_1) + \sin 2\pi(x_0 + x_1) \right\}, \\ \\ V_{poly}(\mathbf{x}) = -\frac{1}{M_{poly}} \left\{ [x_0^2(1-x_0)^2(x_0 - \frac{3}{4})(\frac{1}{4} - x_0)] [x_1^2(1-x_1)^2] \right\}, \\ \text{or} \\ V_{ff}(\mathbf{x}) = -\frac{1}{2} \left\{ \frac{1}{2}(c(x_0) + c(x_1)) + c(x_0 + x_1) \right\}, \\ \\ \text{with} \quad c(x) = \begin{cases} 1 - 24x^2 + 32x^3 & \text{if } x \bmod 1 \leq \frac{1}{2}, \\ 9 - 48x + 72x^2 - 32x^3 & \text{if } x \bmod 1 > \frac{1}{2}. \end{cases} \end{cases} \quad (2.14)$$

Call the first perturbation the *trigonometric* perturbation, the second the *polynomial* perturbation⁵ and the third the *fast-Froeschlé*. The constants M_{trig} and M_{poly} are chosen so that $\max_{\mathbf{x} \in \mathbf{T}^n} |V(\mathbf{x})| = 1$. $V_{ff}(\mathbf{x})$ is a polynomial approximation to a potential originally introduced as a model of star motion in elliptical galaxies [Fro71]. The real Froeschlé map has cosines where ours has $c(x)$ and has three independent constants,

⁵The x_i appearing in the definition of V_{poly} are all taken mod 1.

one for each of the terms. Since its introduction the map has been popular as a model for chaotic Hamiltonian dynamics e.g., [Fro72,Fro73,KnBg85,KM88,MMS89].

All our examples use “standard-like” perturbations, ones where $V_\epsilon(\mathbf{x}, \mathbf{x}')$ depends on \mathbf{x} but not on its successor, \mathbf{x}' . We made this choice of perturbation because it simplifies the map. Using (2.4) we obtain

$$\begin{aligned}\mathbf{p}'(\mathbf{x}, \mathbf{p}) &= \mathbf{p} - \epsilon \frac{\partial V}{\partial \mathbf{x}}(\mathbf{x}), \\ \mathbf{x}'(\mathbf{x}, \mathbf{p}) &= \mathbf{x} + \mathbf{p} - \epsilon \frac{\partial V}{\partial \mathbf{x}}(\mathbf{x}).\end{aligned}\tag{2.15}$$

2.2.2 shapes of orbits and Lyapunov exponents

Figures (2.7) - (2.16) present several families of approximate Birkhoff orbits. Each orbit is displayed as a pair of projections; one, on the left, is the projection into the angular coordinates, the other, on the right, shows the momenta. Both projections are computed from a p, q -periodic state that is an approximate solution to the Euler-Lagrange equation (2.10). The angular projection of a point \mathbf{x}_j is an ordered pair $(\theta_{j,0}, \theta_{j,1})$, with

$$\theta_{j,i} = x_{j,i} \bmod 1;$$

The horizontal is the θ_0 direction and the vertical the θ_1 ; both angles lie between 0.0 and 1.0. The momenta, which are calculated as

$$\mathbf{p}_j = -\frac{\partial H_\epsilon}{\partial \mathbf{x}}(\mathbf{x}_j, \mathbf{x}_{j+1}),\tag{2.16}$$

are arranged similarly; the horizontal is the p_0 direction and the vertical the p_1 .

measures of quality

Beside each pair of projections appears the rotation vector, in the form $(p_0, p_1)/q$, and two measures of the quality of the orbit, *shadow* and *grad size*. The first of these

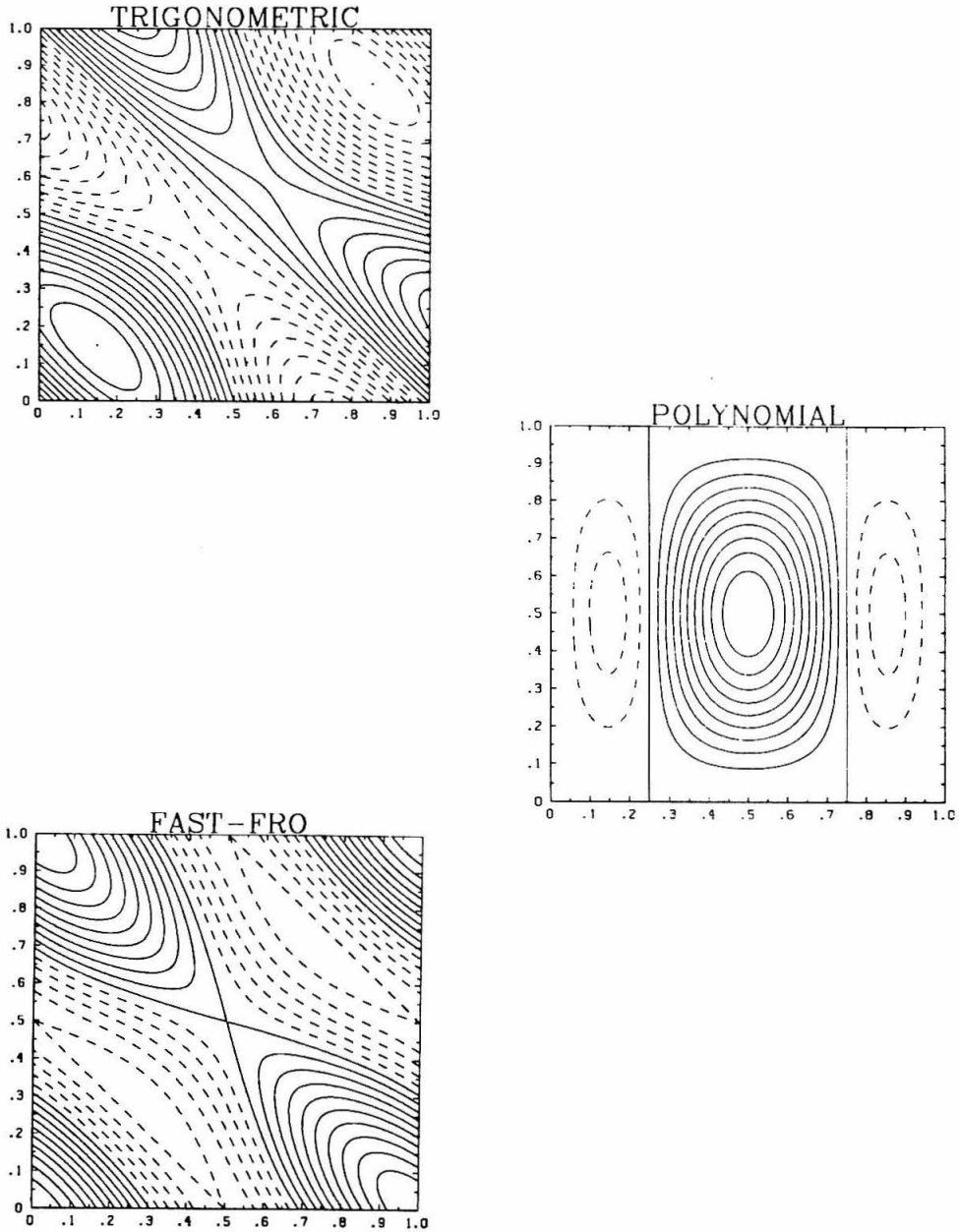


Figure 2.5: Contour maps of $-V_\epsilon(\mathbf{x})$ for the (a) trigonometric, (b) polynomial, and (c) fast-Froeschlé perturbations. The contour interval is 0.1 and the contours corresponding to negative values are dashed.

measures how closely our orbit, which has its momenta given by (2.16), approaches the ideal

$$\begin{aligned} (\mathbf{x}_{j+1}, \mathbf{p}_{j+1}) &= F_\epsilon(\mathbf{x}_j, \mathbf{p}_j), \\ &= (\mathbf{x}'(\mathbf{x}_j, \mathbf{p}_j), \mathbf{p}'(\mathbf{x}_j, \mathbf{p}_j)); \end{aligned}$$

the value of *shadow* is

$$\begin{aligned} &\max_{0 \leq j \leq q-1} \| (\mathbf{x}_{j+1}, \mathbf{p}_{j+1}) - F_\epsilon(\mathbf{x}_j, \mathbf{p}_j) \| \\ &= \max_{0 \leq j \leq q-1} \sqrt{\| \mathbf{x}_{j+1} - \mathbf{x}'(\mathbf{x}_j, \mathbf{p}_j) \|^2 + \| \mathbf{p}_{j+1} - \mathbf{p}'(\mathbf{x}_j, \mathbf{p}_j) \|^2} \\ &= \max_{0 \leq j \leq q-1} \sqrt{\sum_{k=0}^1 (x_{j+1,k} - x'(\mathbf{x}_j, \mathbf{p}_j)_k)^2 + (p_{j+1,k} - p'(\mathbf{x}_j, \mathbf{p}_j)_k)^2}. \end{aligned}$$

Most of the states displayed here have *shadow* $\approx 10^{-6}$. The other measure, *grad size*, is

$$\left[\frac{1}{q} \sum_{i=0}^{q-1} \left\| \frac{\partial L_{p,q}}{\partial \mathbf{x}_i} \right\|^2 \right]^{\frac{1}{2}};$$

it is the norm of the gradient of the action functional, scaled by the length of the state.

shapes

We display orbits for all three perturbations and for two rotation vectors, (1432,1897)/2513 and (2330,377)/3770. The first is an approximation to an irrational vector called the *spiral mean*, the second approximates $(\frac{1}{10}, \gamma)$, where γ is the golden mean. Both approximations come from the Farey triangle scheme of Kim and Ostlund, [KimOst86], see appendix A for details.

For small ϵ , the orbits are well distributed over the angular variables and the momenta look as though they lie on a torus. With increasing perturbation the orbits abruptly contract and concentrate along one-dimensional filaments. The system of filaments depends on both the perturbation and the rotation vector; in figure (2.7b)

the (1432,1897)/2513 orbit has contracted onto a system of three curves, each of which winds around the torus once in each angular direction; we will call these curves of type (1,1). In figure (2.12b) the same rotation vector and the polynomial perturbation lead to a union of seven curves, each of type (0,1). On the other hand, this same perturbation forces the (2330,377)/3770 state to concentrate along a single curve of type (4,1).

Lyapunov exponents

The qualitative behaviour of the orbits is correlated with their stability properties. The Lyapunov exponents measure the exponential rate of divergence of nearby trajectories (see, e.g., [Osc68]) and, for a periodic orbit, are just the eigenvalues⁶ of

$$DF_{\epsilon,(\mathbf{x}_0,\mathbf{p}_0)}^q = DF_{\epsilon,(\mathbf{x}_{q-1},\mathbf{p}_{q-1})} \circ DF_{\epsilon,(\mathbf{x}_{q-2},\mathbf{p}_{q-2})} \circ \cdots \circ DF_{\epsilon,(\mathbf{x}_0,\mathbf{p}_0)} \quad (2.17)$$

where $DF_{\epsilon,(\mathbf{x},\mathbf{p})}$ is the Jacobian of the map. From 2.15 we can calculate

$$DF_{\epsilon,(\mathbf{x},\mathbf{p})} = \begin{bmatrix} \frac{\partial \mathbf{x}'}{\partial \mathbf{x}} & \frac{\partial \mathbf{x}'}{\partial \mathbf{p}} \\ \frac{\partial \mathbf{p}'}{\partial \mathbf{x}} & \frac{\partial \mathbf{p}'}{\partial \mathbf{p}} \end{bmatrix} = \begin{bmatrix} \mathbf{I} - \frac{\partial^2 V_\epsilon}{\partial \mathbf{x}^2} & -\mathbf{I} \\ -\frac{\partial^2 V_\epsilon}{\partial \mathbf{x}^2} & \mathbf{I} \end{bmatrix}$$

where \mathbf{I} is the d -dimensional identity matrix and $\partial^2 V_\epsilon / \partial \mathbf{x}^2$ is the Hessian of the perturbation. Each of the $DF_{\epsilon,(\mathbf{x}_i,\mathbf{p}_i)}$ is a real symplectic matrix and so the entire product is real and symplectic too. The eigenvalues of $DF_{\epsilon,(\mathbf{x}_0,\mathbf{p}_0)}^q$ thus occur in reciprocal pairs $(\lambda_0, 1/\lambda_0)$ and $(\lambda_1, 1/\lambda_1)$, [Arn78]; for the unperturbed map, all four are equal to one. As the perturbation increases, both pairs leave the unit circle. At about the same parameter value for which the first pair departs perceptibly from the circle, the minimizing state contracts along the filaments. The eigenvector corresponding to the largest exponent projects to a vector transverse to the filaments. For large enough perturbation both pairs are non-zero and the distribution along the direction of the

⁶The accurate, direct calculation of the matrix product in (2.17) is usually not possible; see appendix A for a discussion.

filaments is also Cantor-like. See figure (2.6) for the exponents of most of the orbits presented here.

The eigenvector corresponding to the largest exponent projects to a vector transverse to the filaments.

2.2.3 non-existence of tori: a prelude

Notice that the very perturbed orbits look as though they are full of holes, as though there are some parts of the torus they cannot visit. One might imagine that this is just a consequence of the finite lengths of our orbits, that if we had orbits with ten times as many points some of them would be bound to land in the holes. We can show that, for sufficiently large perturbations, the holes are genuine; there are neighborhoods that all minimizing Birkhoff orbits must avoid.

Suppose $V_\epsilon(\mathbf{x})$ is a C^2 , standard-like perturbation to the generating function $H_0(\mathbf{x}, \mathbf{x}') = \frac{1}{2} \|\mathbf{x}' - \mathbf{x}\|$. Suppose further that $V_\epsilon(\mathbf{x})$ has a minimum at $\mathbf{x} = \mathbf{x}_{min}$. Then there is an ϵ_c , such that for $\epsilon > \epsilon_c$, all minimizing states must avoid a region containing \mathbf{x}_{min} .

Proof A globally minimizing state, X , must be an extremum of $L_{p,q}$ such that every small, local, variation, $\mathbf{x}_i \rightarrow \mathbf{x}_i + \delta$ increases the action. That means that X must satisfy the Euler-Lagrange equations (2.10) and also that each matrix

$$\frac{\partial^2 L_{p,q}}{\partial \mathbf{x}_i^2} = \begin{bmatrix} 2 - \epsilon \frac{\partial^2 V}{\partial \mathbf{x}_0^2}(\mathbf{x}_i) & -\epsilon \frac{\partial^2 V}{\partial \mathbf{x}_0 \partial \mathbf{x}_1}(\mathbf{x}_i) \\ -\epsilon \frac{\partial^2 V}{\partial \mathbf{x}_0 \partial \mathbf{x}_1}(\mathbf{x}_i) & 2 - \epsilon \frac{\partial^2 V}{\partial \mathbf{x}_1^2}(\mathbf{x}_i) \end{bmatrix}, \quad (2.18)$$

is positive definite. Because \mathbf{x}_{min} is a minimum, the eigenvalues, $\mu_0(\epsilon) \leq \mu_1(\epsilon)$, of the Hessian of $-V_\epsilon(\mathbf{x}_{max})$ are negative. If one of them is less than -2 then (2.18) cannot be satisfied. Since the μ_i are decreasing functions of ϵ we need only find that value, ϵ_c , for which $\mu_0(\epsilon_c) = -2$.

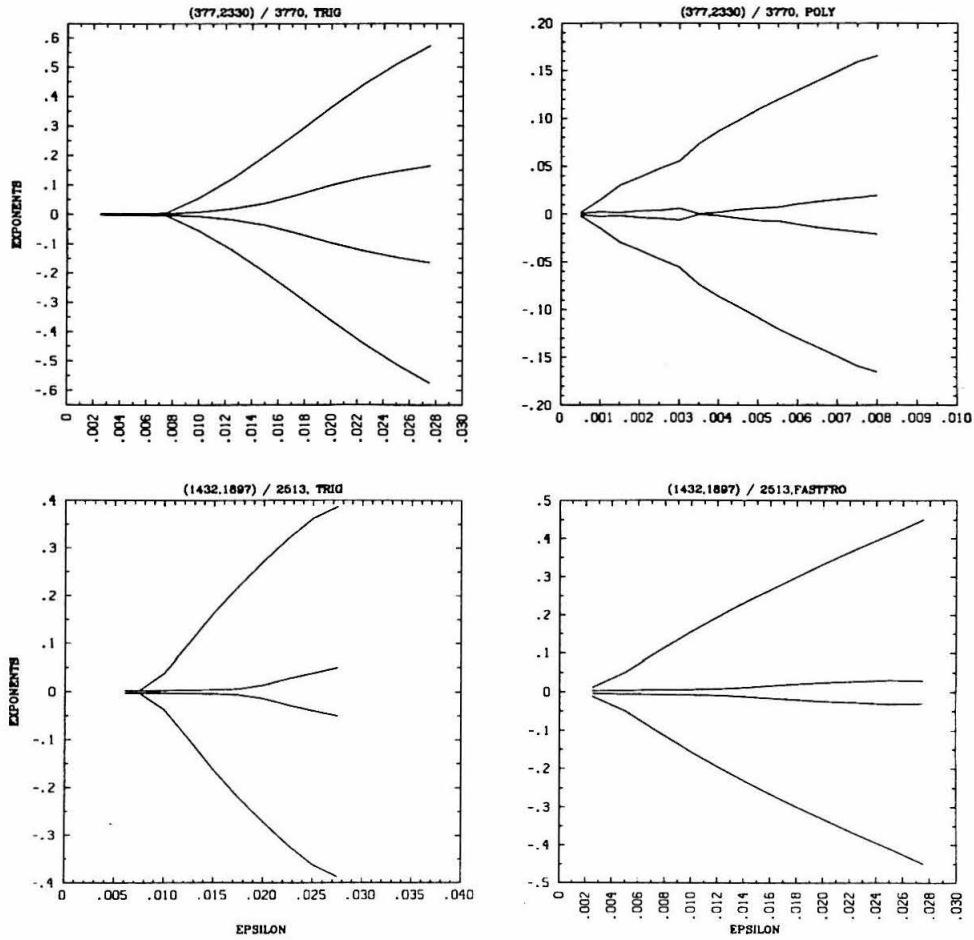


Figure 2.6: *The Lyapunov exponents for the rotation vector $(377, 2330)/3770$ and the trigonometric and polynomial perturbations. Also those for the vector $(1432, 1897)/2513$ with the trigonometric and fast-Froeschlé perturbations.*

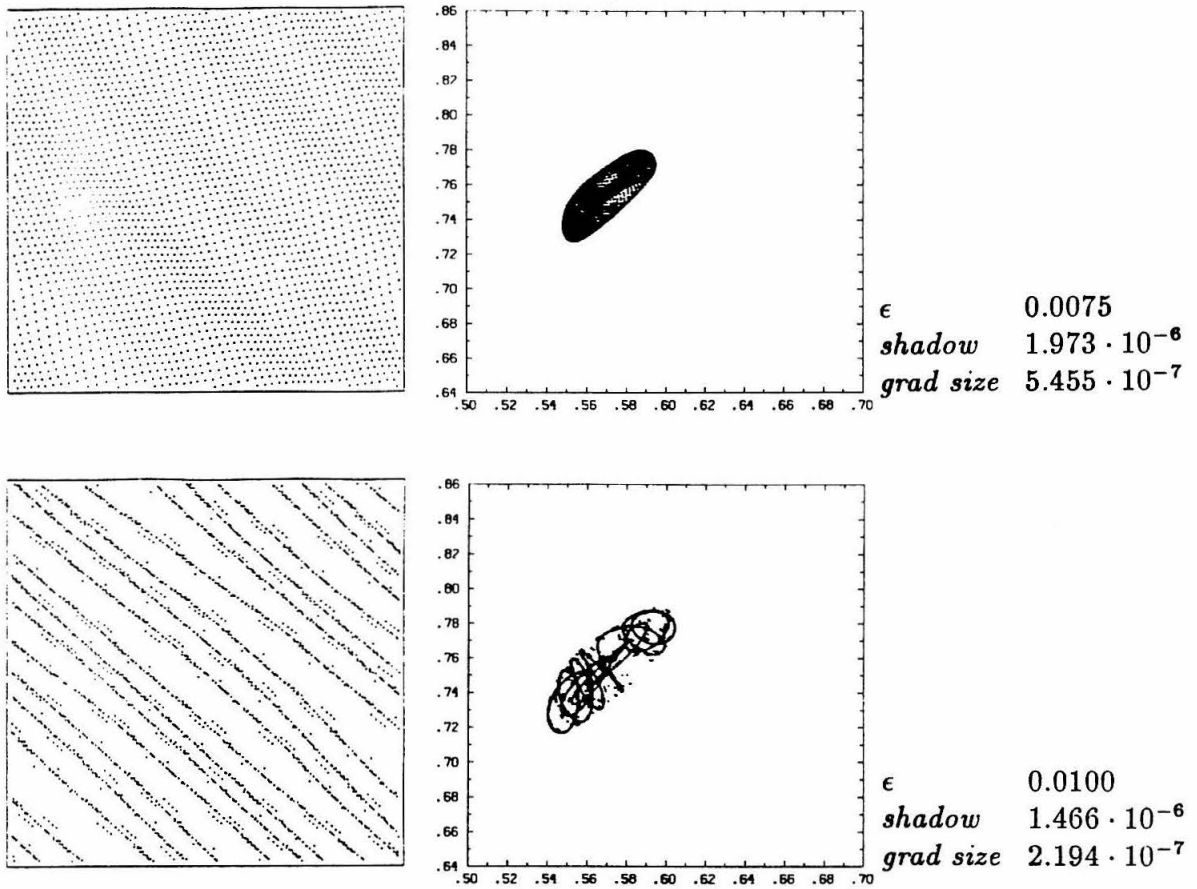


Figure 2.7: *Birkhoff orbits for the trigonometric perturbation and the rotation vector $(1432, 1897)/2513$. This panel illustrates the collapse along filaments. Notice how the $\epsilon = 0.0075$ state has momenta seeming to lie on a smooth surface.*

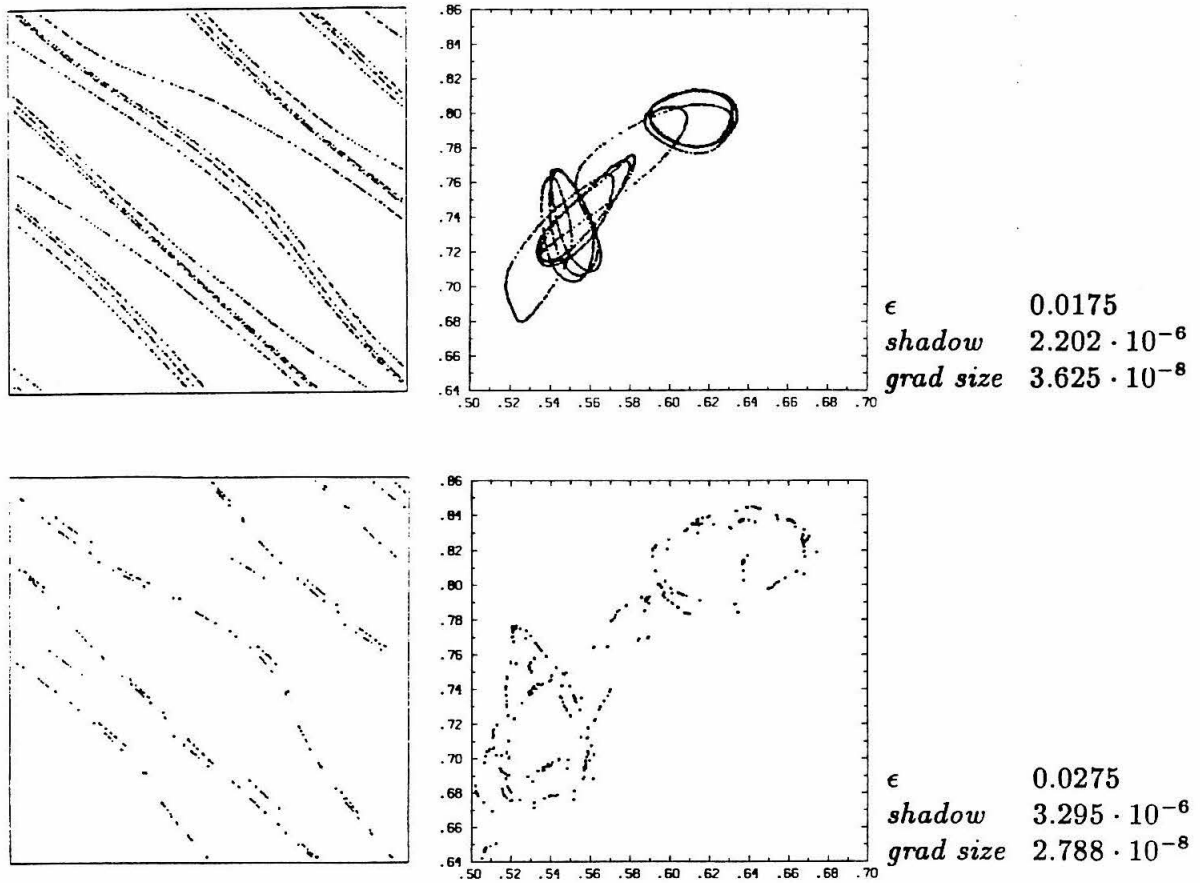


Figure 2.8: *Birkhoff orbits for the trigonometric perturbation and the rotation vector $(1432, 1897)/2513$. This pair shows the appearance of Cantor-like clumping along the filaments.*

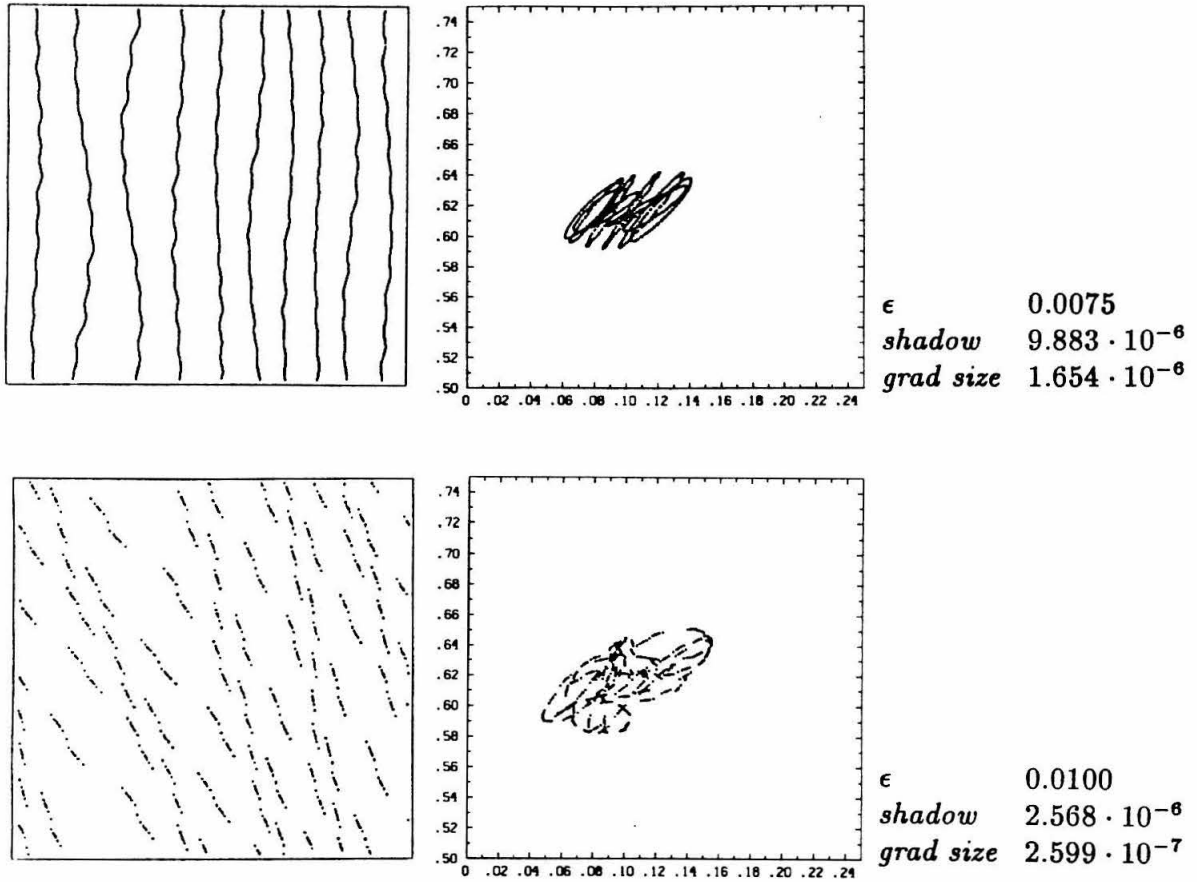


Figure 2.9: *Weakly perturbed Birkhoff orbits for the trigonometric perturbation and the rotation vector $(377, 2330)/3770$.*

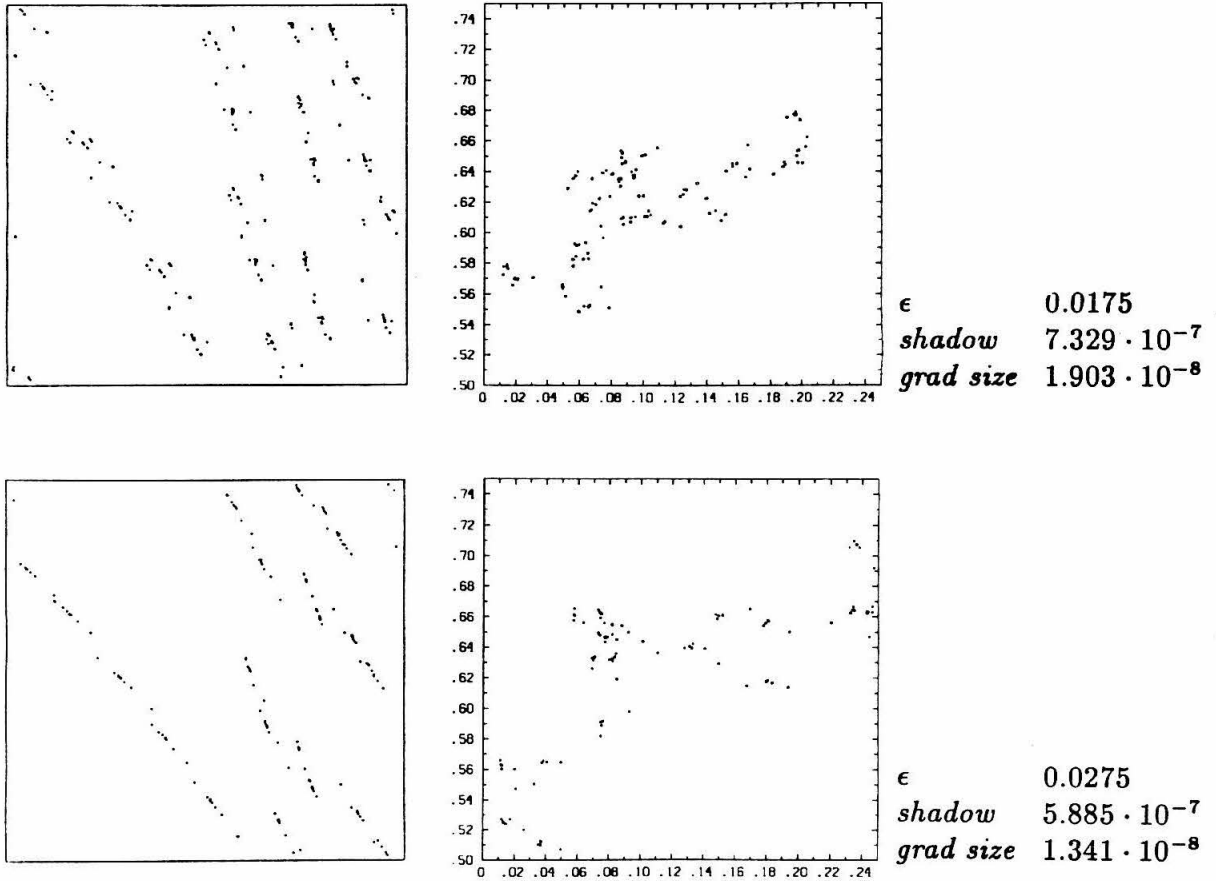


Figure 2.10: *Strongly perturbed Birkhoff orbits for the trigonometric perturbation and the rotation vector $(377, 2330)/3770$.*

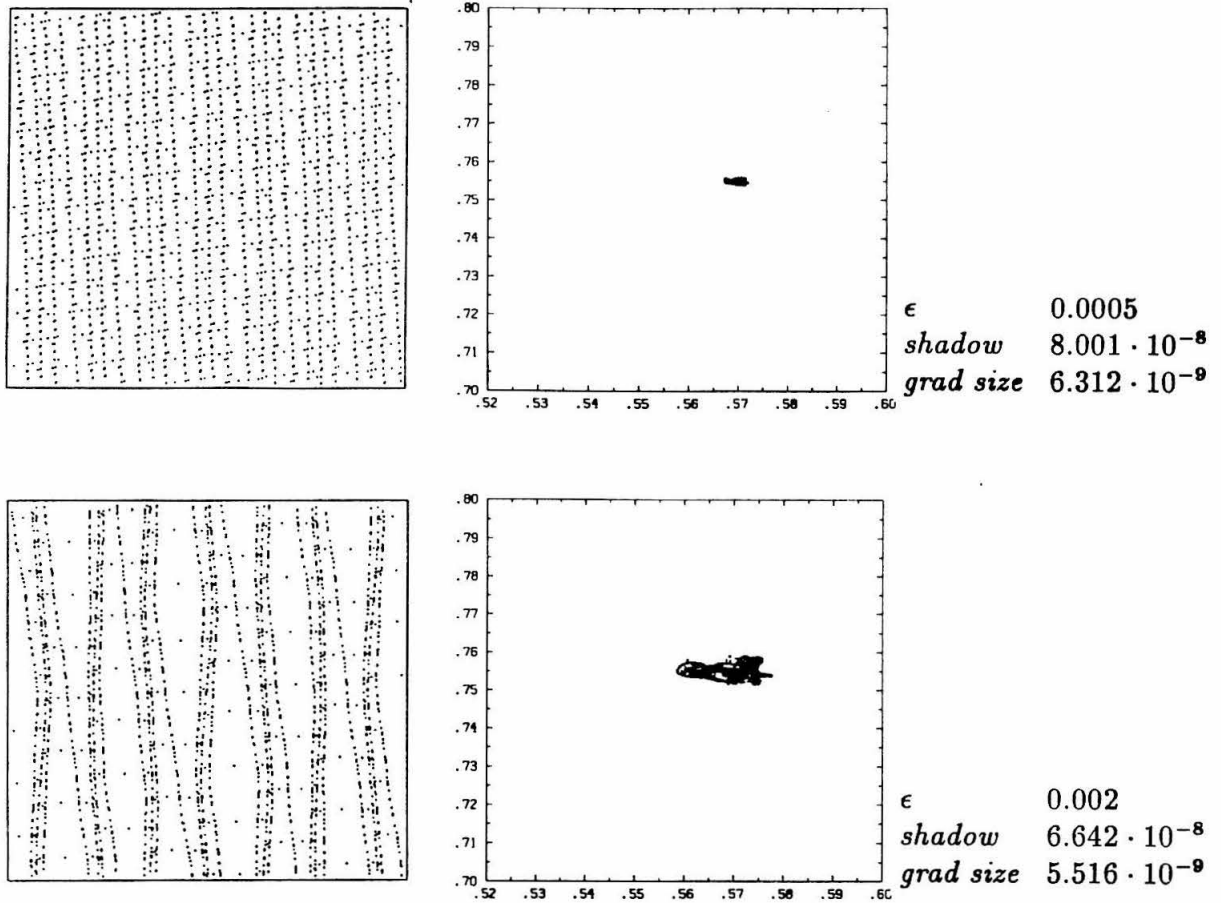


Figure 2.11: *Birkhoff orbits for the polynomial perturbation and the rotation vector $(1432, 1897)/2513$. Note that the momenta remain very near their unperturbed values.*

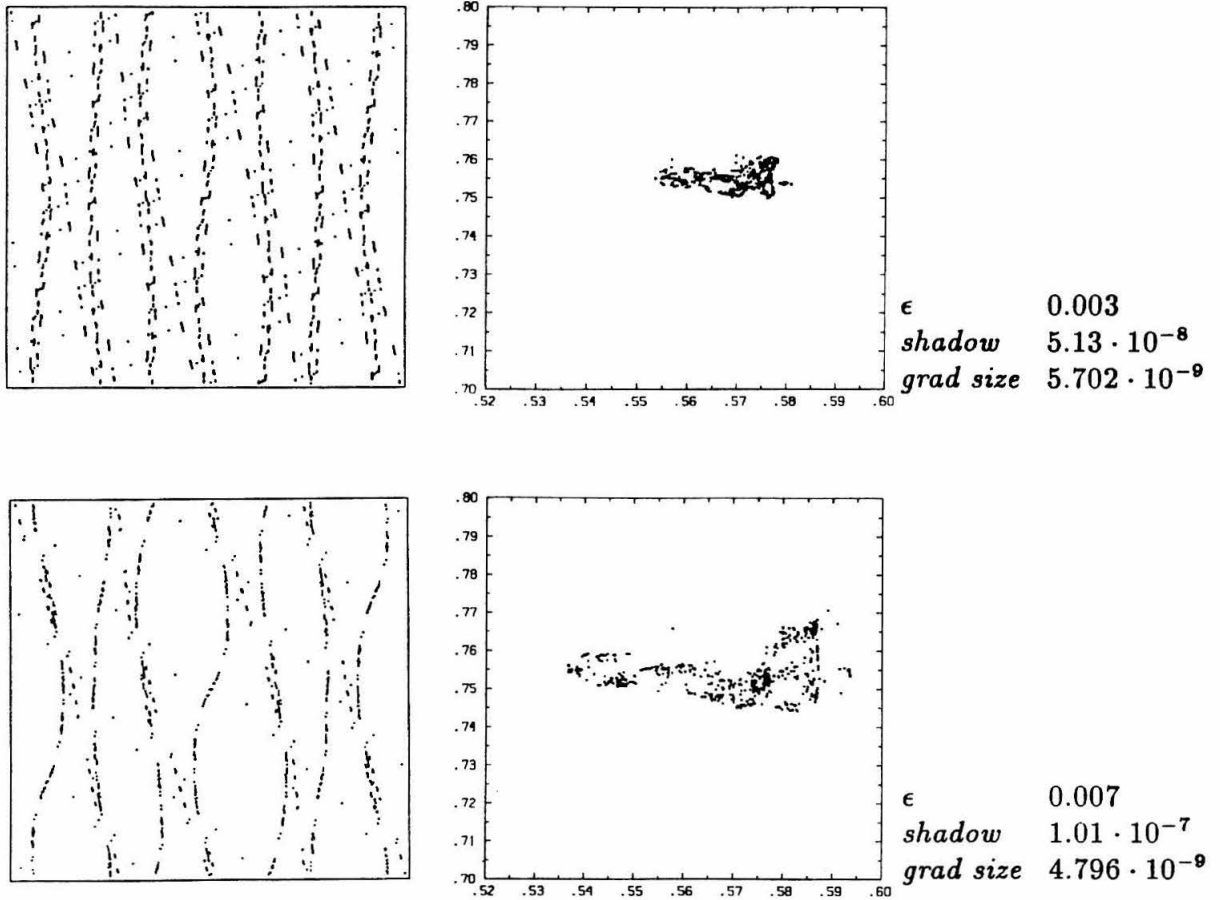


Figure 2.12: Birkhoff orbits for the polynomial perturbation and the rotation vector $(1432, 1897)/2513$. This pair shows the appearance of Cantor-like clumping along the filaments.

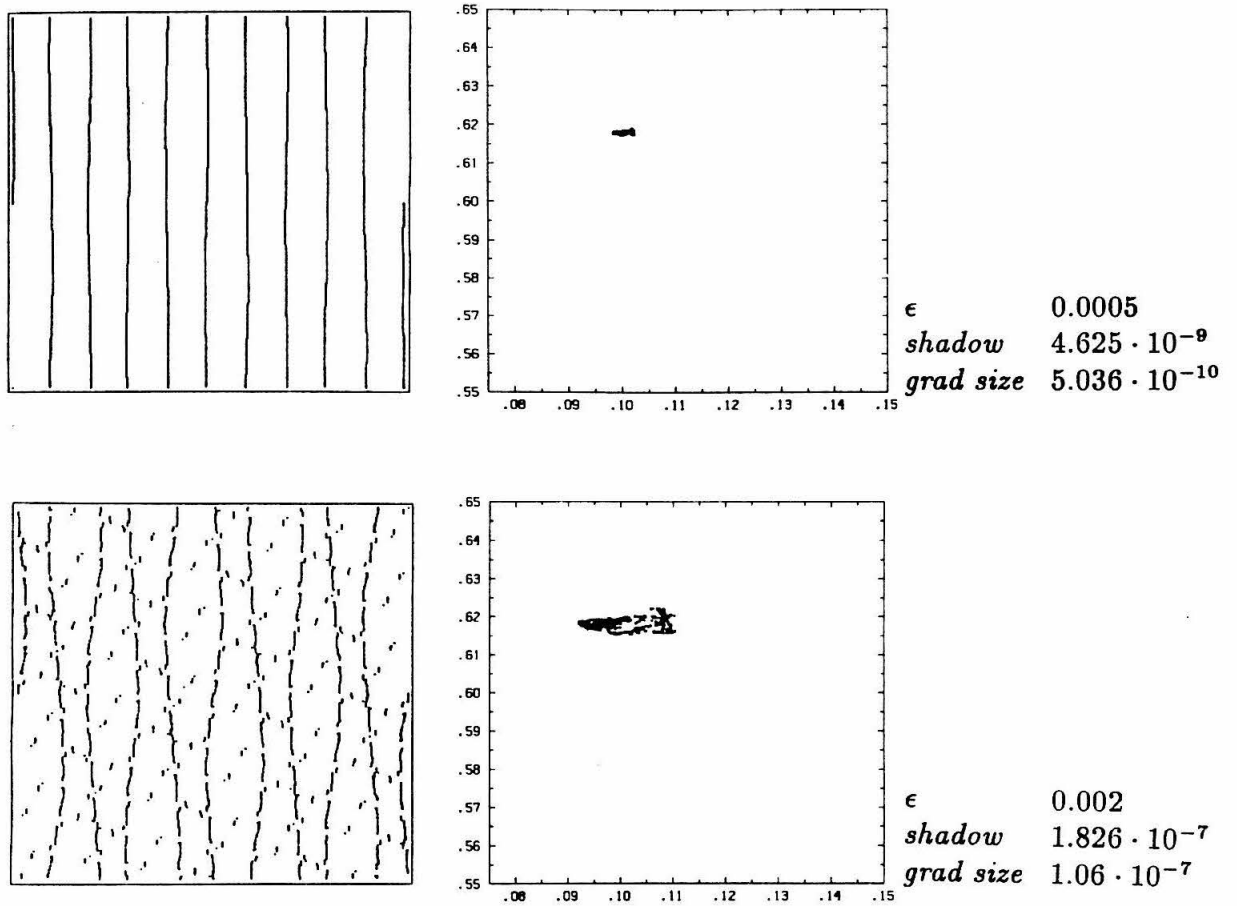


Figure 2.13: *Birkhoff orbits for the polynomial perturbation and the rotation vector (977, 2330)/9770).*

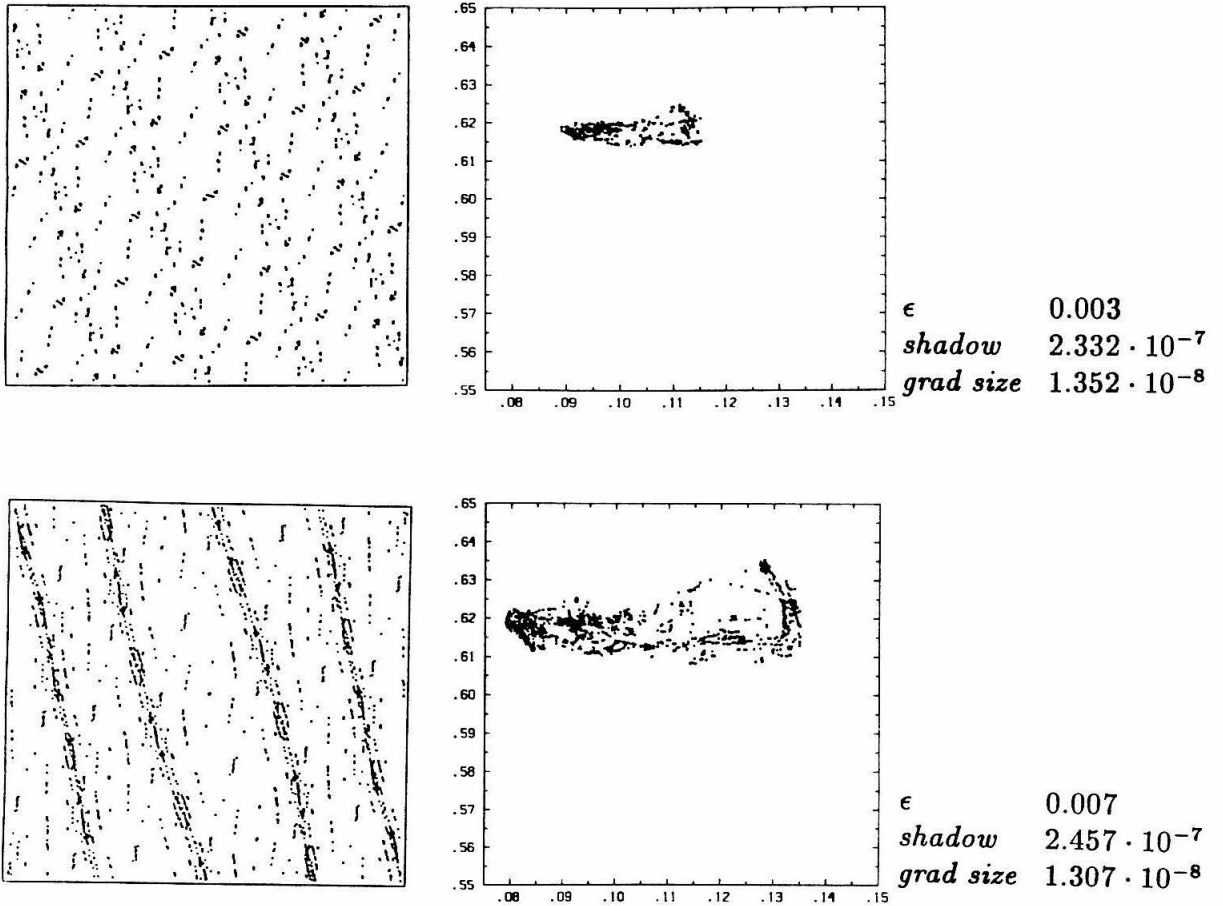


Figure 2.14: *Birkhoff orbits for the polynomial perturbation and the rotation vector $(377, 2330)/3770$.*

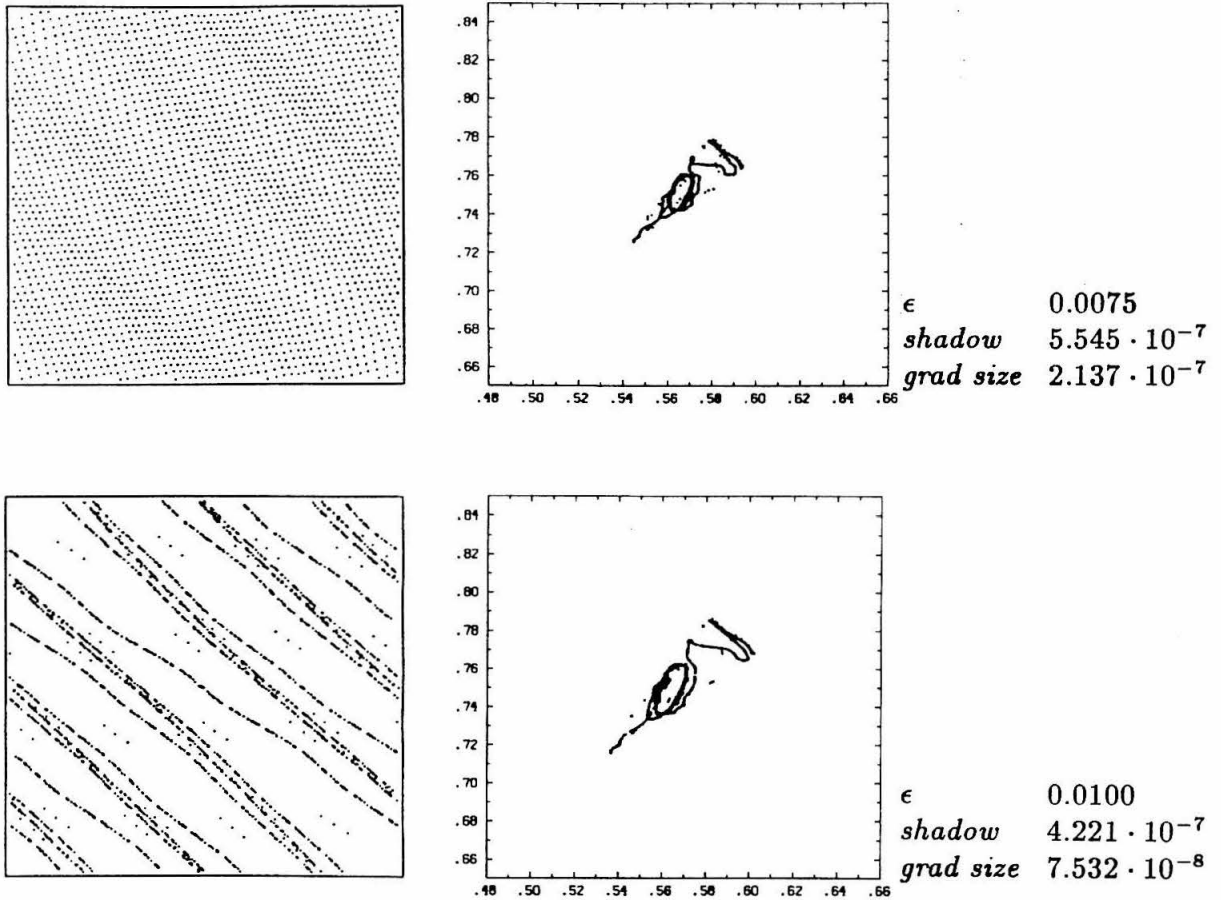


Figure 2.15: *Birkhoff orbits for the fast-Froeschlé perturbation and the rotation vector $(1432,1897)/2513$. Notice how even the $\epsilon = 0.0075$ state seems to have its moment concentrated on a curve.*

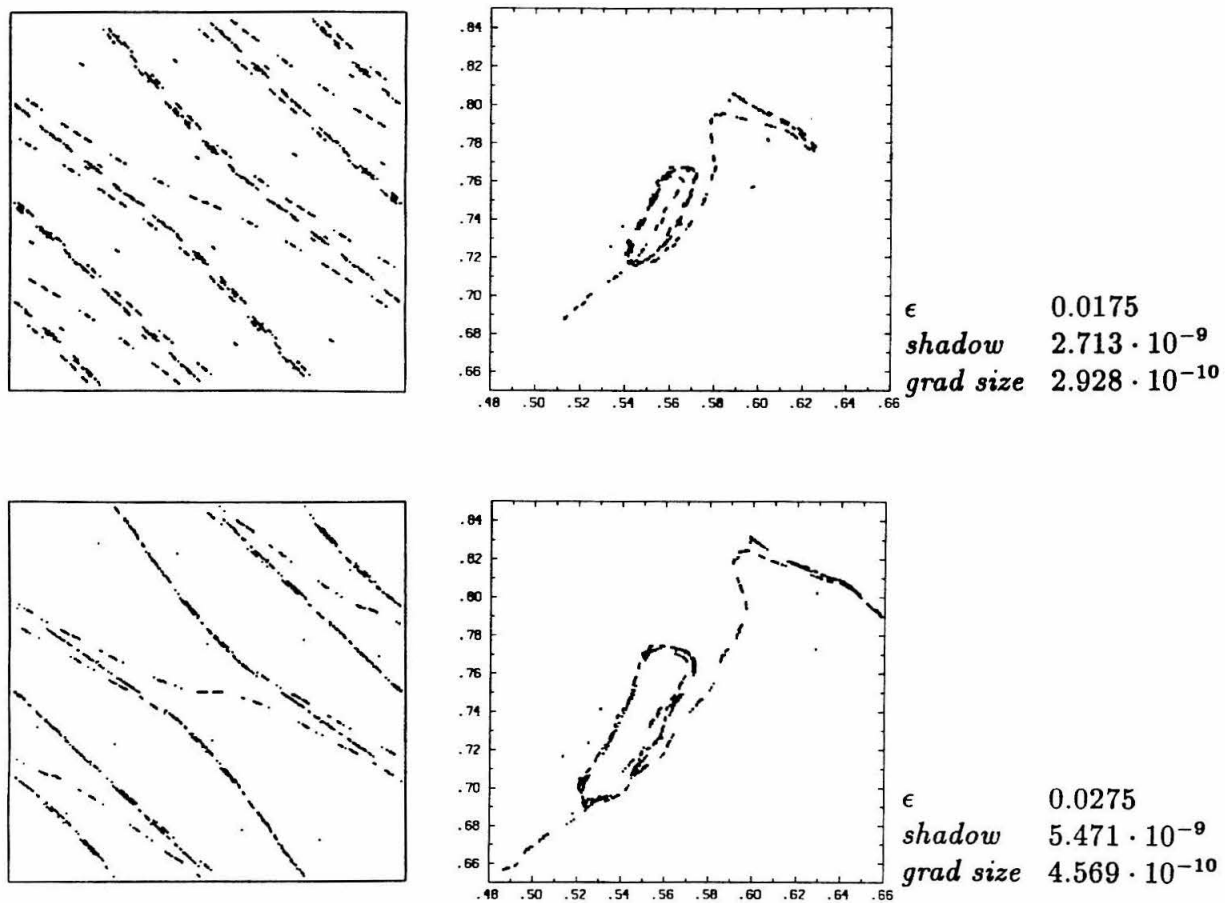


Figure 2.16: *Birkhoff orbits for the fast-Froeschlé perturbation and the rotation vector $(1432, 1897)/2513$.*

For the trigonometric perturbation $\epsilon_c \approx 0.03856$; for the polynomial perturbation $\epsilon_c \approx 0.04167$. The appearance of the states suggests that neither of these is a very good estimate; the region near the maximum is completely devoid of points long before $\epsilon = \epsilon_c$. The real interest of an argument like the one above is that it can provide an estimate of the size of perturbation needed to destroy all the original invariant tori; since the whole next chapter is devoted to such estimates, we leave the subject for now.

2.2.4 smoothness

We would like to be able to say that very long periodic orbits approximate a Cantor set that we could view as the tattered remnant of an invariant torus. Such a remnant should have a kind of smoothness; two points that lie very close to each other in the angular variables should not have wildly different momenta. What we need is a result like the theorem of Birkhoff, generalized by Katok [Kat82], which says that for points in a Mather set, the momenta are Lipschitz functions of the coordinates, i.e., $\| \mathbf{p}_i - \mathbf{p}_j \| \leq C \| \mathbf{x}_i - \mathbf{x}_j \|$ where C is a constant. Katok and Bernstien [KB87] looked for such a result and, as mentioned above, were able to show that, except perhaps at one point, the momenta are Hölder continuous with index $1/2$, that is,

$$\| \mathbf{p}_i - \mathbf{p}_j \| \leq C \| \mathbf{x}_i - \mathbf{x}_j \|^\alpha \quad \alpha = \frac{1}{2}.$$

for some constant C independent of the \mathbf{x}_i .

Hoping to verify or improve their estimate, we computed pairs $(L, \| \Delta \mathbf{x} \|)$, where $L = \| \Delta \mathbf{p} \| / \| \Delta \mathbf{x} \|$, and displayed them on logarithmic axes. If some kind of Hölder continuity applies, then

$$L = \frac{\| \Delta \mathbf{p} \|}{\| \Delta \mathbf{x} \|} \leq C \| \Delta \mathbf{x} \|^{1-\alpha},$$

so

$$\log L \leq \log C + (\alpha - 1) \log \| \Delta \mathbf{x} \|.$$

We can tell whether our orbits are compatible with Lipschitz continuity by looking at the upper envelope of $(L, \|\Delta \mathbf{x}\|)$. If the envelope is a decreasing function of $\|\Delta \mathbf{x}\|$ then the Hölder index is less than one and the momenta are not Lipschitz functions. If the envelope is flat or sloping upward then the continuity is Lipschitz or better. Figure (2.17) shows some collections of $(L, \|\Delta \mathbf{x}\|)$ pairs. The results are ambiguous at best. For very small perturbations, the upper envelope has a positive slope, see figure (2.17 parts a and b). For intermediate values of ϵ , those for which the orbit has contracted into filaments but has not yet begun to concentrate in points, the situation looks worse; the largest values of L occur for the smallest values of $\|\Delta \mathbf{x}\|$, see figures (2.17 parts c and d). This would seem to doom any hope that p is a Lipschitz function of \mathbf{x} . Note, however, that the upper envelope has a slope of -1 . This suggests that $\|\Delta \mathbf{p}\| \approx \text{const}$. On the other hand, we have, from Katok and Bernstien, that \mathbf{p} is Hölder $\frac{1}{2}$. It is thus possible that the lack of smoothness may come from not having enough points. At very large ϵ , those for which the orbit has contracted into a few small clumps, $(L, \|\Delta \mathbf{x}\|)$ begins to have an increasing envelope again. Unfortunately, it is just at these very short distances that we must begin to doubt the quality of our orbits. Typically we have $\text{shadow} = 10^{-6}$ and so must expect the \mathbf{x} s, \mathbf{p} s and their differences to be uncertain at about that level too.

Finally, we note that the uncertainty in the \mathbf{p} s could explain the behavior at intermediate ϵ . If the components of \mathbf{p} s are uncertain beyond σ_p , their differences are uncertain to $\sqrt{2}\sigma_p$. Then, no matter what the continuity properties of p , for small enough $\|\Delta \mathbf{x}\|$ we should expect to see $\|\Delta \mathbf{p}\| \approx \text{const}$. This explanation is not completely satisfactory in that it fails to explain why some of the graphs in figure 2.17 seem to have two different populations of constant $\|\Delta \mathbf{p}\|$ s.

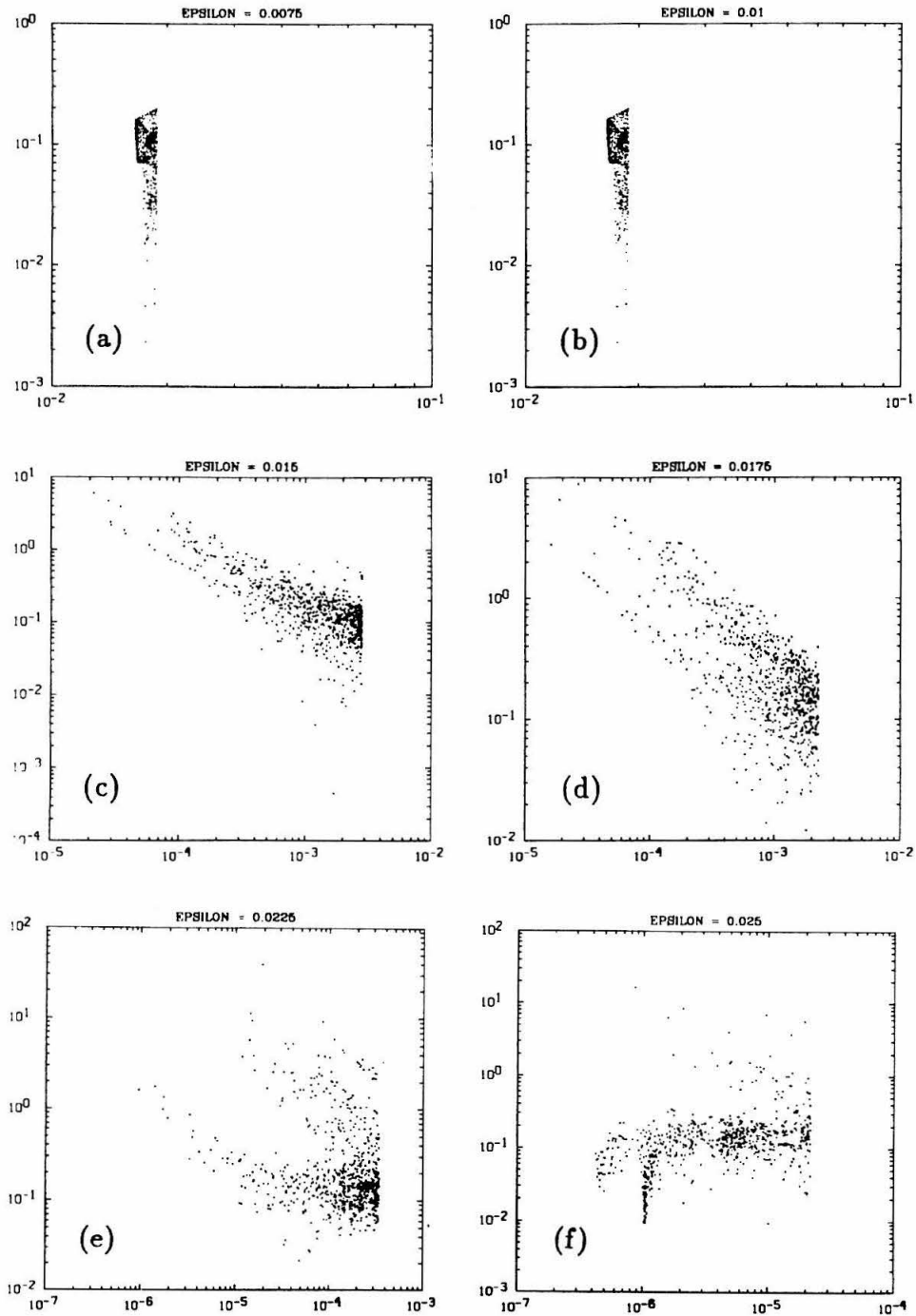


Figure 2.17: Pairs $(L, \|\Delta \mathbf{x}\|)$ calculated for the 800 most closely spaced pairs of points in states of the rotation vector $(1432, 1897)/2513$ with the trigonometric perturbation.

2.3 Hedlund's examples

In this section we will worry about whether the shapes of our states have anything to say about the shapes of much longer states with similar rotation vectors. A central premise of our program of rational approximation is that they do; unfortunately, except for the two-dimensional case (twist maps on the cylinder), we cannot prove this. We cannot even show that states with the *same* rotation vector must have the same shape. Consider the family of minimizing states with rotation vectors,

$$\frac{\mathbf{p}_0}{q_0}, \frac{2\mathbf{p}_0}{2q_0}, \dots, \frac{n\mathbf{p}_0}{nq_0}, \dots \quad n \in \mathbf{Z}^+,$$

where \mathbf{p}_0/q_0 is in lowest terms. For each of these states there is certainly one solution to the Euler-Lagrange equation that is just a concatenation of n copies of the \mathbf{p}_0/q_0 minimizing state. But there may also be other solutions, some of which may have lesser total action.

To see how this can happen, we consider the problem of finding *minimal geodesics*, curves of smallest possible length, on either the two- (or three-) dimensional torus. This problem arises, for example, in the motion of a free particle in a system with periodic boundary conditions and may be reduced to a symplectic map *via* a surface of section, but in the discussion below it will be simpler to think about continuous time and smooth trajectories. We will work with two different representations of the problem, one on the two- (or three-) dimensional torus and another made by periodically extending the torus to get the plane (or \mathbf{R}^3). In either representation, we will allow the metric to be other than the usual Euclidean one.

In the \mathbf{R}^n version of the problem, a minimal geodesic is a curve, $\gamma : \mathbf{R} \rightarrow \mathbf{R}^n$, parameterized in terms of, say, arc length and for which every finite segment is the shortest possible curve connecting its endpoints. Our special interest will be the *periodic geodesics*; on the torus these are curves that wind around and eventually

begin to retrace themselves. In \mathbf{R}^n they appear as curves for which $\exists \tau \in \mathbf{R}$ such that

$$\gamma(t + \tau) = \gamma(t) + \mathbf{m}, \quad \mathbf{m} \in \mathbf{Z}^n \quad (2.19)$$

and we may classify them according to m , which gives the number of times γ winds around each of the coordinate directions on the torus before repeating itself. Hedlund studied these curves on the two-dimensional torus and, in [Hed32], showed that for every pair $(m_0, m_1) \in \mathbf{Z}^2$, there is a minimal periodic geodesic that winds m_0 times around the θ_0 direction and m_1 times in the θ_1 direction before closing.

He also made an observation that connects the geodesic problem to the problem of finding Birkhoff periodic orbits. He asked whether, for example, the minimizing periodic geodesic for the pair (10,20) could be other than the curve which traces 10 times over the (1,2) geodesic. He found that it could not. The corresponding statement for Birkhoff orbits is that the pathology outlined at the beginning of the section does not occur for two-dimensional twist maps of the annulus.

In the last section of his paper, Hedlund demonstrated that one cannot expect the analogous result in higher dimension. He presented an explicit example of a metric on \mathbf{T}^3 for which the shortest geodesic of type (ni, nj, nk) is not n copies of the shortest (i, j, k) geodesic. Victor Bangert [Bang87] has proved that a metric on \mathbf{T}^n has at least $n + 1$ minimal geodesics and has given some principles for the design of Hedlund-type examples.

Figures (2.18) and (2.19) contain the main ideas. Bangert sets up the metric so it has certain non-intersecting lattices of “tunnels,” tubes in the middle of which the metric is so small that the length of a segment is, at most, say, 1/100 of its Euclidean length. Outside the tunnels the metric is such that the length of a segment is a bit longer than its Euclidean length. In Bangert’s examples the tunnels run along the lines $(0, t, \frac{1}{2})$, $(\frac{1}{2}, \frac{1}{2}, t)$, and $(t, 0, 0)$, $t \in \mathbf{R}$ and along all their \mathbf{Z}^n translates. Under these rather severe conditions he is able to show that a minimizing geodesic must spend essentially all its time inside the tunnels, venturing out only to leap from one

system of tunnels to another.

A minimizing, periodic geodesic then has only three short segments lying outside the tunnels, no matter how long it is. Note that such a geodesic strays a long way from the straight line that connects its endpoints; the latter is a minimizing periodic geodesic for the flat, Euclidean metric. In the language of Birkhoff orbits, Hedlund's pathology would occur if some few p - q periodic states turned out to have such tiny actions that all very long states would be composed of a few segments, with each segment containing many copies of the few economical states. Although we cannot preclude this possibility, we feel it is unlikely. Hedlund and Bangert's examples require that the curves through the tunnels be much, much shorter than their Euclidean lengths, consequently, their metrics are very far from flat. By contrast, our generating functions are close to the unperturbed ones. We might thus hope that our minimizing states are obliged to stay close to the unperturbed states. Katok has shown, in [Kat88], that if the perturbed states stay within some bounded distance of the unperturbed distance and if the bound is independent of the length of the state, then Hedlund's pathology does not occur.

We undertook two studies to investigate these issues. In the first, figure (2.20), we measured the deviation of our minimizing states from the straight line connecting x_0 to x_q . The distance always remains smaller than the diameter of the torus, $1/\sqrt{2}$. In the second study we used the Farey triangle algorithm of Kim and Ostlund, (see appendix A), to get a sequence of rotation vectors tending to $(377, 2330)/3770$. The states for these vectors are displayed in figure 2.21. The longest orbits look very much like the shortest. We also did some experiments on families of rotation vectors of the form⁷ $n\mathbf{p}_0/nq_0$; The longer states were indistinguishable from the shorter ones.

⁷An unperturbed minimizing state is n copies of the unperturbed p_0/q_0 state and our procedures for constructing perturbed minimizing states are such that this shorter, internal periodicity would be retained throughout the calculation. We tried to circumvent this problem by adding a small, random displacement to each of the points in the starting guess, see appendix A.

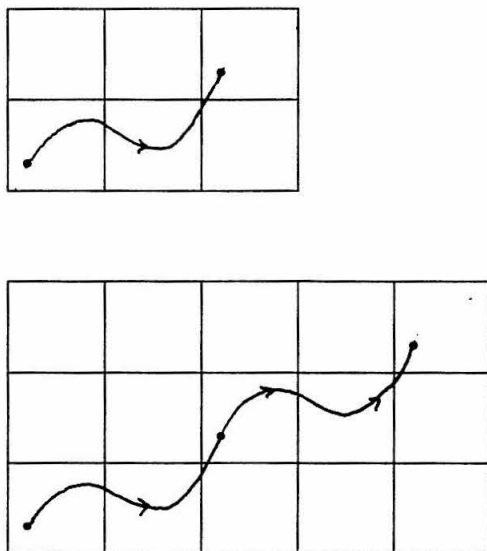


Figure 2.18: *Some minimizing periodic geodesics for the two-dimensional torus; the shortest curve of type $(2,4)$ is just 2 copies of the shortest one of type $(1,2)$.*

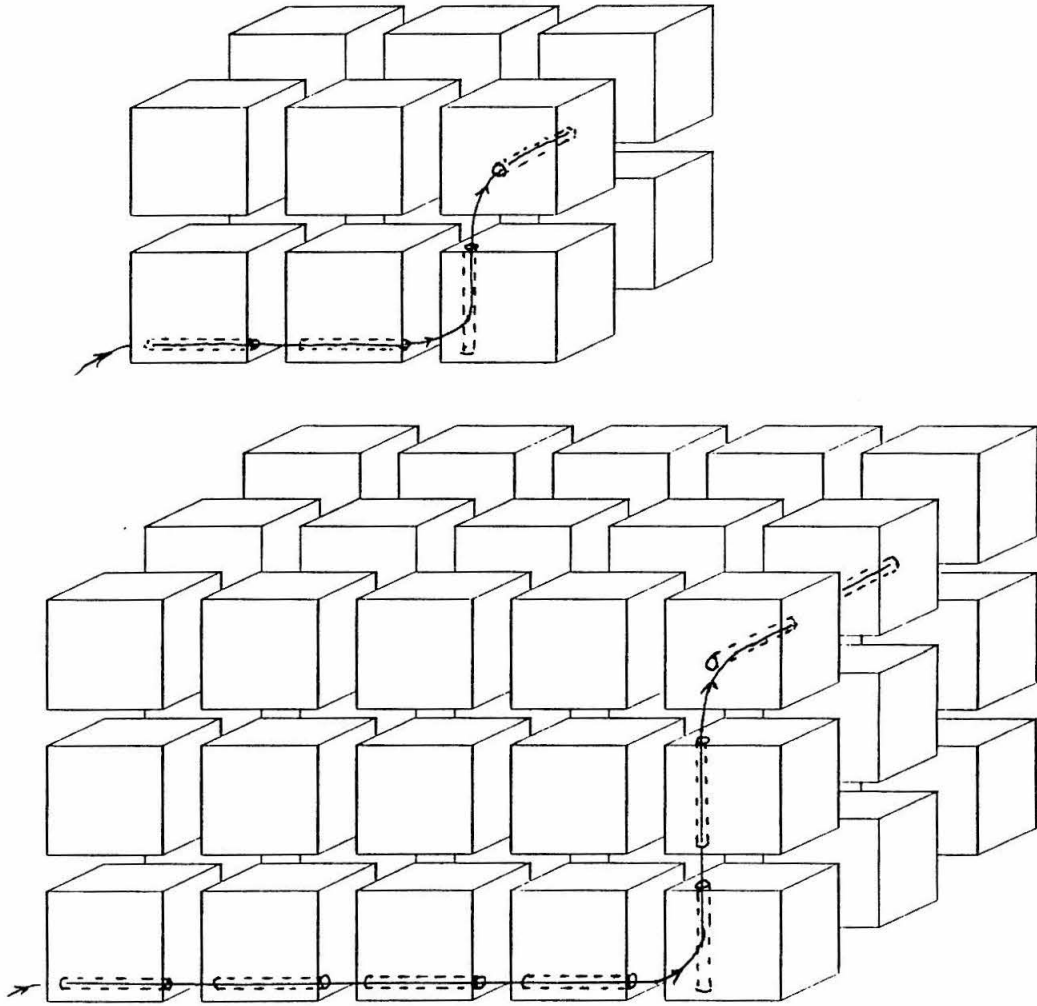


Figure 2.19: *Some minimizing periodic geodesics for a Hedlund example on the three-dimensional torus; the shortest curve of type $(2,4,2)$ is not 2 copies of the shortest one of type $(1,2,1)$.*

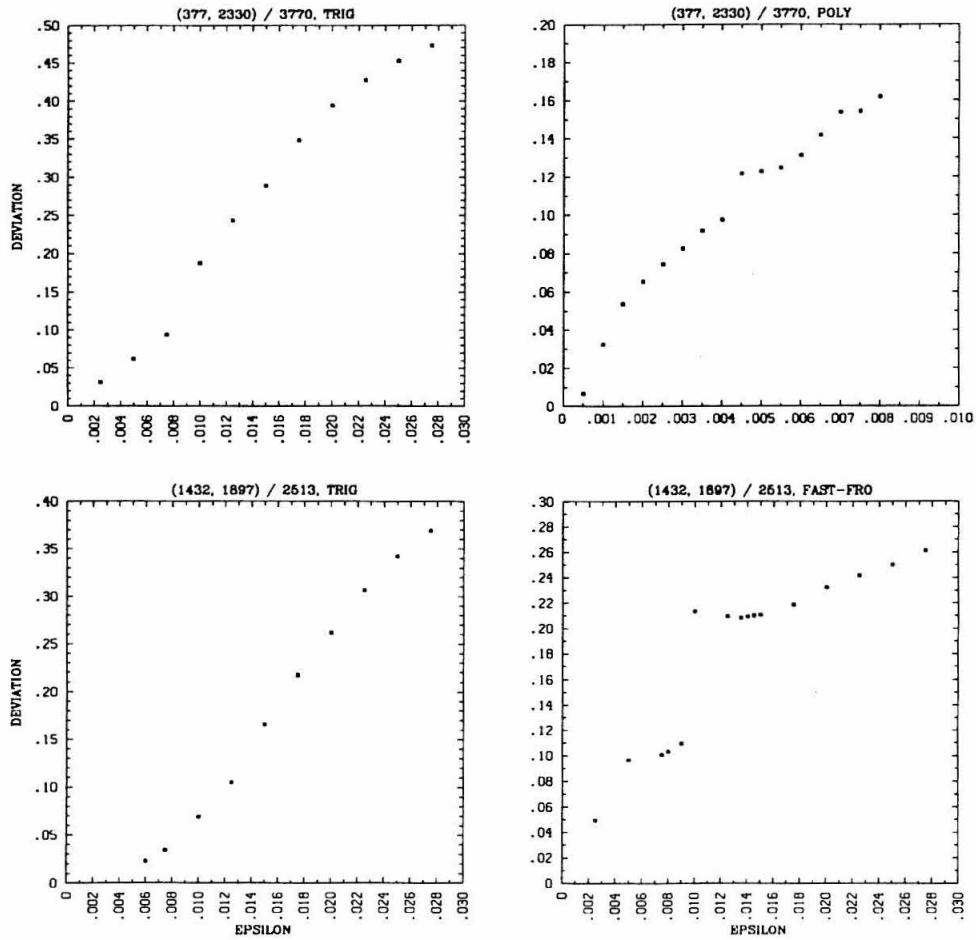


Figure 2.20: *The largest displacement between a point in a perturbed minimizing state and the position it would occupy in the absence of the perturbation. Note the abrupt jumps in the deviations for the fast-Froeschlé example.*

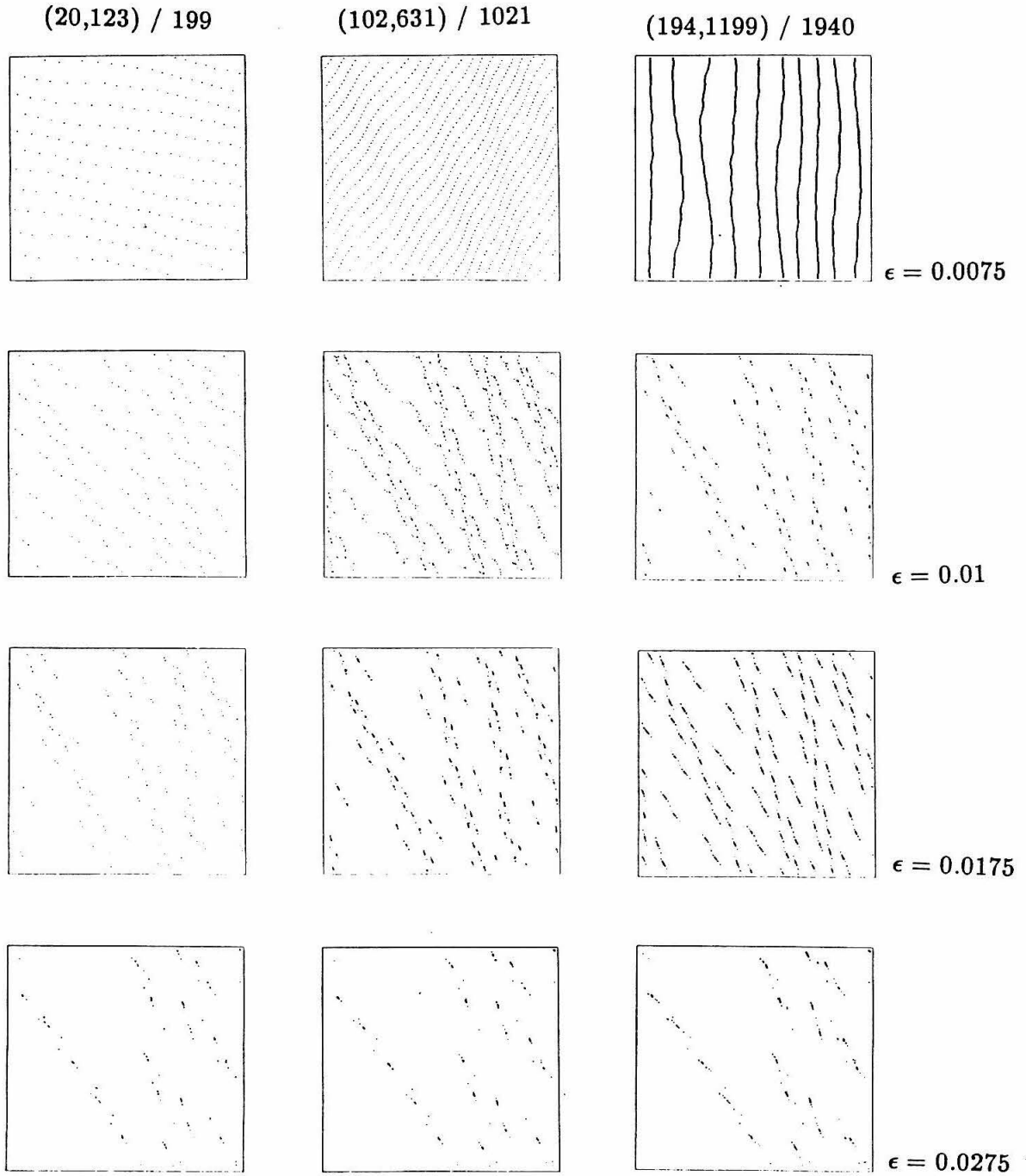


Figure 2.21: A series of orbits whose rotation vectors approximate $(377, 2330) / 3770$.

Chapter 3

The Frontier of Chaos

Our first investigations aimed at the question “What remains after invariant tori have been destroyed?” Our next set asks the more basic “How could we tell if the tori were there?” To answer this question we might follow Kolmogorov, Arnold and Moser and seek to find perturbations so small that some tori would be guaranteed to exist. Conversely, we could try to find perturbations so large that no invariant tori remain. Numerical evidence suggests that the first approach will be hard; tori seem to persist well beyond the point where traditional KAM arguments break down.¹ We will adopt the latter strategy; we will try to fill in the blanks in the following “converse KAM” theorem :

Theorem *For the n -dimensional symplectic twist map $F_\epsilon : \mathbf{A}^n \rightarrow \mathbf{A}^n$,*

$$F_\epsilon(x, r) = (x', r') = \boxed{\phantom{\text{expression}}}$$

depending on the parameters, ϵ , we are guaranteed that no KAM tori exist for any $\epsilon \in S_F = \{\boxed{\phantom{\text{set}}}\}$.

Proof

¹Several authors have now proved machine-assisted, constructive KAM theorems for specific maps; these are in much better agreement with non-rigorous numerical predictions. See e.g., [CC88], [Rana87], and [LR88].

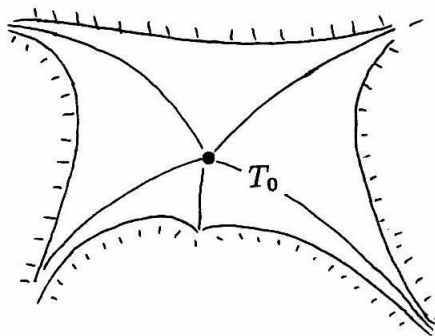


Figure 3.1: *The space of near-integrable maps, showing the frontier of non-integrability around T_0 , an integrable system.*

Herman, in [Herm83] first saw that one might get a better notion of where invariant tori exist by looking at the edge of the region where they do not. He considered maps, $T_\epsilon : \mathbf{T} \times \mathbf{R} \rightarrow \mathbf{T} \times \mathbf{R}$, of the form²

$$T_\epsilon(x, p) = (x', p') = (x + p, p + \epsilon f(x + p)), \quad (3.1)$$

small perturbations to the integrable system, and envisioned a kind of cartography of non-integrability. By choosing different f s he could consider different directions in the space of perturbations. For each fixed f he could increase the value of ϵ until it reached a size, $\epsilon = \epsilon_c(f)$, such that no invariant tori remained. By calculating pairs $(f, \epsilon_c(f))$ he could map out the edge of non-integrability, the frontier of chaos.

We will concentrate on ways to get rigorous bounds for $\epsilon_c(f)$ but will not make a very extensive survey³ of f s. The rest of the chapter is organized by dimension of the phase space and sharpness of non-existence criteria. In the next section we review converse KAM theorems for area-preserving twist maps on the cylinder, and in section 3.2 we explain how to prove them with a digital computer. In 3.3 we formulate some criteria for higher-dimensional systems and finally, in section 3.4, apply them to an example.

²Our examples are not of this form, but, after a change of coordinates, their inverses are.

³Jacob Wilbrink, in [Wilb87], used a non-rigorous existence criterion to survey a whole one parameter family of maps.

3.1 Converse KAM results on the cylinder

Many of the ideas presented here originated with Herman's paper [Herm83]. Katok, at the end of his paper [Kat83], discusses the distribution of points in minimizing states and explains a way to prove the non-existence of circles. Mather used similar techniques to make applications to the standard map, [Ma84], and to billiards, [Ma82b]. He also introduced a different, more generally applicable criterion based on the existence of action-minimizing states. MacKay and Percival augmented Herman's argument with rigorous computation and discovered a connection between Herman's work and Mather's action criterion.⁴ The presentation below owes a great deal to their excellent paper, [MP85], and to [Strk88], which came out of Stark's thesis.

3.1.1 definitions and a first criterion

We will study maps given by (3.1) and try to find criteria that preclude the existence of the kind of tori produced by the KAM theory. We cannot, of course, rule out the existence of tori in the broadest sense. No matter how large the perturbation, some tori may remain in the islands around elliptic periodic points. In the two-dimensional case we will restrict our attention to the kind of circles that wind once around the cylinder; such circles⁵ can be smoothly deformed into the curve $p = 0$. In higher dimension we will consider those tori that can be smoothly deformed into the torus $p = (0, 0, \dots, 0)$.

Maps given by (3.1) are automatically area and orientation preserving. We will add the further restrictions that the perturbation, f , be differentiable, periodic, and

⁴Recently, Rafael de la Llave (personal communication) has developed an extremely promising criterion based on the construction of hyperbolic orbits.

⁵These circles are also called *rotational* because the restriction of the map to such a circle gives a motion conjugate to a rotation.

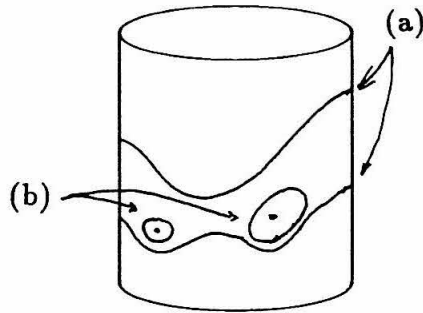


Figure 3.2: *The cylinder and several invariant circles, some (a) rotational and some (b) encircling a periodic orbit.*

have average value zero, i.e.,

$$f(x) = f(x + 1), \quad \int_0^1 f(x) dx = 0.$$

The restriction on the average value is essential; if it is not met T_ϵ has no invariant tori at all. To see why, consider a curve, $(x, \Gamma_0(x))$, and its image, $(x, \Gamma_1(x))$, where Γ_1 is given implicitly by

$$\Gamma_1(x') = p'(x, \Gamma_0(x))$$

or

$$\Gamma_1(x + \Gamma_0(x)) = \Gamma_0(x) + \epsilon f(x). \quad (3.2)$$

Preservation of area and orientation guarantee that the area between the two is independent of Γ_0 since, if we consider another curve, Γ'_0 , and its image, Γ'_1 , we can write

$$\int_0^1 \Gamma'_0 - \Gamma_0 = \int_0^1 \Gamma'_1 - \Gamma_1 \quad \text{so} \quad \int_0^1 \Gamma'_0 - \Gamma'_1 = \int_0^1 \Gamma_0 - \Gamma_1$$

and hence we can calculate it for any curve we like. Using $\Gamma_0(x) = p_0$ and equation (3.2) we get

$$\Gamma_1(x + p_0) = p_0 + \epsilon f(x), \quad \text{or} \quad \Gamma_1(x) = p_0 + \epsilon f(x - p_0).$$

Thus we find

$$\Delta\Gamma(x) \equiv \Gamma_1(x) - \Gamma_0(x) = \epsilon f(x - p_0).$$

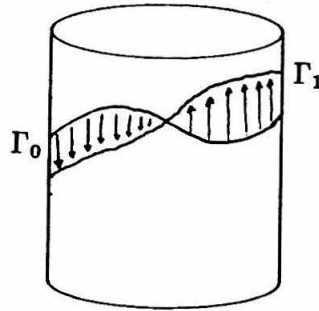


Figure 3.3: A curve and its image. The area between the two is shaded.

The area between the two curves is then

$$\int_0^1 \Delta\Gamma(x)dx = \int_0^1 \epsilon f(x - p_0),$$

the average value of f . Now suppose Γ_0^{inv} is an invariant circle. That means $\Gamma_1^{inv} = \Gamma_0^{inv}$. Then

$$\int_0^1 \Delta\Gamma(x)dx = 0$$

and we have our first and simplest test for the non-existence of invariant circles. Unfortunately this is not a very decisive criterion; it leaves open the possibility of circles for any value of k in the Taylor-Chirikov standard map. To do any better we must more carefully consider the geometry of invariant circles, a task we turn to next.

3.1.2 Lipschitz cone families and their refinement

The first thing to notice is that invariant circles divide the cylinder into two disjoint pieces. Orbits that begin below an invariant circle must always remain below it. One might hope to turn this observation into a non-existence criterion, say, by starting an orbit at some point (θ_0, p_0) and evolving it forward. If the orbit eventually attains arbitrarily large momenta then the map has no invariant circles. Chirikov [Chkv79] calls orbits with indefinitely increasing momentum “accelerator modes” and notes that they exist in the standard map for $k \geq 2\pi$.

Rigorous implementation of this strategy is hard. The simple calculation described

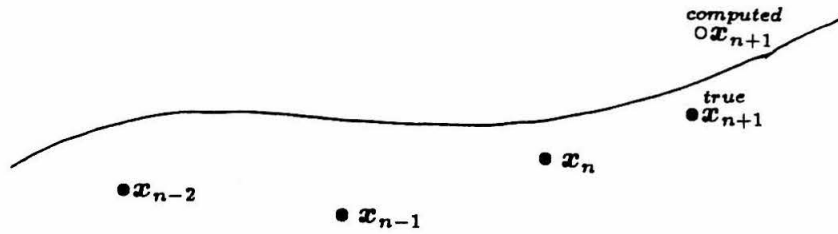
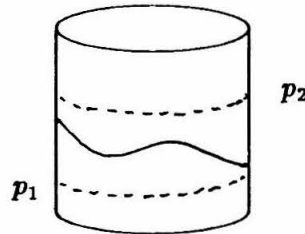


Figure 3.4: *Numerical error may carry a point across an invariant circle.*

above does not work because one can never be sure that a computational error will not carry the orbit across a genuine invariant circle. Simply following an orbit cannot establish the non-existence of circles. One might instead try to follow an orbit and say that if it never rises above a certain momentum $p = p_{max}$ then it must be trapped beneath an invariant circle. That is, one might try to prove the *existence* of circles.

From an analytic point of view this seems like a good idea. A theorem of Birkhoff [Birk22] says that if the twist map is continuously differentiable and if there are two values of the momentum, p_1 and p_2 , $p_1 < p_2$, such that any orbit that begins with momentum less than p_1 never attains a momentum greater than p_2 , then there is an invariant circle somewhere in the band $p_1 < p < p_2$. Further, the circle⁶ is the graph of some Lipschitz function, $\Gamma(\theta)$.

Figure 3.5: *If orbits with initial momentum less than p_1 never rise above $p = p_2$ there is an invariant circle.*



Despite this analytic support, we cannot get a good existence criterion either. Not only is computational error again a problem, but we must also worry about the cantori. Although they are not true barriers to the diffusion of phase points, they

⁶[Ma84] gives a sketch of the proof of this theorem.

can be formidable partial barriers.⁷ Even if we could calculate an orbit with perfect precision we could never be sure that it was permanently trapped below a particular p_{max} . To get a really useful criterion we must pay closer attention to Birkhoff's theorem, particularly to the part where he tells us that rotational invariant circles are the graphs of Lipschitz functions.

Suppose the invariant circle has rotation number ω , then we will say that it is the graph of $\Gamma_\omega(\theta)$. Since Γ_ω is Lipschitz we have

$$|\Gamma_\omega(\theta + \Delta\theta) - \Gamma_\omega(\theta)| \leq L |\Delta\theta|, \quad (3.3)$$

where L is a constant independent of θ . On the graph this means that a vector tangent to the circle is confined inside a cone, see figure (3.6). Since Γ_ω is only a Lipschitz function it need not have a well-defined tangent at every point. That is, although (3.3) implies that both the right and left limits,

$$\begin{aligned} (\Gamma'_\omega)_{right} &\equiv \lim_{\Delta\theta \searrow 0} \frac{|\Gamma_\omega(\theta + \Delta\theta) - \Gamma_\omega(\theta)|}{|\Delta\theta|} \\ (\Gamma'_\omega)_{left} &\equiv \lim_{\Delta\theta \nearrow 0} \frac{|\Gamma_\omega(\theta + \Delta\theta) - \Gamma_\omega(\theta)|}{|\Delta\theta|} \end{aligned}$$

must exist, they need not be the same. Nonetheless, both limits must be smaller than L , and so both the vectors $(1, (\Gamma'_\omega)_{left})$ and $(1, (\Gamma'_\omega)_{right})$ are in the cones⁸ pictured in figure (3.6).

The constant L is a property of Γ_ω and is defined only along the curve. We could, instead, draw a cone at every point, (θ, p) , such that if an invariant circle passes through (θ, p) its tangent must lie inside. We will call such a system of cones a *cone family* and represent it with two θ -periodic functions, $L_+(\theta, p)$ and $L_-(\theta, p)$; a vector tangent to a circle through (θ, p) may only have slope, ℓ , with $L_-(\theta, p) \leq \ell \leq L_+(\theta, p)$.

⁷For the golden cantorus of the standard map, with $k = 1.0$, [MMP84] find the mean crossing time to be on the order of 10^6 iterations.

⁸Indeed, a Lipschitz function is absolutely continuous and so has a derivative defined almost everywhere, see e.g., [Ttch39].

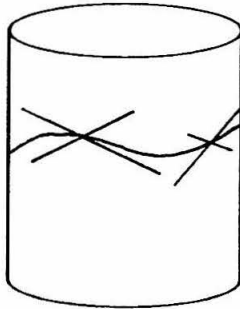


Figure 3.6: An invariant curve and with some Lipschitz cones.

The simplest possible cone family is

$$L_-(\theta, p) = L_{0-}, \quad L_+(\theta, p) = L_{0+}. \quad (3.4)$$

We will call this a *naive* or *uniform* cone family. We can always get such a family by taking, at the worst, $-L_{0-} = L_{0+} = \infty$. Often, as we shall see, we can do much better.

Each tangent vector lying inside the cone family is ostensibly a permissible tangent to an invariant curve but the dynamics may preclude some of the slopes permitted by the naive cone condition. Consider the action of the map on a tangent vector, say the vector ν with footpoint (θ, p) .

$$\nu' = DT_{\epsilon, (\theta, p)} \nu$$

is its image and has footpoint (θ', p') . We can apply the map DT_{ϵ} to all the vectors allowed by the Lipschitz cone at some point $z_n = (\theta_n, p_n)$ and examine their images at $z_{n+1} = (\theta_{n+1}, p_{n+1}) = T_{\epsilon}(z_n)$. In this way we can use the map on tangent vectors to define a map on cones. The image of the cone from z_n will not usually coincide with the cone at z_{n+1} . This means we can eliminate part of the cone at z_n , for if there were an invariant graph above θ_n its tangent vector would have to be one of the ones whose images lie inside the naive cone at z_{n+1} . We could make a similar argument involving DT_{ϵ}^{-1} and z_{n-1} and so refine the cone at z_n even further, see figure (3.7).

More formally, we can use the map to recursively define a sequence of cone families,

$C_n(\theta, p) \equiv \{L_{n-}(\theta, p), L_{n+}(\theta, p)\}$ by

$$\begin{aligned} C_0 &= \{L_{0-}, L_{0+}\} \\ C_{n+1}(\theta, p) &= DT_\epsilon^{-1} \{C_n(T_\epsilon(\theta, p))\} \cap C_n(\theta, p) \cap DT_\epsilon^1 \{C_n(T_\epsilon^{-1}(\theta, p))\} \end{aligned} \quad (3.5)$$

where C_0 is the naive cone family, (3.4). The vectors permitted by the n th cone family have n allowed images and preimages. For twist maps this refinement procedure produces increasingly restrictive cone families [Strk88]. If it ever happens that $C_n(\theta, p)$ is empty, i.e. that the intersection in (3.5) contains no vectors, then no invariant circle can pass through the point (θ, p) .

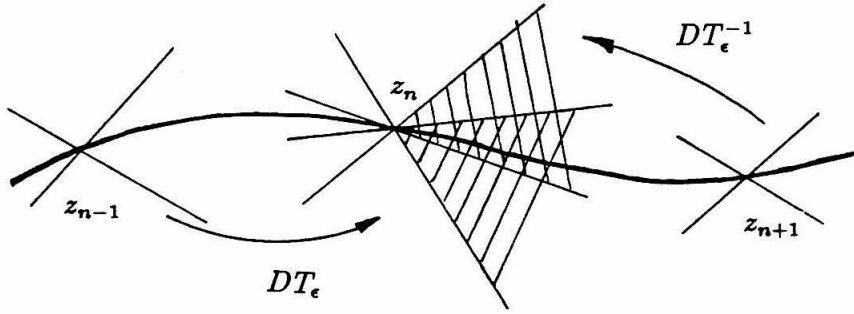


Figure 3.7: *Refining the cone family. The inverse image of the cone at z_{n+1} and the forward image of the cone at z_{n-1} intersect in a new, smaller cone at z_n .*

Cone crossing arguments turn out to be quite successful, though they need a little more elaboration to be suitable for computation. So far we have seen how to prove that no invariant circle can pass through a particular point, now let us use this to prove non-existence of circles. Because a rotational invariant circle must cross every vertical line, we can establish non-existence by proving that no circle can cross a particular vertical line $\{(\theta, p) | \theta = \theta_0, p \in [0, 1]\}$. To do that we divide the phase space up into finitely many pieces. For example, each piece might be a rectangle of the form $R_{ij} = \{(\theta, p) | p \in [p_j, p_{j+1}] \theta \in [\theta_j, \theta_{j+1}]\}$. We can use this decomposition to construct a sequence of piecewise constant cone families, see figure (3.8).

$$C_n(R_{ij}) \equiv \{L_{n-}(R_{ij}), L_{n+}(R_{ij})\} \quad C_0(R_{ij}) = \{-L, +L\}$$

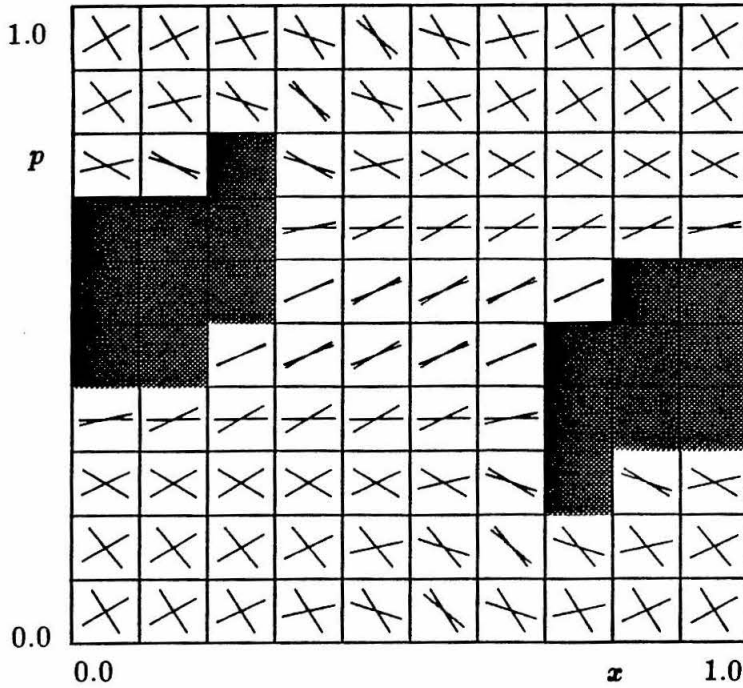


Figure 3.8: A piecewise constant cone family for the standard map with $k = 1.0$. No invariant circles can pass through the shaded squares.

$$L_{n-}(R_{ij}) = \text{l.b.}_{R_{ij}} L_{n-}(\theta, p),$$

$$L_{n+}(R_{ij}) = \text{u.b.}_{R_{ij}} L_{n+}(\theta_0, p). \quad (3.6)$$

where the notations “u.b.” and “l.b.” mean “upper bound” and “lower bound.” If the rectangles are small enough, refinements like (3.6) can eventually produce a whole vertical strip of empty cones.

Finally, we note that the foregoing serves to prove non-existence for a single map. In practice one wants non-existence results for a whole class of maps, for example, for all the standard maps with parameters $k_{min} \leq k \leq k_{max}$. One need only modify (3.6) a little, taking the bounds over both R_{ij} and k .

Stark has shown that such a program, allied with some extra observations, can reveal non-existence of circles with only a finite amount of work. He shows, for example, that if one has a family of maps depending on parameters and one studies a compact set of the parameters for which no invariant circles exist, then the cone-crossing criterion will demonstrate their non-existence after only a finite amount of

computation.⁹

3.1.3 some new coordinates and two more criteria

Here we will begin to explain one way to implement the ideas of the previous section on a digital computer. In the process we will reformulate the cone-crossing criterion in a way that obscures its geometric origin¹⁰ but reveals a connection to minimizing states. The first step is to recast the map in terms of delay coordinates; we have been considering $T_\epsilon(\theta, p) = (\theta', p')$, let us now speak of $g_\epsilon : \mathbf{T} \times \mathbf{T} \mapsto \mathbf{T} \times \mathbf{T}$ so that $g_\epsilon(\theta_n, \theta_{n+1}) = (\theta_{n+1}, \theta_{n+2})$ where the θ 's are angular coordinates of successive points in an orbit. We will also need a lift of g , $G_\epsilon : \mathbf{R} \times \mathbf{R} \rightarrow \mathbf{R} \times \mathbf{R}$, $G_\epsilon(u, v) = (u', v')$. As before, T_ϵ and G_ϵ are related by an action generating function, $H_\epsilon(u, v)$, where

$$\begin{aligned} H_\epsilon(x_n, x_{n+1}) &= \frac{1}{2}(x_{n+1} - x_n)^2 - \epsilon V(x_{n+1}), & V(x) &= - \int_0^x f(y) dy, \\ \partial_1 H_\epsilon(x_n, x_{n+1}) &= -p_n, \\ \partial_2 H_\epsilon(x_n, x_{n+1}) &= p_{n+1}, \end{aligned}$$

and

$$\begin{aligned} G_\epsilon(x_{n-1}, x_n) &\equiv (x_n, x_{n+1}), \\ x_{n+1} &= x'(x_n, p_n), \\ &= x'(x_n, \partial_2 H_\epsilon(x_{n-1}, x_n)). \end{aligned}$$

In terms of these coordinates an invariant circle appears as a curve $x_{n+1} = \gamma(x_n)$ satisfying

$$\begin{aligned} \gamma(u+1) &= \gamma(u) + 1, \\ G_\epsilon(x_n, \gamma(x_n)) &= (x_{n+1}, x_{n+2}) = (\gamma(x_n), \gamma(\gamma(x_n))). \end{aligned}$$

The most naive Lipschitz cone, (3.4) with $L_{0\pm} = \pm\infty$, appears here as $0 \leq \ell \leq \infty$

⁹Here “finite” means that one could do the calculations to some finite precision and refine the cone families for some finite number of steps.

¹⁰See [MP85] for a more direct implementation.

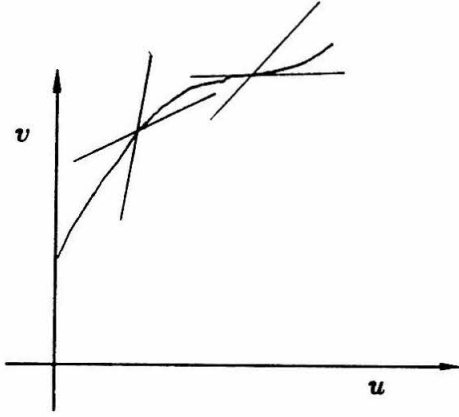


Figure 3.9: *An invariant curve and some Lipschitz cones in the delay coordinate system.*

where ℓ is the slope of γ . The lower bound of zero is just the requirement that the original map, when restricted to an invariant curve, be order preserving.

For examples like (3.1) u' and v' have very simple forms:

$$\begin{aligned} u'(u, v) &= v, \\ v'(u, v) &= v + (v - u) + \epsilon f(v), \\ &= 2v - u + \epsilon f(v). \end{aligned} \tag{3.7}$$

G_ϵ 's action on tangent vectors is equally simple:

$$\begin{bmatrix} \delta u' \\ \delta v' \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ -1 & 2 - \epsilon \frac{d^2 V}{dx^2} \end{bmatrix} \begin{bmatrix} \delta u \\ \delta v \end{bmatrix}. \tag{3.8}$$

For later convenience we will refer to $2 - \epsilon \frac{d^2 V}{dx^2}(x)$ as $\beta(x)$.

If we take a tangent vector, $[1, \ell]$, representing a slope of ℓ then (3.8) tells us that its image will represent a slope ℓ' given by:

$$\begin{aligned} \ell' &= \frac{\delta v'}{\delta u'}, \\ &= \frac{\beta(v)\delta v}{\delta v} - \frac{\delta u}{\delta v}, \\ &= \beta(v) - \frac{1}{\ell}. \end{aligned} \tag{3.9}$$

Preservation of order requires that both ℓ and ℓ' be positive. Combining this with (3.9) we obtain our first real criterion.

Criterion 1 *If there are any values $v \in [0, 1]$ for which $\beta(v) < 0$ then the map $G_\varepsilon(u, v)$ to which β corresponds has no rotational invariant circles. For the standard map this criterion says $k_c \leq 2$.*

We can squeeze one further analytic criterion out of (3.9) by noticing that ℓ' will surely be negative if ever ℓ is very small, and that, always, $\ell' < \max_{v \in [0, 1]} \beta(v)$. Suppose we have m and M such that $0 \leq m \leq \beta(v) \leq M$ holds everywhere. Then

$$\ell' \leq M - \frac{1}{\ell} \quad (3.10)$$

and $\ell' \geq 0$ together imply

$$0 \leq M - \frac{1}{\ell} \quad \text{or} \quad \ell \geq \frac{1}{M}. \quad (3.11)$$

Inequality (3.11) is a global restriction on slopes, a new lower bound for the uniform Lipschitz cone family. We could thus run through the argument again, this time requiring $\ell' \geq \frac{1}{M}$. Having done that we would have a better, narrower cone family and could repeat the argument yet again ... better to carry this process straight to its conclusion and realize that our estimates will stop improving when we find a slope, ℓ_- , such that

$$\ell_- = M - \frac{1}{\ell_-}.$$

This has two roots. The least of them is just the ℓ_- we wanted; the larger one is a global upper bound on slopes. It comes from the remark above, that $\ell' \leq M$. Since every vector tangent to an invariant curve is the image of some other tangent we can conclude $\ell \leq M$. Once that's done we can argue $\ell' \leq M - \frac{1}{M}$ and so on. Finally we attain

$$\ell_- \leq \ell \leq \ell_+ \quad \text{where} \quad \begin{aligned} \ell_- &= \frac{M - \sqrt{M^2 - 4}}{2}, \\ \ell_+ &= \frac{M + \sqrt{M^2 - 4}}{2}. \end{aligned} \quad (3.12)$$

Armed with this best of all possible uniform cones, we are able to make a genuine, dynamical cone crossing argument.

Criterion 2 (“Mather $\frac{4}{3}$ ”) *If $m \leq \beta(v) \leq M$ and ℓ_+ and ℓ_- are the bounds of the uniform cone family given by (3.12), then there are no rotational circles if*

$$\ell_- > m - \frac{1}{\ell_+}. \quad (3.13)$$

Remark *For the standard map, $m = (2 - k)$ and $M = (2 + k)$ and so (3.13) implies that $k_c \leq \frac{4}{3}$.*

Proof The idea is to concentrate on those states that contain the point where β attains its minimum, where $\beta(v) = m$. Visits to this point are most punishing to the slopes of tangent vectors; they lead to the smallest possible values of ℓ' in (3.9). If m is so small that even the slope from the upper edge of the uniform family, ℓ_+ , is diminished to an untenable value, then certainly no others can survive.

3.1.4 non-existence for minimalists

We will now reformulate Criterion 2 in the language of minimizing states. The new version will prove more fruitful for higher-dimensional generalizations. Here again we follow MacKay and Percival, who demonstrated that their cone crossing criterion is equivalent to the action-difference criterion put forward by Mather in [Ma86].

We begin by assuming that an invariant circle exists, then we deduce some facts about the minimizing orbits lying on it. Then, to prove non-existence, we will do a calculation that contradicts these facts. Define a *minimizing state* to be sequence $\{\dots x_{n-1}, x_n, x_{n+1}, \dots\}$ such that every finite segment x_n, x_{n+1}, \dots, x_m is a minimum of the action functional,

$$W_{m,n}(X) = \sum_{j=m}^{n-1} H_\epsilon(x_j, x_{j+1}), \quad (3.14)$$

where H_ϵ is the action-generating function and we consider variations that leave x_n and x_m fixed. Mather’s action-difference idea is to note that if an irrational invariant

circle exists, then every orbit on it is minimizing and has the same action. That is, if we take two states arising from orbits on the circle, $X^a = \{\dots, x_0^a, x_1^a, \dots\}$ and $X^b = \{\dots, x_0^b, x_1^b, \dots\}$ and take the limit

$$\lim_{n \rightarrow \infty} \sum_{j=-n}^{n-1} H_\epsilon(x_j^a, x_{j+1}^a) - H_\epsilon(x_j^b, x_{j+1}^b) \quad (3.15)$$

it should come out to be zero.¹¹ He suggests that to test the existence of an invariant circle having irrational rotation number ω one should approximate ω by a sequence of rational numbers, $\frac{p_n}{q_n}$, and use the rational numbers to construct the two sequences of Birkhoff periodic orbits, the minimax and minimizing orbits. These sequences accumulate on two distinct sets on the putative invariant circle. If the circle is really present, orbits on the two sets should have the same action and so the limit

$$\Delta W_\omega \equiv \lim_{\substack{p_n, q_n \\ \frac{p_n}{q_n} \rightarrow \omega}} \Delta W_{p_n, q_n} = W_{(p_n, q_n) \text{ minimax}} - W_{(p_n, q_n) \text{ minimizing}} \quad (3.16)$$

should tend to zero. If it tends to some other value then no circle with rotation number ω exists. Rather than trying to calculate the limit in (3.16), we will exploit the fact that every state $X = \{\dots, x_{-1}, x_0, x_1, \dots\}$ arising from an orbit $\{\dots, (x_{-1}, p_{-1}), (x_0, p_0), (x_1, p_1), \dots\}$ lying in an invariant circle must be minimizing; every finite segment snipped out of such a state must be a non-degenerate minimum over all segments having the same endpoints¹².

The foregoing suggests a strategy for proving converse KAM theorems. One chooses an auspicious starting point, x_0 , for which the perturbation to the generating function is large, and considers every possible state containing it. This is not quite so huge a task as it sounds. Since the map, $G_\epsilon(u, v)$, determines the whole state

¹¹Showing that the action difference (3.15) vanishes is different, and harder, than showing that the *average* values of the actions are the same. While the latter follows from the ergodicity of irrational rotation, Mather's result requires a more delicate examination of the action functional. See [Ma86] for details.

¹²The reader may wonder why the states lying on an invariant circle do not belong to a one parameter family, and ask how they can lead to non-degenerate minima. The answer is that we consider only variations that leave the endpoints of finite segments fixed; if we allowed them to move the minima would be degenerate.

once, say, x_0 and x_1 have been given, we need only consider all possible successors, x_1 . For each x_1 we work out the state, X , and the variation of the action over finite segments, $\{x_{-1}, x_0, \dots, x_n\}$,

$$\begin{aligned}\delta W_{-1,n} &= \sum_{j=1}^{n-1} \frac{\partial W_{-1,n}}{\partial x_j} \delta x_j + \frac{1}{2} \delta \mathbf{x}^T \mathbf{D}^2 W_{-1,n} \delta \mathbf{x} \\ &= 0 + \frac{1}{2} \sum_{j,k=1}^{n-1} \frac{\partial^2 W_{-1,n}}{\partial x_j \partial x_k} \delta x_j \delta x_k.\end{aligned}$$

The term linear in δx_j is automatically zero because X is a minimizing state. For our examples, (3.1), the quadratic term can be represented by the symmetric matrix,

$$\mathbf{D}^2 W_{-1,n} = \begin{bmatrix} 2 + \epsilon \frac{df}{dx}(x_0) & -1 & 0 & \dots & \dots & 0 \\ -1 & 2 + \epsilon \frac{df}{dx}(x_1) & -1 & \dots & \dots & 0 \\ \vdots & & & \ddots & & \vdots \\ \vdots & & & & \ddots & \vdots \\ 0 & \dots & \dots & -1 & 2 + \epsilon \frac{df}{dx}(x_{n-2}) & -1 \\ 0 & \dots & \dots & \dots & -1 & 2 + \epsilon \frac{df}{dx}(x_{n-1}) \end{bmatrix},$$

which we shall call $M_n(X)$, or M_n for short.

If X is minimizing then M_n is positive definite. Since M_n is so simple it is easily rendered into diagonal form, a form that makes it simple to calculate the determinant.

We can write

$$\begin{bmatrix} 2 + \epsilon \frac{df}{dx}(x_0) & -1 & 0 & 0 & \dots \\ -1 & 2 + \epsilon \frac{df}{dx}(x_1) & -1 & 0 & \dots \\ 0 & -1 & 2 + \epsilon \frac{df}{dx}(x_2) & -1 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix} \rightarrow \begin{bmatrix} d_0 & 0 & 0 & 0 & \dots \\ 0 & d_1 & 0 & 0 & \dots \\ 0 & 0 & d_2 & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

where the d_j are computed recursively using

$$\begin{aligned}d_0 &= 2 + \epsilon \frac{df}{dx}(x_0), \\ d_{j+1} &= \beta(x_{j+1}) - \frac{1}{d_j}, \quad \text{where } \beta(x_{j+1}) = 2 + \epsilon \frac{df}{dx}(x_{j+1}).\end{aligned}\tag{3.17}$$

If ever one of the d_j is negative we may conclude that M_j is not positive definite and so does not arise from a minimizing state. Notice the similarity between the evolution equation for the diagonal entries, (3.17), and the one for slopes, (3.9). As we refined the limits on slopes, so we can refine those on diagonal entries. We obtain a d_- such that if $d_j < d_-$ then some later d_k , $k > j$ is sure to be negative. We also get d_+ , a global upper bound on the d_j . We can thus modify (3.17) so that we begin with $d_{-1} = d_+$, so $d_0 = \beta(x_0) - \frac{1}{d_+}$. The original prescription corresponds to taking $d_{-1} = \infty$.

3.2 Rigorous computing

In this section we will see how to implement the action criterion of the last section on a digital computer. Since we will eventually want to treat maps in spaces of arbitrary dimension we will outline some of the procedures in greater generality than required for the cylinder. The most important part will be a technique for rigorously bounding the image of a set.

3.2.1 two reductions and a plan

As in section (3.1.2), we need only show that no invariant circle crosses a particular vertical line. In the language of the previous section this means our problem is reduced to showing that some particular x_0 cannot appear as a member of any minimizing state. We can get a further reduction by noticing that our examples satisfy

$$p'(\theta, p + 1) = p'(\theta, p) + 1;$$

their dynamical structure is periodic in p as well as in θ . So, if an invariant circle passes through the point (θ, p) , there is also one through $(\theta, p + 1)$; if no invariant circles pass through some vertical segment $I_0 \equiv \{(\theta, p) | \theta = \theta^*, p \in [0, 1]\}$, then there

cannot be any at all. Studying a segment like I_0 is equivalent to studying a collection

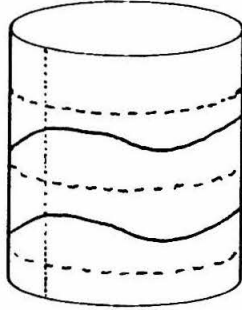


Figure 3.10: *Rotational invariant circles must cross every vertical line, and, for our examples, must be periodic in p as well as θ .*

of states $\{X \mid x_0 = x^*, x_1 \in [0, 1]\}$, where x^* is a lift of θ^* . With these reductions in hand, we are ready to plan the main computation. Our goal will be to prove:

Theorem

There is an $x^ \in [0, 1]$ and an interval of parameter values, $I_\epsilon \equiv [\epsilon_-, \epsilon_+]$, such that none of the maps, G_ϵ , $\epsilon \in I_\epsilon$, have a minimizing state with $x_0 = x^*$.*

Plan for the proof:

- (i) Formally extend the phase space to include the parameter ϵ and use the map $G_\epsilon(u, v)$ to define a new one, $G : \mathbf{R} \times \mathbf{R} \times \mathbf{R} \rightarrow \mathbf{R} \times \mathbf{R} \times \mathbf{R}$, where

$$G(\epsilon, u, v) = (\epsilon, G_\epsilon(u, v)). \quad (3.18)$$

- (ii) Select a starting point x^* . For examples (3.1) we will want x^* such that $\beta(x^*)$ is a minimum, a choice that is independent of ϵ .

- (iii) Divide the interval $[0, 1]$ into a collection of closed intervals, I_j , $\bigcup_{j=1}^N I_j = [0, 1]$. Using the I_j , which should intersect only at their endpoints, we can construct a collection of sets in the extended phase space, $S_j \equiv \{(\epsilon, u, v) \mid \epsilon \in I_\epsilon, u = x^*, v \in I_j\}$. In practice, this division is done by the program itself. It begins by trying to prove the theorem on the whole interval at once, and gets either, “Yes, the theorem is true,” or “Maybe it’s true.” If the answer is “maybe” it splits the interval

in half and tries the two pieces separately. If one of them yields “maybe” it gets subdivided too The process of subdivision will go on forever if the theorem is false, but if it is true the work of Stark suggests that the cutting will stop after finitely many steps.

- (iv) For each piece I_j , try to prove that no minimizing state with $x_0 = x^*$ can have $x_1 \in I_j$.

The last step is where the computation comes in; we will use an argument like the one at the end of section (3.1.4), but here we calculate upper bounds¹³ \bar{d}_k for the k th diagonal entry in (3.17).

$$\begin{aligned} \bar{d}_0 &= \text{u.b.}_{\epsilon \in I_\epsilon} \beta(x^*) - \frac{1}{d_+}, \\ \bar{d}_1 &= \text{u.b.}_{(\epsilon, u, v) \in S_j} \beta(v) - \frac{1}{\bar{d}_0}, \\ \bar{d}_2 &= \text{u.b.}_{(\epsilon, u, v) \in G(S_j)} \beta(v) - \frac{1}{\bar{d}_1}, \\ &\vdots \\ \bar{d}_{n+1} &= \text{u.b.}_{(\epsilon, u, v) \in G^n(S_j)} \beta(v) - \frac{1}{\bar{d}_n}. \end{aligned} \tag{3.19}$$

Finding a way to calculate the kind of bound that appears in the definition of \bar{d}_2 , an upper bound over an image of S_j , is the last hurdle in the argument. What we need is a procedure to rigorously bound the image of a set. In the next section we will explain a quite general scheme due to MacKay and Percival.

3.2.2 bounding images of prisms

For concreteness, and to get an algorithm straightforward enough to be realized as a computer program, we will concentrate on sets with a prescribed form, parallelepipeds, or *prisms* for short. An n -dimensional prism is specified by a center

¹³We will often want to evaluate upper bounds, as opposed to maxima. The former are realizable on computers, the latter may not be.

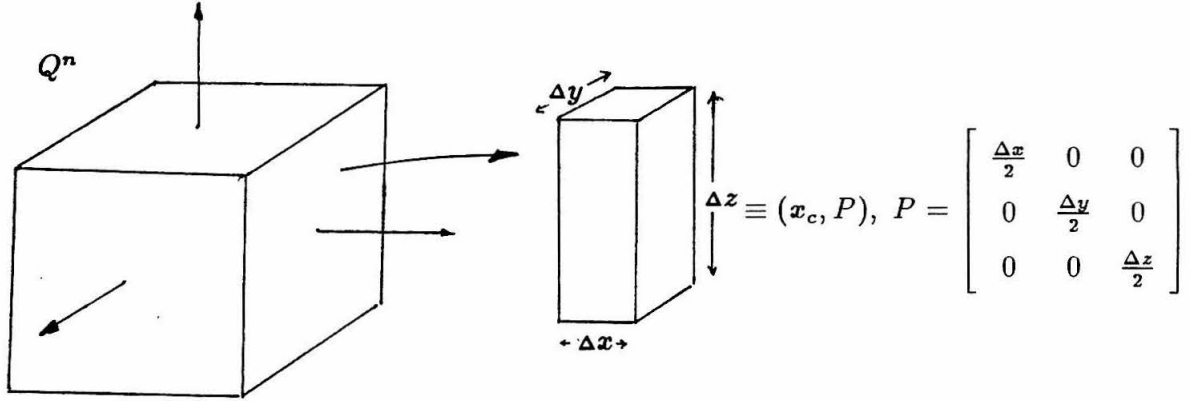


Figure 3.11: The n -dimensional hypercube Q^n is mapped to the prism by the matrix P .

point, x_c , and an $n \times n$ matrix, P . The prism is the set

$$\{x \in \mathbf{R}^n | x = x_c + P\eta, \eta \in Q^n\}, \quad (3.20)$$

where Q^n is the n -dimensional hypercube, $\{\eta \in \mathbf{R}^n | -1 \leq \eta_j \leq 1\}$, see figure (3.11).

Our principal technical tool is the following result.

Lemma ([MP85]) *Suppose $\Phi : \mathbf{R}^n \rightarrow \mathbf{R}^n$ is a C^1 map. Then the Φ - image of the prism $S \equiv (x_c, P)$ is contained in the prism (x_c', P') where x_c' is arbitrary, $P' = A \circ W$ for an arbitrary invertible matrix A , and W the diagonal matrix*

$$W = \begin{bmatrix} w_1 & 0 & \cdots & 0 \\ 0 & w_2 & \cdots & 0 \\ \vdots & & \ddots & \vdots \\ 0 & 0 & \cdots & w_n \end{bmatrix}$$

with

$$w_j = \text{u.b.} \left(|(\Phi(x_c) - x_c')_j| + \text{u.b.}_{x \in S} \sum_{k=1}^n |[A^{-1} \circ D\Phi_x \circ P]_{jk}| \right). \quad (3.21)$$

Remark *The lemma seems unnecessarily general; we are left to choose the matrix A and the new center point, x_c completely arbitrarily. If we choose them unwisely the*

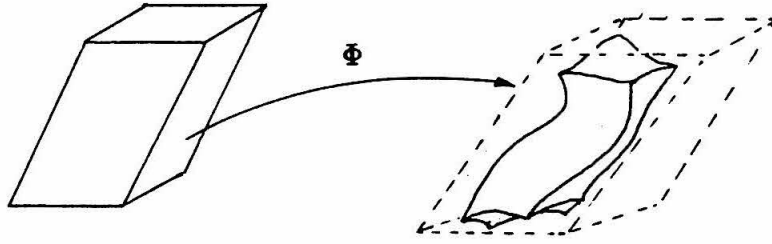


Figure 3.12: A prism, its image, and a prism bounding the image.

new prism will surround the image of S , but may be much larger than necessary. Usually we will want

$$\mathbf{x}_c' \approx \Phi(\mathbf{x}_c), \quad \text{and} \quad A \approx D\Phi_{\mathbf{x}_c} \circ P.$$

The freedom allowed by the lemma will make it easy to handle errors in computing $\Phi(\mathbf{x}_c)$ and cases where $D\Phi_{\mathbf{x}_c}P$ is singular or nearly singular.

Example (Proof of the lemma for one-dimensional maps)

We start in with a one-dimensional example, see figure (3.13). Here the map is some C^1 function, $\phi : \mathbf{R} \rightarrow \mathbf{R}$, and a prism, S , is just an interval $x_c - \Delta x \leq x \leq x_c + \Delta x$. We can use the computer to find $\bar{\phi}(x)$, a numerical approximation to $\phi(x)$ for which $|\phi(x) - \bar{\phi}(x)| \leq \delta$. Then, choosing $x_c' = \bar{\phi}(x_c)$ and¹⁴ $A = \phi'(x_c)\Delta x$, we find

$$\begin{aligned} \text{u.b. } |x_c' - \phi(x_c)| &\leq \delta, \\ A^{-1} &= \frac{1}{\phi'(x_c)\Delta x}, \\ W &= \frac{\delta}{|\phi'(x_c)\Delta x|} + \text{u.b.}_{x \in S} \left| \frac{\phi'(x)\Delta x}{\phi'(x_c)\Delta x} \right|, \\ &= \frac{\delta}{|\phi'(x_c)\Delta x|} + \text{u.b.}_{x \in S} \left| \frac{\phi'(x)}{\phi'(x_c)} \right|, \end{aligned}$$

and

$$P' \equiv \Delta x' = A \circ W \geq \delta + \Delta x (\max_{x \in S} |\phi'(x)|). \quad (3.22)$$

¹⁴The choice of A is meant to suggest the form required by the higher-dimensional theorem. If $\phi'(x_c) = 0$ we will have to make another choice; any constant will do.

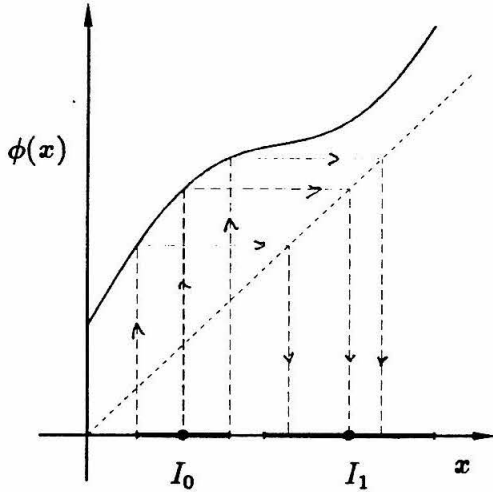


Figure 3.13: *The bounding lemma applied to a lift of the circle map, $\phi(x) = x + \Omega + \frac{\epsilon}{2\pi} \sin(2\pi x)$, with $\Omega = 0.3$, $\epsilon = 0.8$. The interval I_1 , at right, is the one given by the lemma; it contains the image of I_0 .*

Now let us check some point $x \in S$, and see that its image is inside the prism $S' = (x'_c, P')$. Since x is in S we can write $x = x_c + \eta \Delta x$ with $-1 \leq \eta \leq 1$. If $\phi(x)$ is in S' , then,

$$x'_c - \Delta x' \leq \phi(x) \leq x'_c + \Delta x' \quad \text{or} \quad |\phi(x) - x'_c| \leq \Delta x'.$$

To see that this is true, consider $\gamma(t) = \phi(x_c + t\eta \Delta x)$. $\gamma(t)$ is a C^1 function from $[0,1]$ to \mathbf{R} with $\gamma(0) = \phi(x_c)$, $\gamma(1) = \phi(x)$. By the Mean Value Theorem there is a $t_0 \in [0,1]$ such that

$$\begin{aligned} \gamma(1) - \gamma(0) &= \frac{d\gamma}{dt}(t_0), \\ \phi(x) - \phi(x_c) &= \frac{d}{dt}(\phi(x_c + t_0\eta \Delta x)), \\ &= \eta \Delta x \phi'(x_c + t_0\eta \Delta x). \end{aligned}$$

Rewriting this,

$$\begin{aligned} |\phi(x) - x'_c| &= |\phi(x_c) - x'_c + \eta \Delta x \phi'(x_c + t_0\eta \Delta x)|, \\ &\leq |\phi(x_c) - x'_c| + |\Delta x \phi'(x_c + t_0\eta \Delta x)|, \\ &\leq \Delta x', \end{aligned} \tag{3.23}$$

even as the lemma claimed.

Proof (The general case)

The argument is much the same as the one-dimensional argument above. Here the assertion of the theorem is that every point in the initial prism, $S = (x_c, P)$, has its image in $S' = (x'_c, P')$. If one writes a point, $x \in S$, as $x = x_c + P\eta$, $\eta \in Q^n$ then the theorem says

$$P'^{-1}(\Phi(x_c + P\eta) - x'_c) = \eta', \quad \eta' \in Q^n. \quad (3.24)$$

If we take (3.24) one component at a time we find

$$|[P'^{-1}(\Phi(x_c + P\eta) - x'_c)]_j| \leq 1. \quad (3.25)$$

To prove this for the j th component we consider a function $\gamma_j : [0, 1] \rightarrow \mathbf{R}$, $\gamma_j(t) = [P'^{-1}\Phi(x_c + tP\eta)]_j$. $\gamma_j(t)$ has the same smoothness as the map and so the Mean Value Theorem says $\exists t_0 \in [0, 1]$ such that

$$\begin{aligned} \gamma_j(1) - \gamma_j(0) &= \frac{d\gamma_j}{dt}(t_0), \\ \text{or } [P'^{-1}(\Phi(x_c + P\eta) - \Phi(x_c))]_j &= [P'^{-1} \circ D\Phi_{(x_c + t_0 P\eta)} \circ P\eta]_j. \end{aligned}$$

Arguing as we did in the sequence (3.23);

$$\begin{aligned} |[P'^{-1}(\Phi(x_c + P\eta) - x'_c)]_j| &= \left| [W^{-1} \circ A^{-1} \{(\Phi(x_c) - x'_c) + D\Phi_{\gamma(t_0)} \circ P\eta\}]_j \right|, \\ &= \frac{1}{w_j} \left| [A^{-1} \{(\Phi(x_c) - x'_c) + D\Phi_{\gamma(t_0)} \circ P\eta\}]_j \right|, \\ &\leq \frac{1}{w_j} \left\{ |[A^{-1}(\Phi(x_c) - x'_c)]_j| \right. \\ &\quad \left. + \sum_{k=1}^n |[A^{-1} \circ D\Phi_{\gamma(t_0)} \circ P]_{jk}| \right\}, \\ &\leq 1, \end{aligned}$$

which is just the thing required by (3.25).

3.2.3 choices for the matrix A

Although we usually take $A \approx D\Phi_{x_c} \circ P$ we may sometimes need to make a different choice to avoid a singular A . Indeed, the very first prisms we consider, the ones of the

form $I_\epsilon \times x^* \times I_j$, have zero width in the u direction and so have singular matrices, P . In this section we will illustrate two schemes for fattening up the matrix $D\Phi_{x_c} \circ P$. The first, the *fixed-form* scheme, is borrowed directly from [MP85]. The second, called the *column-rotor*, is a slight generalization of theirs. These techniques have not been carefully optimized and are probably not the best. They work well enough and, in any case, are not the most time consuming part of the algorithm.

Fattener 1 (fixed-form) Require the new matrix to have a particular form. Suppose, for example, that the initial prism, P , and the derivative of the map, $D\Phi_{x_c}$, are

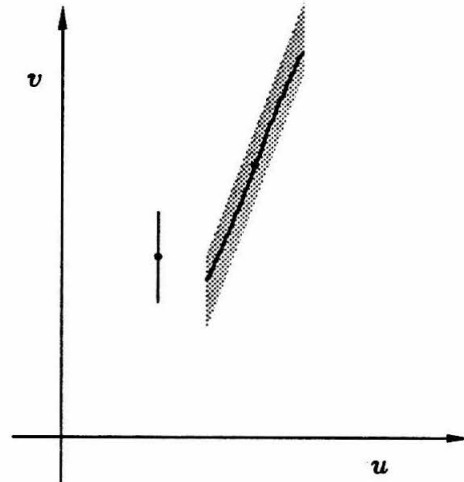
$$P = \begin{bmatrix} 0 & 0 \\ 0 & \frac{\Delta y}{2} \end{bmatrix}, \quad D\Phi_{x_c} = \begin{bmatrix} 0 & 1 \\ -1 & \beta(x_c) \end{bmatrix}, \quad \text{and so} \quad D\Phi_{x_c} \circ P = \begin{bmatrix} 0 & \frac{\Delta y}{2} \\ 0 & \frac{\Delta y}{2} \beta(x_c) \end{bmatrix},$$

We might then look for a matrix A of the form

$$A = \begin{bmatrix} 0 & a_{12} \\ 1 & a_{22} \end{bmatrix}.$$

Figure (3.14) shows an application of this scheme.

Figure 3.14: *The fixed-form fattener applied to the image of a singular, vertical prism. The map is the delay-embedded version of the standard map with $k = 0.8$. The new prism, shown in grey, fits snugly in the u direction but is much more generous in the v direction.*



Fattener 2 (column-rotor) This method deals with matrices whose columns, when viewed as vectors, are all very nearly parallel. Such matrices will be close to singular,

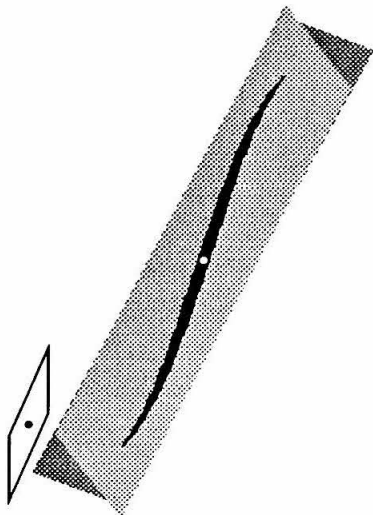


Figure 3.15: *The column-rotor scheme applied to a narrow prism. The initial prism is at the lower left; it is outlined in black and its center is marked with a dot. The prism's true image is solid black. A bounding prism, produced with the column-rotor scheme using an angle of 27° , is shown in light grey, the darker prism beneath used an angle of 90° .*

and must be expected to arise if the dynamics are hyperbolic. If we neglect the fattening steps, the matrix of the prism bounding $\Phi^n(S_0)$ looks like

$$P_n \approx D\Phi_{\Phi^{n-1}(x_c)} \circ D\Phi_{\Phi^{n-2}(x_c)} \circ \cdots \circ D\Phi_{x_c} \circ P. \quad (3.26)$$

If any of the Lyapunov exponents are positive the columns of the matrix product (3.26) will be nearly parallel to each other and to the eigenvector corresponding to the largest eigenvalue of $D\Phi_{x_c}^n$. The idea of this scheme is to rotate the columns with respect to one another so as to guarantee a certain minimum angle between each pair. In two dimensions, (see figure (3.15)), this is an entirely satisfactory program. In three and more dimensions it is possible to find linearly dependent collections of column vectors each pair of which is separated by a sizable angle - one could have a triple of coplanar vectors, for example. Such collections do not seem to arise in our calculations, and we have made no special provisions to avoid them. The details of column rotation are described in appendix B.

3.3 On to higher dimension

Here we develop some new results. The forms of the arguments will be much the same as in the preceding sections, but the maps, tori, and cones will exist in higher-dimensional spaces. The general results for higher-dimensional invariant tori are not so strong as for circles on the cylinder, so we must make a few new restrictions and will obtain somewhat weaker results. We will see how to generalize the cone-crossing and action criteria and then show an application to the example with the trigonometric perturbation, (2.14).

3.3.1 maps and tori

As above, we will consider only small perturbations of integrable systems. We will have $2n$ -dimensional symplectic maps, $f_\epsilon : \mathbf{T}^n \times \mathbf{R}^n \rightarrow \mathbf{T}^n \times \mathbf{R}^n$, of the form

$$\begin{aligned} f_\epsilon(\boldsymbol{\theta}, \mathbf{p}) &= (\boldsymbol{\theta}'(\boldsymbol{\theta}, \mathbf{p}), \mathbf{p}'(\boldsymbol{\theta}, \mathbf{p})) \\ \boldsymbol{\theta}' &= \boldsymbol{\theta} + \mathbf{p} - \frac{\partial V_\epsilon}{\partial \boldsymbol{\theta}} \\ \mathbf{p}' &= \mathbf{p} - \frac{\partial V_\epsilon}{\partial \boldsymbol{\theta}} \end{aligned} \tag{3.27}$$

where $V_\epsilon(\boldsymbol{\theta}) : \mathbf{T}^n \rightarrow \mathbf{R}$ is some periodic function with at least two continuous derivatives and ϵ is drawn from some, perhaps multi-dimensional, parameter space. We will work mostly with a lift, $F_\epsilon : \mathbf{R}^n \times \mathbf{R}^n \rightarrow \mathbf{R}^n \times \mathbf{R}^n$. As we noted in chapter 2, maps like (3.27) are the higher dimensional analogs of standard-type maps.

The generating function for a map like (3.27) is

$$\begin{aligned} H_\epsilon(\mathbf{x}, \mathbf{x}') &= \frac{1}{2} \|\mathbf{x} - \mathbf{x}'\|^2 - V_\epsilon(\mathbf{x}) \\ &= \sum_{j=1}^n (x'_j - x_j)^2 - V_\epsilon(\mathbf{x}). \end{aligned} \tag{3.28}$$

Although $H_\epsilon(\mathbf{x}, \mathbf{x}')$ is formally very similar to the generating functions used earlier in the chapter it is not quite the same; the perturbation, V_ϵ , depends on \mathbf{x} rather

than \mathbf{x}' . As we shall see, this makes no real difference in the formulation of non-existence criteria. We make this small change because the examples of chapter 2 have generating functions like (3.28).

As on the cylinder, we will not be able to prove the non-existence of all possible types of tori, only those that are invariant graphs, sets of the form $\{(\boldsymbol{\theta}, \mathbf{p}) \mid \boldsymbol{\theta} \in \mathbf{T}^n, \mathbf{p} = \boldsymbol{\psi}(\boldsymbol{\theta})\}$ for some $\boldsymbol{\psi} : \mathbf{T}^n \rightarrow \mathbf{R}^n$. In higher dimension we must add the further requirement that the graphs be *Lagrangian*, that is, they must have¹⁵

$$\frac{\partial \psi_i}{\partial \theta_j} = \frac{\partial \psi_j}{\partial \theta_i}. \quad (3.29)$$

On the cylinder we have the mighty theorem of Birkhoff to assure us that any rotational invariant circle must be a graph. Unfortunately, for $n > 1$ we have no such assurance; there may be “accidental” invariant tori that are graphs, but not Lagrangian graphs, and there may even be rotational invariant tori that are not graphs at all. Still, (3.29) is not a disastrous restriction. Our techniques are fully complementary to traditional KAM theory in that constructive versions of KAM produce just the sort of tori we can preclude, invariant, Lagrangian graphs.

Herman, in [Herm88], has announced some results along the lines of a higher-dimensional version of Birkhoff’s theorem, but they are not so comprehensive as the original. He has, however, shown that a Lagrangian graph, invariant under a map like (3.27), is Lipschitz. This will prove helpful when we try to obtain global inequalities like (3.12).

3.3.2 Lipschitz cones: old formulae in new guises

Both the cone-crossing and action minimizing criteria have higher-dimensional analogs. We will briefly examine the former because of its intuition-pleasing geometric roots,

¹⁵Equivalently, a Lagrangian torus is one on whose tangent space the symplectic two-form, $\omega = \sum_{j=1}^n dp_j \wedge d\theta_j$, vanishes.

then concentrate on the latter. Most of the formulae will bear a strong formal resemblance to the ones from the first part of the chapter.

As on the cylinder, we begin by switching to a map g acting on the delay coordinates, $g_\epsilon(\boldsymbol{\theta}_i, \boldsymbol{\theta}_{i+1}) = (\boldsymbol{\theta}_{i+1}, \boldsymbol{\theta}_{i+2})$, and a lift, $G_\epsilon : \mathbf{R}^n \times \mathbf{R}^n \rightarrow \mathbf{R}^n \times \mathbf{R}^n$ with $G_\epsilon(\mathbf{u}, \mathbf{v}) = (\mathbf{u}', \mathbf{v}')$. In these coordinates the derivative of the map is

$$DG_\epsilon = \begin{bmatrix} \frac{\partial \mathbf{u}'}{\partial \mathbf{u}} & \frac{\partial \mathbf{u}'}{\partial \mathbf{v}} \\ \frac{\partial \mathbf{v}'}{\partial \mathbf{u}} & \frac{\partial \mathbf{v}'}{\partial \mathbf{v}} \end{bmatrix} = \begin{bmatrix} 0 & \mathbf{I} \\ -\mathbf{I} & 2\mathbf{I} - \frac{\partial^2 V_\epsilon}{\partial \mathbf{x}^2}(\mathbf{v}) \end{bmatrix}, \quad (3.30)$$

where \mathbf{I} is the $n \times n$ identity matrix and $\frac{\partial^2 V_\epsilon}{\partial \mathbf{x}^2}$ is the matrix of second partial derivatives of V_ϵ . An invariant graph, $\mathbf{p} = \boldsymbol{\psi}(\boldsymbol{\theta})$, appears as a hypersurface

$$\begin{aligned} \mathbf{v} &= \boldsymbol{\Lambda}(\mathbf{u}), \\ &= \mathbf{u} + \boldsymbol{\psi}(\mathbf{u}) - \frac{\partial V_\epsilon}{\partial \mathbf{x}}(\mathbf{u}). \end{aligned}$$

$V_\epsilon(\mathbf{u})$ and $\boldsymbol{\psi}(\mathbf{u})$ are periodic extensions and $\boldsymbol{\Lambda}(\mathbf{u} + \mathbf{m}) = \boldsymbol{\Lambda}(\mathbf{u}) + \mathbf{m} \forall \mathbf{m} \in \mathbf{Z}^n$. The geometric object corresponding to a vector tangent to an invariant circle is now a hyperplane tangent to the graph. A vector, $(\delta \mathbf{u}, \delta \mathbf{v})$, lying in this hyperplane has

$$\delta \mathbf{v} = \mathbf{L} \delta \mathbf{u} \quad \text{where} \quad \mathbf{L} = \begin{bmatrix} \frac{\partial \Lambda_1}{\partial u_1} & \frac{\partial \Lambda_1}{\partial u_2} & \cdots \\ \frac{\partial \Lambda_2}{\partial u_1} & \frac{\partial \Lambda_2}{\partial u_2} & \cdots \\ \vdots & \vdots & \ddots \end{bmatrix} \quad (3.31)$$

so that the tangent plane is the subspace spanned by the n vectors

$$\begin{aligned} &(1, 0, \dots, 0, \frac{\partial \Lambda_1}{\partial u_1}, \frac{\partial \Lambda_2}{\partial u_1}, \dots, \frac{\partial \Lambda_n}{\partial u_1}), \\ &(0, 1, \dots, 0, \frac{\partial \Lambda_1}{\partial u_2}, \frac{\partial \Lambda_2}{\partial u_2}, \dots, \frac{\partial \Lambda_n}{\partial u_2}), \\ &\vdots \end{aligned}$$

These are conveniently represented in block form as $[\mathbf{I}, \mathbf{L}]$ where \mathbf{I} is the $n \times n$ identity matrix and \mathbf{L} is as in equation(3.31). The action of the map on the hyperplane is

given by

$$DG_\epsilon \circ \begin{bmatrix} \mathbf{I} \\ \mathbf{L} \end{bmatrix} = \begin{bmatrix} 0 & \mathbf{I} \\ -\mathbf{I} & \boldsymbol{\beta} \end{bmatrix} \begin{bmatrix} \mathbf{I} \\ \mathbf{L} \end{bmatrix} = \begin{bmatrix} \mathbf{L} \\ \boldsymbol{\beta}\mathbf{L} - \mathbf{I} \end{bmatrix}, \quad (3.32)$$

where $\boldsymbol{\beta} = 2\mathbf{I} - \frac{\partial^2 V_\epsilon}{\partial \mathbf{x}^2}(\mathbf{v})$. The new tangent hyperplane must then have

$$\mathbf{L}' = \boldsymbol{\beta} - \mathbf{L}^{-1}. \quad (3.33)$$

In the two-dimensional slope evolution equation, (3.9), existence of an invariant circle meant both the slopes ℓ and ℓ' had to be positive. Here the existence of an invariant Lagrangian graph implies that the matrices \mathbf{L} and \mathbf{L}' are positive definite. On the cylinder we were able to study equation (3.9) and obtain a narrower global Lipschitz cone; where first we had $0 \leq \ell \leq \infty$ we eventually got $\ell_- \leq \ell \leq \ell_+$, with ℓ_\pm given by equation (3.12). There is a higher-dimensional analog of this best global Lipschitz cone, but we defer it until section 3.3.4.

3.3.3 minimalism revisited

We now turn to the higher-dimensional generalization of the action criterion. The arguments below come mostly from MacKay, Meiss, and Stark, [MMS89], Katok, [Kat88], and Herman, [Herm88]. The first thing we need is a higher-dimensional version of the theorem of Mather that told us that invariant circles are composed entirely of minimizing orbits. The necessary result, which says that every orbit on an invariant Lagrangian graph is minimizing, has been proven by Katok, [Kat88], and by MacKay, Meiss and Stark, [MMS89]. With this result in hand we can proceed as before. We consider finite segments, $\mathbf{x}_{-1}, \mathbf{x}_0, \dots, \mathbf{x}_n$ taken out of minimizing states. The action functional is still

$$\begin{aligned} W_{-1,n} &= \sum_{j=-1}^{n-1} H_\epsilon(\mathbf{x}_j, \mathbf{x}_{j+1}), \\ &= \sum_{j=-1}^{n-1} \frac{1}{2} \|\mathbf{x}_{j+1} - \mathbf{x}_j\|^2 - V_\epsilon(\mathbf{x}_j). \end{aligned}$$

and the second variation of $W_{-1,n}$ is, in block form,

$$\begin{bmatrix} \beta(\mathbf{x}_0) & -\mathbf{I} & 0 & 0 & \cdots & 0 \\ -\mathbf{I} & \beta(\mathbf{x}_1) & -\mathbf{I} & 0 & \cdots & 0 \\ 0 & -\mathbf{I} & \beta(\mathbf{x}_2) & -\mathbf{I} & & 0 \\ \vdots & & \ddots & \ddots & \ddots & \vdots \\ 0 & & & & -\mathbf{I} & \beta(\mathbf{x}_{n-2}) & -\mathbf{I} \\ 0 & & \cdots & & 0 & -\mathbf{I} & \beta(\mathbf{x}_{n-1}) \end{bmatrix},$$

which is readily block-diagonalized to

$$\begin{bmatrix} \mathbf{d}_0 & 0 & \cdots \\ 0 & \mathbf{d}_1 & \cdots \\ \vdots & \vdots & \ddots \end{bmatrix}.$$

The diagonal blocks, \mathbf{d}_j , are given recursively by

$$\begin{aligned} \mathbf{d}_0 &= \beta(\mathbf{x}_0), \\ \mathbf{d}_{j+1} &= \beta(\mathbf{x}_{j+1}) - \mathbf{d}_j^{-1}, \quad \beta(\mathbf{x}_{j+1}) = 2\mathbf{I} - \frac{\partial^2 V_\epsilon}{\partial \mathbf{x}^2}(\mathbf{x}_{j+1}). \end{aligned} \quad (3.34)$$

Our concern is that the \mathbf{d}_j be positive definite. It is here that blithe, formal, generalization fails us; there are no sensible formal analogs for results like equations (3.10), (3.12) and (3.13). Instead we need to invent a way to test whether the least eigenvalue of \mathbf{d}_j is positive. We will develop a whole suite of estimates for this eigenvalue, then use them and a plan like the one in section 3.2.1 to prove the non-existence of Lagrangian graphs.

All the matrices we will be discussing are real and symmetric, hence, Hermitian. For a particular matrix, M , we will need to define $\lambda_-(M)$, the least eigenvalue of M , $\lambda_+(M)$, the largest eigenvalue, and $\text{Tr}[M] = \sum_{j=1}^{\dim(M)} M_{jj}$, the trace. The following lemma will be our main tool.

Lemma *For real, symmetric, $n \times n$, positive definite matrices β , \mathbf{d} , and \mathbf{d}' with*

$$\mathbf{d}' = \beta - \mathbf{d}^{-1} \quad (3.35)$$

the following suite of inequalities hold:

$$\lambda_-(\mathbf{d}') \leq \frac{1}{n} \text{Tr}[\boldsymbol{\beta}] - \frac{n}{\text{Tr}[\mathbf{d}]}, \quad (3.36)$$

$$\lambda_-(\mathbf{d}') \leq \lambda_+(\boldsymbol{\beta}) - \frac{1}{\lambda_-(\mathbf{d})}, \quad (3.37)$$

$$\lambda_-(\mathbf{d}') \leq \lambda_-(\boldsymbol{\beta}) - \frac{1}{\lambda_+(\mathbf{d})}. \quad (3.38)$$

Proof The first inequality, which is due to Herman, comes from the observations that for a positive definite, Hermitian matrix, M , $\lambda_-(M) \leq \frac{1}{n} \text{Tr}[M]$ and $\text{Tr}[M^{-1}] \leq \frac{n^2}{\text{Tr}[M]}$. Both these inequalities are strict except for the degenerate case where all the eigenvalues are the same. The other two inequalities, which are ours, depend on

$$\lambda_+(M) = \max_{\nu \in \mathbf{R}^n, \|\nu\|=1} \langle \nu, M\nu \rangle$$

and

$$\lambda_-(M) = \min_{\nu \in \mathbf{R}^n, \|\nu\|=1} \langle \nu, M\nu \rangle,$$

where the norm and inner product are the usual Euclidean norm in \mathbf{R}^n and ordinary dot product, $\langle \mathbf{u}, \mathbf{v} \rangle = \sum_{j=1}^n u_j v_j$. Given these equations we can obtain inequalities about the least eigenvalue of \mathbf{d}' in (3.35) by evaluating $\langle \nu, \mathbf{d}'\nu \rangle$ on particular vectors. If, for example, one takes ν to be the unit eigenvector corresponding to the smallest eigenvalue of \mathbf{d} one finds

$$\begin{aligned} \lambda_-(\mathbf{d}') \leq \langle \nu, \mathbf{d}'\nu \rangle &= \langle \nu, \boldsymbol{\beta}\nu \rangle - \langle \nu, \mathbf{d}^{-1}\nu \rangle, \\ &= \langle \nu, \boldsymbol{\beta}\nu \rangle - \frac{1}{\lambda_-(\mathbf{d})}, \\ &\leq \lambda_+(\boldsymbol{\beta}) - \frac{1}{\lambda_-(\mathbf{d})}. \end{aligned}$$

This is inequality (3.37) of the lemma. Inequality (3.38) comes from an identical argument with ν the unit eigenvector corresponding to the least eigenvalue of $\boldsymbol{\beta}$.

3.3.4 global estimates: narrowing the cones

Here we see how to use our inequalities to reduce the range of permissible $\lambda_-(\mathbf{d}_j)$. On the face of it, we must allow $0 \leq \lambda_-(\mathbf{d}) \leq \infty$, but inequalities (3.36) and (3.37) have the correct form to allow an iterative refinement like the one in section 3.1.3. Since $\text{Tr}[\boldsymbol{\beta}(\mathbf{v})]$, and $\lambda_+(\boldsymbol{\beta}(\mathbf{v}))$ are continuous, \mathbf{Z}^n -periodic functions, they have well-defined minima and maxima, say,

$$\begin{aligned} t &\leq \text{Tr}[\boldsymbol{\beta}] \leq T, \\ b &\leq \lambda_+(\boldsymbol{\beta}) \leq B. \end{aligned}$$

Inequalities (3.36) and (3.37) then imply that the \mathbf{d}_j from a minimizing state must satisfy

$$\begin{aligned} \text{Tr}_{\min} \leq \text{Tr}[\mathbf{d}_j] \leq \text{Tr}_{\max}, \quad \text{with} \quad \text{Tr}_{\min} &= \text{l.b.} \left\{ \frac{T - \sqrt{T^2 - 4n^2}}{2} \right\}, \\ \text{Tr}_{\max} &= \text{u.b.} \left\{ \frac{T + \sqrt{T^2 - 4n^2}}{2} \right\}, \end{aligned} \quad (3.39)$$

and

$$\begin{aligned} \lambda_{-\min} \leq \lambda_-(\mathbf{d}_j) \leq \lambda_{-\max}, \quad \text{with} \quad \lambda_{-\min} &= \text{l.b.} \left\{ \frac{B - \sqrt{B^2 - 4}}{2} \right\}, \\ \lambda_{-\max} &= \text{u.b.} \left\{ \frac{B + \sqrt{B^2 - 4}}{2} \right\}. \end{aligned} \quad (3.40)$$

We can also get some analytic use out of inequality (3.38) by combining it with (3.40).

$$\begin{aligned} \lambda_+(\mathbf{d}) &\leq \text{Tr}[\mathbf{d}] - (n-1)\lambda_-(\mathbf{d}) \\ &\leq \text{Tr}[\mathbf{d}] - (n-1)\lambda_{-\min}. \end{aligned}$$

Hence,

$$\begin{aligned} \lambda_-(\mathbf{d}') &\leq \lambda_-(\boldsymbol{\beta}) - \frac{1}{\lambda_+(\mathbf{d})} \\ &\leq \lambda_-(\boldsymbol{\beta}) - \frac{1}{\text{Tr}[\mathbf{d}] - (n-1)\lambda_{-\min}}. \end{aligned} \quad (3.41)$$

This profusion of inequalities makes possible a whole host of “Mather $\frac{4}{3}$ ” arguments; Herman, in [Herm88], gave the one based on (3.36) and (3.39). In the next section we show how to apply his criterion, along with other, new ones, to a specific example.

3.4 A converse KAM theorem

Here we use the arguments above on a specific system, the trigonometric example from chapter 2. We will use the same example to illustrate some¹⁶ of the issues in proving a machine-assisted converse KAM theorem and will show the results of several calculations.

3.4.1 analytic preliminaries

The plan for a converse KAM theorem, section 3.2.1, requires a starting point, \mathbf{x}^* , and the constants t , T , b , and B from equations (3.39) and (3.40). For the example at hand,

$$\begin{aligned} \beta(\mathbf{v}) &= 2\mathbf{I} - \epsilon \frac{\partial^2 V_{trig}}{\partial \mathbf{x}^2}, \\ &= 2\mathbf{I} - \frac{\epsilon}{M_{trig}} \begin{bmatrix} \left\{ \frac{\sin 2\pi v_0}{2} + \sin 2\pi(v_0 + v_1) \right\} & \sin 2\pi(v_0 + v_1) \\ \sin 2\pi(v_0 + v_1) & \left\{ \frac{\sin 2\pi v_1}{2} + \sin 2\pi(v_0 + v_1) \right\} \end{bmatrix} \end{aligned}$$

and so

$$\mathrm{Tr}[\beta(\mathbf{v})] = 4 - \frac{\epsilon}{M_{trig}} \left\{ \frac{1}{2} \{ \sin 2\pi v_0 + \sin 2\pi v_1 \} - 2 \sin 2\pi(v_0 + v_1) \right\} \quad (3.42)$$

$$\lambda_-(\beta(\mathbf{v})) = \frac{1}{2} \left\{ \frac{\mathrm{Tr}[\beta(\mathbf{v})] - \frac{\epsilon}{M_{trig}} \sqrt{\frac{1}{4} (\sin 2\pi v_0 + \sin 2\pi v_1)^2 + 4 \sin^2 2\pi(v_0 + v_1)}}{\frac{\epsilon}{M_{trig}}} \right\} \quad (3.43)$$

¹⁶Appendix B gives a detailed discussion of the algorithms used and includes a specification of the functions and data structures. The code itself is in appendix C.

Both $\text{Tr}[\beta]$ and $\lambda_-(\beta)$ achieve their extrema on the line $v_0 = v_1$. The symmetries of V_ϵ also ensure that

$$\begin{aligned} t - 4 &= \epsilon \min \text{Tr} \left[\frac{\partial^2 V_{trig}}{\partial \mathbf{x}^2} \right] = -\epsilon \max \text{Tr} \left[\frac{\partial^2 V_{trig}}{\partial \mathbf{x}^2} \right] = 4 - T \\ b - 2 &= \epsilon \min \lambda_- \left(\frac{\partial^2 V_{trig}}{\partial \mathbf{x}^2} \right) = -\epsilon \max \lambda_- \left(\frac{\partial^2 V_{trig}}{\partial \mathbf{x}^2} \right) = 2 - B \end{aligned}$$

We find the approximate positions of the extrema using Newton's method, then evaluate the bounds t , T etc... From these we can calculate the ranges of permissible $\lambda_-(\mathbf{d}_j)$.

The choice of the starting point, \mathbf{x}^* , depends on which of the inequalities (3.36) - (3.38) we expect to be most fruitful. Good use of inequality (3.36) would require that \mathbf{x}^* be a place where $\text{Tr}[\beta]$ attains its minimum; this choice immediately gives $\epsilon_c \leq 0.0435$. Best use of inequalities (3.37) and (3.38) requires \mathbf{x}^* at a place where

$$\lambda_-(\beta) = b. \quad (3.44)$$

This turns out to be the best choice; it immediately gives $\epsilon_c \leq 0.0278$. Note that we need not be particularly rigorous about finding \mathbf{x}^* . Indeed, we are free to choose it anywhere we like; we just get much better results if (3.44) is satisfied.

3.4.2 the computations

Once \mathbf{x}^* is chosen, we can set up the extended phase space, $I_\epsilon \times \mathbf{R}^n \times \mathbf{R}^n$, extend G_ϵ to G as in (3.18), and proceed with a proof. The plan is the same as in section 3.2.1, except that here the role of the intervals, I_j , is played by rectangles in the unit square. That is, we first ask "Can any $\mathbf{x} \in [0, 1] \times [0, 1]$ follow \mathbf{x}^* in a minimizing state?" If the answer is "no" then we are finished, if not we cut the square in half and ask the same question for each piece. Once the rectangle of potential successors is smaller than the whole square we can iterate the argument for several steps, bounding image prisms as in section 3.2.2. This yields a sequence of prisms in the extended phase

space, S_0, S_1, \dots , with

$$\begin{aligned} S_0 &= I_\epsilon \times \{\mathbf{x}^*\} \times \{\text{successor rectangle}\} \equiv (\mathbf{x}_{\epsilon,0}, P_0) \\ S_1 &= (\mathbf{x}_{\epsilon,1}, P_1) \supset G(S_0) \\ &\vdots \end{aligned}$$

Beginning with

$$\text{u.b. } \lambda_-(\mathbf{d}_{-1}) \equiv \lambda_{-max} \quad \text{and} \quad \text{u.b. } \text{Tr}[\mathbf{d}_{-1}] \equiv \text{Tr}_{max}$$

we proceed, at each step evaluating the whole suite

$$\lambda_-(\mathbf{d}_{j+1}) \leq \underset{(\epsilon, \mathbf{u}, \mathbf{v}) \in S_{j+1}}{\text{u.b.}} \left(\frac{1}{n} \text{Tr}[\boldsymbol{\beta}(\mathbf{v})] \right) - \frac{n}{\text{u.b.}(\text{Tr}[\mathbf{d}_j])} \quad (3.45)$$

$$\lambda_-(\mathbf{d}_{j+1}) \leq \underset{(\epsilon, \mathbf{u}, \mathbf{v}) \in S_{j+1}}{\text{u.b.}} (\lambda_+(\boldsymbol{\beta}(\mathbf{v}))) - \frac{1}{\text{u.b.}(\lambda_-(\mathbf{d}_j))} \quad (3.46)$$

$$\lambda_-(\mathbf{d}_{j+1}) \leq \underset{(\epsilon, \mathbf{u}, \mathbf{v}) \in S_{j+1}}{\text{u.b.}} (\lambda_-(\boldsymbol{\beta}(\mathbf{v}))) - \frac{1}{\text{u.b.}(\text{Tr}[\mathbf{d}_j]) - \lambda_{-min}} \quad (3.47)$$

and choosing the best upper bound. Computing (3.45) automatically gives the bound on $\text{Tr}[\mathbf{d}_j]$ used in (3.47). These estimates do not, of course, keep improving forever. Eventually either one of the u.b. $\lambda_-(\mathbf{d}_j)$ falls below λ_{-min} or one of the prisms S_j gets so large that the inequalities (3.45) - (3.46) are vacuous. At that point one either quits or cuts the initial prism in half¹⁷ and starts over.

3.4.3 results

Table (3.1) summarizes our results. We were able to show that the last few of the minimizing states of section 2.2.2 persist beyond the point where no invariant tori remain.

The figures on the following pages show some of the systems of prisms used in the proofs. The dark grey rectangles are sets that cannot contain a successor to \mathbf{x}^* , the

¹⁷The choice of which cut to make, whether along the ϵ , v_0 , or v_1 axis, depends on the shape of the final S_j .

u.b. $\epsilon_c \leq$	<i>longest</i>	<i>deepest</i>	<i>prisms</i>	<i>time (sec.)</i>
0.0278	3	10	39	500
0.0276	4	11	64	759
0.0274	4	13	156	2698
0.0272	6	21	933	~

Table 3.1: A sequence of bounds on ϵ_c and some details about the computations that verified them. The table includes: *longest*, the length of the longest sequence of image prisms considered; *prisms* the total number of prisms on which the algorithm succeeded; *deepest*, the number of refining cuts needed to make the smallest successful prism and *time* the execution time in seconds. All computations were done on a Sun4.

light grey regions may be ignored on account of symmetry, (see section 3.4.4). As one might expect, those states that go from \mathbf{x}^* to neighborhoods near the the maximum of V_{trig} , (those that correspond to rectangles in the upper right corner), are harder to prove non-minimizing. To succeed on such a rectangle the program must extend the corresponding state far enough to evaluate several u.b. $\lambda_-(\mathbf{d}_j)$. Since the prism-bounding algorithm always gives an S_{j+1} bigger than the true image of S_j , the initial prisms must be small.

3.4.4 using symmetry

In figures (3.16) – (3.18) we were able to ignore about half the possible successors. To see why, notice that V_{trig} is unchanged by the interchange of its v_0 and v_1 arguments. Two segments, such as $\{\dots, \mathbf{x}^*, \mathbf{x}_1, \mathbf{x}_2, \dots\}$ and $\{\dots, \mathbf{x}^*, \mathbf{x}'_1, \mathbf{x}'_2, \dots\}$ in figure (3.19), will have the same action because they are each other's images under the interchange $x_{j,0} \rightleftharpoons x_{j,1}$. Here, the interchange is just a reflection about the line¹⁸ $x_0 = x_1$. So,

¹⁸One must take some care here. The interchange is really a reflection through the diagonal line containing \mathbf{x}^* . Our program always arranges that \mathbf{x}^* is in the square $[0, 1] \times [0, 1]$ and on the line $x_0 = x_1$.

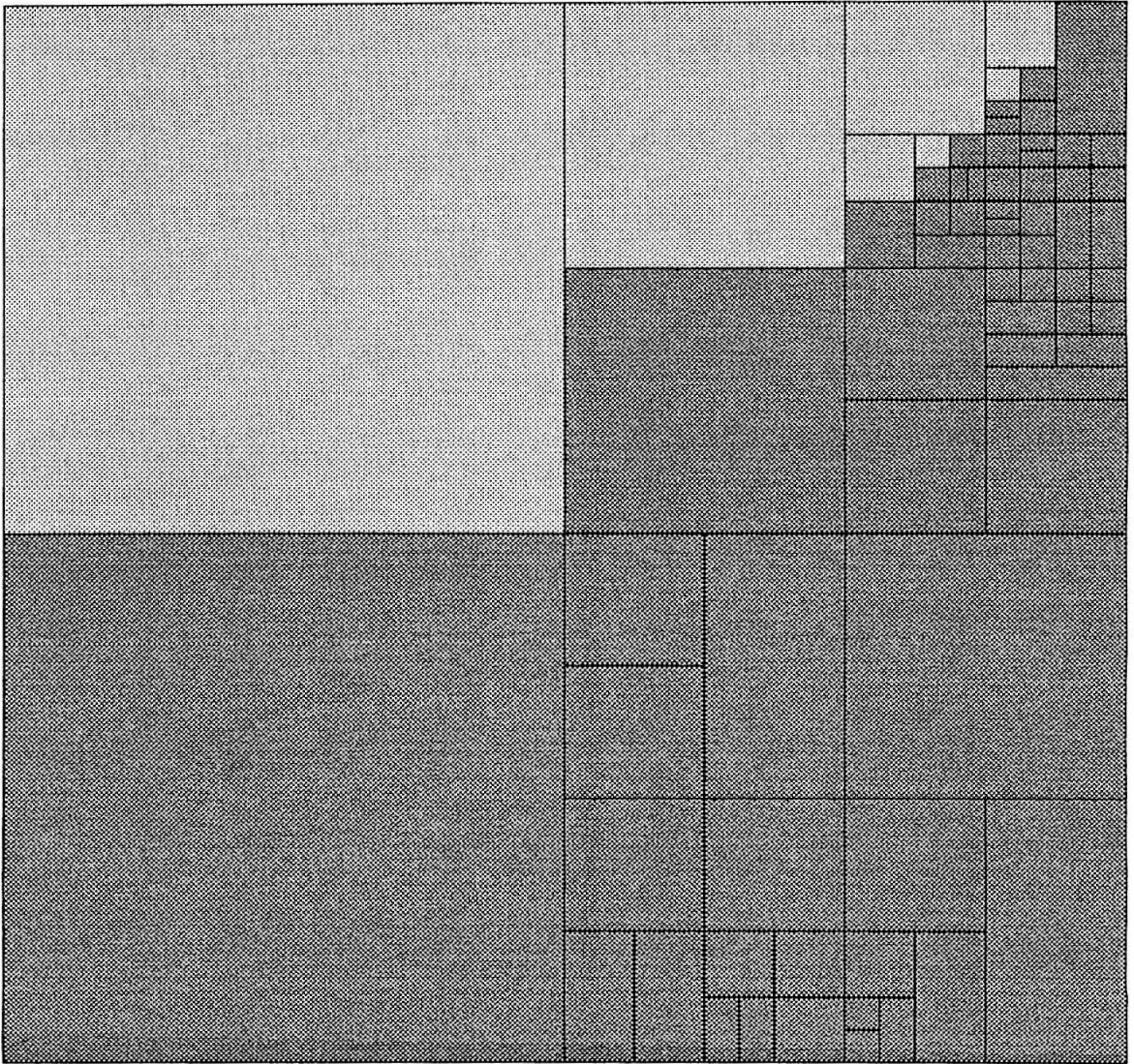


Figure 3.16: *The system of prisms used to show $\epsilon_c \leq 0.0276$.*

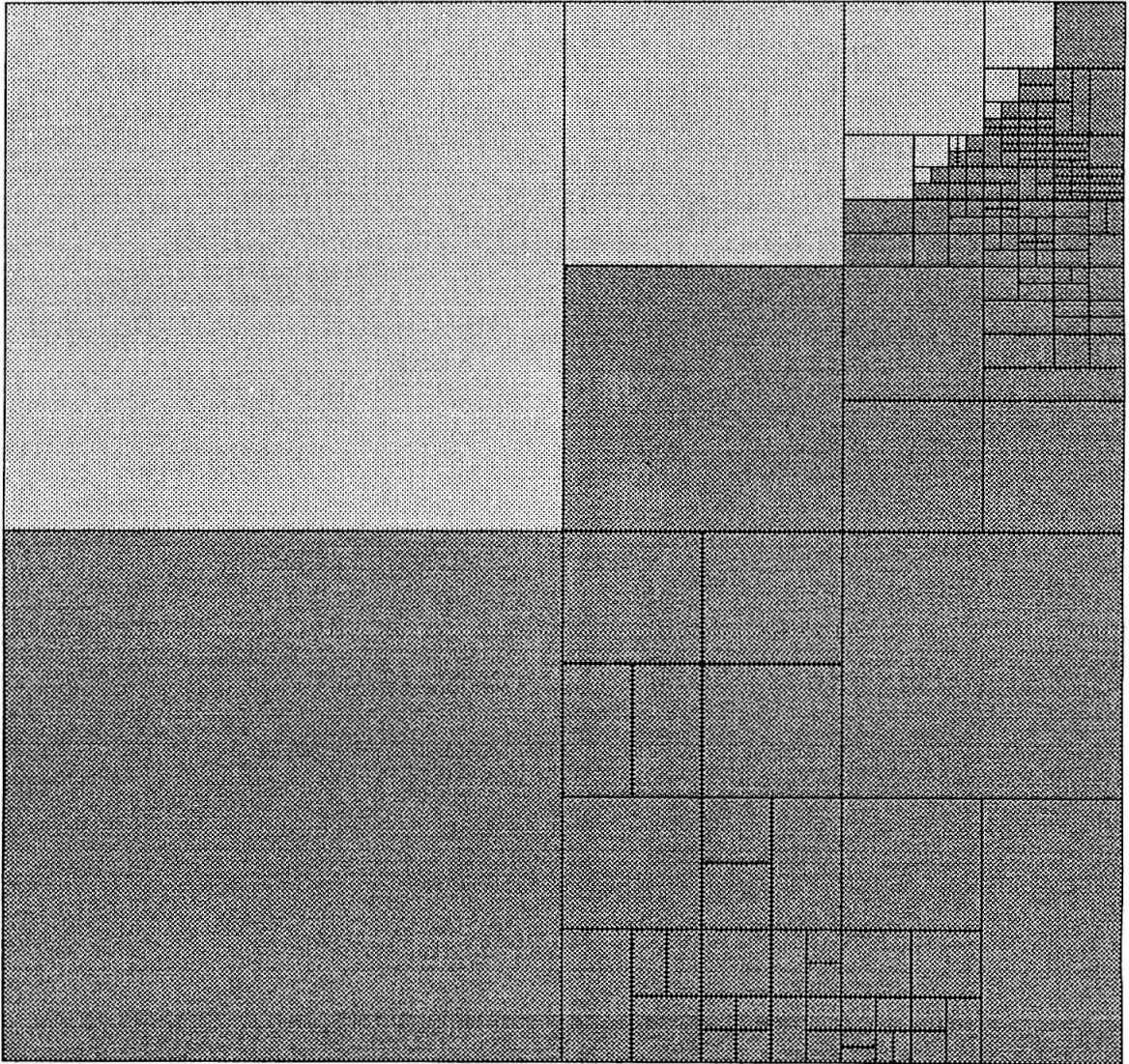


Figure 3.17: $\epsilon_c \leq 0.0274$

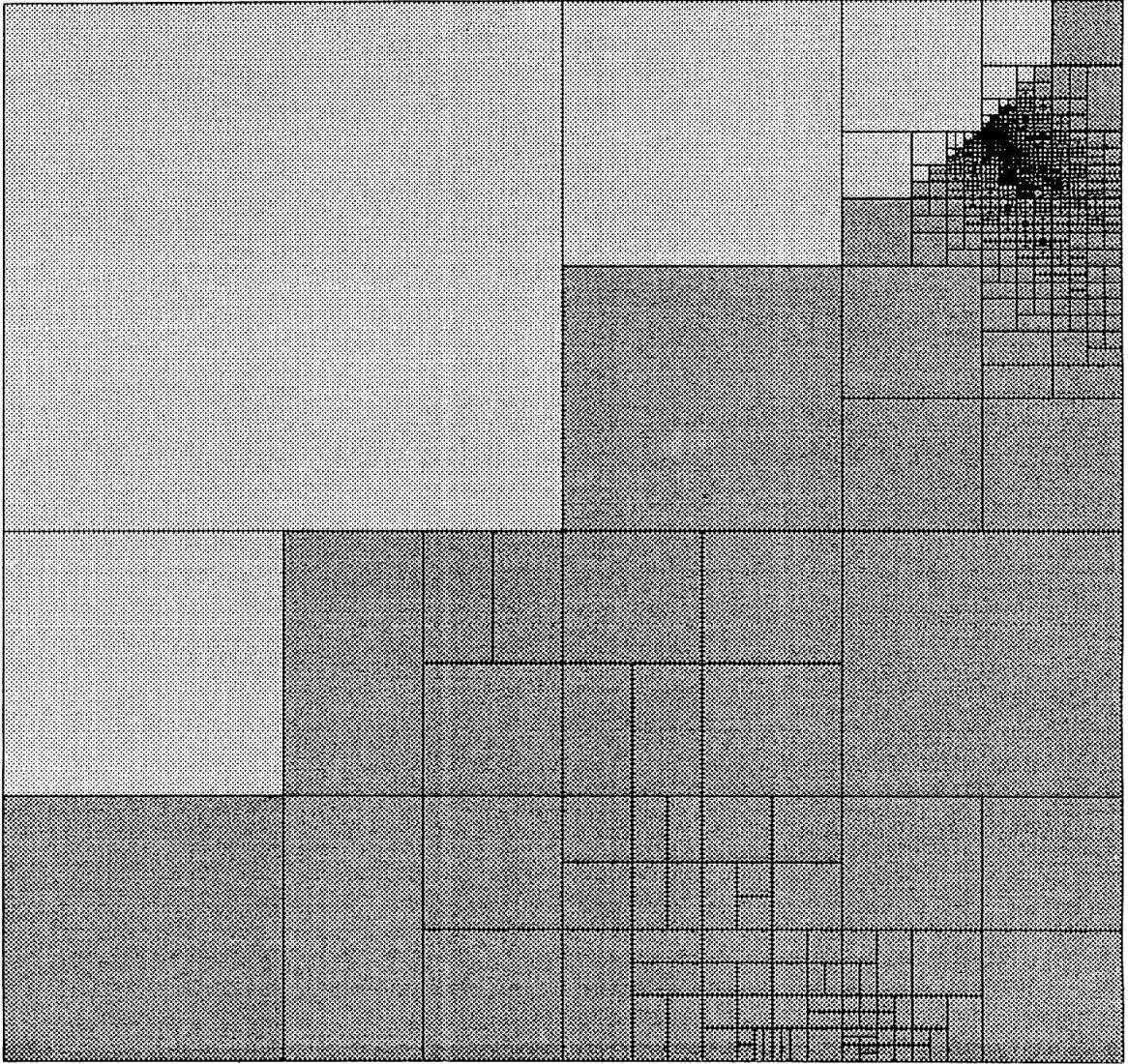


Figure 3.18: $\epsilon_c \leq 0.0272$

referring to figure (3.19), if we prove that no minimizing state can pass from \boldsymbol{x}^* through the box around \boldsymbol{x}_1 , we are automatically assured that none can go through the box around \boldsymbol{x}'_1 either.

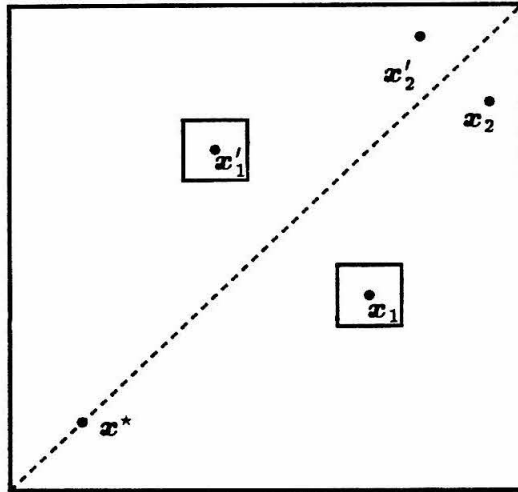


Figure 3.19: *Two symmetrically related states have the same action.*

Appendix A

Approximate Numerical Methods

In this appendix we review the numerical methods used to obtain the results of chapter 2. The first section describes the methods used to calculate the minimizing states; the next section discusses Kim and Ostlund's scheme for approximating irrational vectors by rational ones and the last section explains how we found the Lyapunov exponents pictured in figure (2.6).

A.1 Methods of minimization

All our minimization schemes solve the Euler-Lagrange equations (2.10). For each rotation vector, \mathbf{p}/q , and perturbation we produce a sequence of states $\{X_0, X_1, \dots, X_k, \dots\}$ each of which satisfies (2.10) for a particular value of $\epsilon = \epsilon_j$. We usually begin with a state whose first point, \mathbf{x}_0 , lies on the minimum of the perturbation to the generating function (that is, on a maximum of $V_\epsilon(\mathbf{x})$) and whose other points are $\mathbf{x}_j = \mathbf{x}_0 + \frac{j}{q}\mathbf{p}$. Such a state is globally minimizing for the unperturbed generating function so we set $\epsilon_0 = 0$. We then increase the size of the perturbation, ϵ_j , in small steps and use X_j as a starting point to calculate X_{j+1} using either a gradient-flow scheme or Newton's

method.

The former involves integrating the system of differential equations

$$\frac{d\mathbf{x}_i}{d\tau} = -\frac{\partial L_{p,q}}{\partial \mathbf{x}_i},$$

through a long interval of the formal “time,” τ . This method is very slow; it crawls down to the minimum with exponentially decreasing speed. On the other hand it is extremely reliable and seems very rarely to converge to a state other than the global minimum. Newton’s method is much faster, but somewhat prone to converge to extrema other than the minimum. It works by producing a sequence of approximate states Y_0, Y_1, \dots according to the recursive scheme :

$$\begin{aligned} Y_0 &= \text{some initial guess}, & Y_{i+1} &= Y_i + D_i \\ D_i &= -\mathbf{H}^{-1}d(L_{p,q}) \end{aligned} \quad (\text{A.1})$$

where \mathbf{H}^{-1} is the inverse of the Hessian of the action functional and $d(L_{p,q})$ is the functional’s gradient. Since \mathbf{H} has $(qd)^2$ entries, solving (A.1) could be an $O((qd)^2)$ process, but our Hessian,

$$\begin{bmatrix} 2\mathbf{I} - \epsilon \mathbf{V}_0 & -\mathbf{I} & 0 & \dots & \dots & -\mathbf{I} \\ -\mathbf{I} & 2\mathbf{I} - \epsilon \mathbf{V}_1 & -\mathbf{I} & \dots & \dots & 0 \\ \vdots & & & \ddots & & \vdots \\ \vdots & & & & \vdots & \\ 0 & \dots & \dots & -\mathbf{I} & 2\mathbf{I} - \epsilon \mathbf{V}_{q-2} & -\mathbf{I} \\ -\mathbf{I} & \dots & \dots & \dots & -\mathbf{I} & 2\mathbf{I} - \epsilon \mathbf{V}_{q-1} \end{bmatrix},$$

where

$$\mathbf{I} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad \mathbf{V}_j \equiv \frac{\partial^2 V}{\partial \mathbf{x}^2}(\mathbf{x}_j) = \begin{bmatrix} \frac{\partial^2 V}{\partial x_0^2} & \frac{\partial^2 V}{\partial x_0 \partial x_1} \\ \frac{\partial^2 V}{\partial x_0 \partial x_1} & \frac{\partial^2 V}{\partial x_1^2} \end{bmatrix}(\mathbf{x}_j),$$

has only a few terms off the diagonal. We implemented two schemes to solve (A.1), one that does Gauss-Jordan elimination [PFTV86] and another, rather more complicated algorithm that generalizes the one-dimensional work of Percival and Metsel [MP87]. We tried the latter because we hoped it would be more numerically stable; it was not, and ran a bit more slowly than the Gauss-Jordan program.

A.2 Rational approximation of irrational vectors

The problem of approximating a single real number by a sequence of rationals is completely solved by the simple continued fraction algorithm [Khin64,Rob78]. We write

$$\omega = a_0 + \frac{1}{a_1 + \frac{1}{a_2 + \frac{1}{a_3 + \frac{1}{a_4 + \dots}}}} \quad (\text{A.2})$$

where the a_i , called the *partial quotients* of ω , are positive integers. We compute them recursively according to

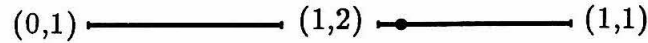
$$\begin{aligned} r_0 &= \omega & a_i &= \text{Int}[r_i] \\ r_{i+1} &= \frac{1}{r_i - a_i}. \end{aligned}$$

If ω is rational then all but finitely many of the a_i are zero, but if ω is irrational then the sequence never terminates. Truncating the expansion (A.2) after finitely many a_i gives a sequence of rational approximations $\frac{p_0}{q_0}, \frac{p_1}{q_1}, \dots$ with many desirable properties. Each $\frac{p_i}{q_i}$ is a best approximation in the sense that the only rationals closer to ω have larger denominators. Further, the sequence contains infinitely many $\frac{p_i}{q_i}$ such that $|\omega - p_i/q_i| \leq 1/\sqrt{5}q^2$. Indeed, the extremely good convergence of this sequence can be a problem. If one wants many approximations with modest denominators one

level 0



level 1



level 2

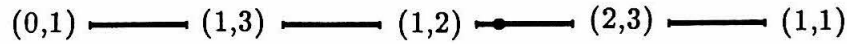


Figure A.1: Several levels of the Farey tree. The solid dot shows the position of the golden mean. Its n th approximation is always the mediant that has the largest sum $p_n + q_n$ of any appearing at the n th level.

must either study numbers that, like the golden mean, have very slowly growing q_i , or introduce other approximation algorithms that produce more slowly converging sequences.

One such algorithm depends on the Farey tree construction of the rationals. In a Farey tree one represents the rational number $\frac{p}{q}$ as an ordered pair (p, q) . The endpoints of the unit interval are thus $(0, 1)$ and $(1, 1)$. The construction proceeds by successively splitting intervals with endpoints (p_l, q_l) and (p_r, q_r) into two *daughter* intervals by inserting an interior point at $((p_l + p_r), (q_l + q_r))$. The number $((p_l + p_r), (q_l + q_r))$ is called the *mediant* of (p_l, q_l) and (p_r, q_r) . A sequence of Farey subdivisions that begins from the unit interval will eventually produce all rational numbers, each rational appearing as a mediant exactly once and in lowest terms. We can use the Farey tree as a tool for rational approximation by choosing p_n/q_n to be the mediant of the n th level interval containing ω . Since an interval in the n th level of the tree has length at most $1/(n + 1)$, the sequence of Farey approximations must eventually converge. Since every sequence of Farey approximation begins with $p_0/q_0 = \frac{1}{2}$ and each subsequent approximation requires only a choice of either the left or right daughter interval, we can represent the sequence of Farey approximations as a binary address. For example, the address *lllll* . . . would indicate that ω lies always

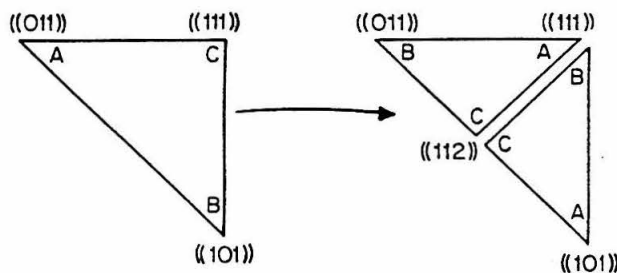


Figure A.2: *The mediant operation that refines Farey triangles. The parent triangle is represented by an equilateral right triangle. The algorithm divides this into two similar, daughter triangles by adding a new point in the middle of the hypotenuse. The coordinates of the new point are sums of the coordinates of the end points of the hypotenuse.* [KimOst86]

between $(0, 1)$ and $(1, n)$.

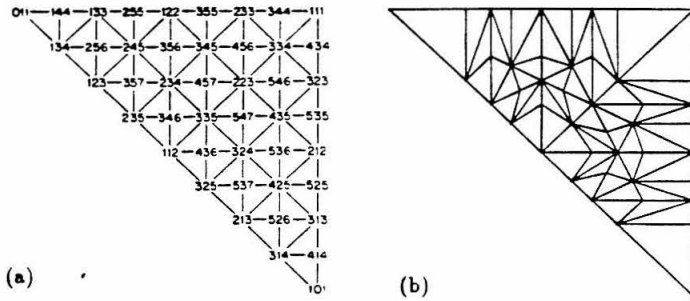
Kim and Ostlund [KimOst86] provide a detailed algorithm for implementing Farey approximation on a computer and generalize the idea to solve the problem of simultaneously approximating two irrationals (ω_0, ω_1) by rationals of the form $(p_0/q, p_1/q)$ ¹, which they represent as the triple (p_0, p_1, q) . To simplify the presentation let us restrict our attention to those vectors for which (ω_0, ω_1) is such that $\omega_0 + \omega_1 \geq 1$; the other case is not very different. The analogs of Farey intervals are *Farey triangles*, see figure A.2, and the act of refinement again involves adding a point obtained by coordinate-wise addition. When the vertices of the Farey triangles are viewed as rational points in \mathbf{R}^2 , the 2-d Farey mediant lies on the line connecting its parents so that the subdivision into triangles represented in figure A.2 reflects a genuine triangular decomposition of the unit square. Successive subdivisions produce every rational vector, though some appear twice.² As in the 1-d Farey approximation scheme, one chooses between a right and left daughter at each level of refinement. Irrational vectors thus have binary addresses. Kim and Ostlund assert that the analog of the

¹These are just the sorts of approximations we want; q is the period of our periodic state.

²Those vertices in the interior of the triangle $(0, 1, 1)$, $(1, 0, 1)$, $(1, 1, 1)$ lie on the hypotenuse of two different Farey triangles.

Figure A.3: *Five levels of the Farey triangulation,*

(a), and (b), *the corresponding partition of the unit square.*



[KimOst86]

golden mean is the vector whose address is $rrrrrrrrr\dots$; they call it the *spiral mean*. Its components are (τ^{-2}, τ^{-1}) , where τ satisfies $\tau^3 - \tau - 1 = 0$. One of the rotation vectors we studied, $(1432, 1897) / 2513$, is an approximation to the spiral mean, and we used the Farey triangle algorithm to produce the approximations used in the sequence of orbits pictured in section 2.3.

A.3 Lyapunov exponents

The Lyapunov exponents displayed in section 2.2.2 were found with the algorithm outlined in [BGGS80]. Their method depends on two observations, the first that one can compute the largest Lyapunov exponent by examining the growth of a vector tangent to an orbit, the second that the Lyapunov exponents are constant on a certain nested family of subspaces of the tangent space. To find all the exponents one selects a family of linearly independent vectors $\nu_0, \nu_1, \dots, \nu_{2d-1} \in TM_{x_0}$ and carries them along the orbit with the tangent map DF . Unless one makes a fantastically improbable choice of initial vectors, each ν_i will grow with an exponential rate λ_{max} ,

$$\lambda_{max} = \frac{1}{q} \log \frac{\|DF_{x_0}^q \nu_i\|}{\|\nu_i\|}, \quad (\text{A.3})$$

equal to the largest Lyapunov exponent. The ν_i will also become more and more nearly parallel because their growth is dominated by that of the eigenvector with the

largest eigenvalue; $DF_{(x_0, p_0)}^q \nu_0$ will be nearly parallel to this eigenvector. If we examine those components of $DF_{(x_0, p_0)}^q \nu_1$ that are perpendicular to $DF_{(x_0, p_0)}^q \nu_0$ we should find that they grow with a rate given by the next to largest Lyapunov exponent. Those components of $DF_{(x_0, p_0)}^q \nu_2$ that are perpendicular to both $DF_{(x_0, p_0)}^q \nu_0$ and $DF_{(x_0, p_0)}^q \nu_1$ should grow with a rate given by the third to largest Lyapunov exponent, and so on.

In practice the $DF_{(x_0, p_0)}^q \nu_i$ are too nearly parallel to permit the direct calculation described above. Instead one carries out the calculation of $DF_{(x_0, p_0)}^q \nu_i$ in q stages, using the definition of $DF_{x_0}^q$, (2.17). Whenever $DF_{(x_0, p_0)}^q \nu_0$ gets larger than some modest limit, one performs a Gram-Schmidt orthogonalization on the vectors, then normalizes each member of the resulting orthogonal collection and keeps a running total of the logarithms of the normalization constants. The Lyapunov exponents are just

$$\lambda_i = \frac{1}{q} \sum_{\text{normalizations}} \log n_i,$$

where n_i is a normalization constant for the i th vector. We adopted the scheme of [BGG80] only after trying a more difficult and time consuming method based on the rate of growth of the volumes of parallelepipeds. Although this original algorithm had a pleasing likeness to the definitions of Oseledec's great paper [Osc68], it gave the same answer as the algorithm described above, but took quite a bit longer.

Appendix B

Converse KAM Methods

The algorithms used to prove the theorems of section 3.4.3 have been implemented in the C programming language. This appendix describes the program in some detail. Section B.1 gives an overview of a typical computation and section B.2 explains how the basic data: numbers, intervals, and prisms, are stored in the computer. Section B.3 carefully describes the crucial algorithms and serves as an introduction to the parts of the code appearing in appendix C.

B.1 What the program does

This section expands on the plan for a proof offered in section 3.2.1. It first discusses the specific map studied, then gives a more detailed sketch of the computation, ending with a typical input file and the resulting output. This section also introduces a convention of typography and one of nomenclature. Under the former, bits of text taken directly from computer programs will be printed in the typewriter typeface. Under the latter, closely related objects will have similar names. For the sake of efficiency, I have written two versions of most functions. The first, quick and sloppy,

is used for exploration. The second, stately and rigorous, verifies any promising results suggested by the first. The quick function usually has some descriptive name, as has `bound_btrace()`, which bounds the trace of the blocks $\beta(\mathbf{x}_i)$. The rigorous version, `Rbound_btrace()`, has almost the same name, but for the prefix, R, connoting rigor. A similar convention applies to names of variables; `minLeastLam` is an approximate value for λ_{-min} , the smallest permissible value for the least eigenvalue of a diagonal block. The rigorous estimate of the same number is called `RminLeastLam`.

B.1.1 the map

The program really works with the three-parameter, four-dimensional, symplectic map,

$$\begin{aligned} \mathbf{y}' &= \mathbf{y} + \mathbf{J}', \\ \mathbf{J}' &= \mathbf{J} - \frac{\partial V_{abc}}{\partial \mathbf{y}}. \end{aligned}$$

Where

$$V_{abc}(\mathbf{y}) = -a \sin(y_0) - b \sin(y_1) - c \sin(y_0 + y_1). \quad (\text{B.1})$$

If one takes $a = b = \frac{4\epsilon\pi^2}{2M_{trig}}$, $c = \frac{4\epsilon\pi^2}{M_{trig}}$ this map is conjugate to the trigonometric example *via* the change of coordinates,

$$\mathbf{x} = \frac{\mathbf{y}}{2\pi}, \quad \mathbf{p} = \frac{\mathbf{J}}{2\pi}.$$

I included the extra parameters because it was easy, and left open the possibility of further work. I used $\mathbf{y} \equiv 2\pi\mathbf{x}$ to avoid having to multiply by 2π so often.

B.1.2 sketch of a computation

This section explains what the program does. First, it reads an input file and invokes a host of initialization functions. These have names like `init...`(`)` and do such things

as initialize variables, allocate memory, and copy the input data to various output files. Next, the program chooses the starting point, \mathbf{x}^* and prepares the first, all-encompassing prism, which then becomes the sole member of a linked list of untested prisms. The rest of the computation is a struggle to get to the end of this list. It grows shorter whenever the prism-testing algorithm succeeds; when the program is able to show that none of the points in a particular prism could follow \mathbf{x}^* in a minimizing state, that prism is removed from the list and forgotten. The list grows longer when the algorithm fails; the offending prism is divided in two by `refinePrism()` and replaced by the resulting pair.

The program tests a prism in several stages; it begins by examining the values of the parameters included in the prism and computing λ_{\min} and Tr_{\min} ; then it invokes a series of prism-testing functions. The first of these, `quick_try()`, tries to show that the state with $\mathbf{x}_0 = \mathbf{x}^*$, $\mathbf{x}_1 = \{\text{center of the prism}\}$ cannot be minimizing. If `quick_try()` fails the prism is judged hopeless and is immediately halved; if `quick_try()` succeeds, the program passes the prism to `try_Prism()`. This function does a full, orbit-following, image-bounding test, but uses only 48-bit, double-precision numbers and does not give rigorous results. If `try_Prism()` succeeds too, then, finally, `Rtry_Prism()` checks the prism rigorously. Eventually the program either reaches the end of the list, and so proves a converse KAM theorem, or founders on a difficult prism and quits.

B.1.3 using the program: a sample

The computation that proved $\epsilon_c \leq 0.0274$ began when I typed:

```
converse <trig274.in >&trig274.out -d30
```

The `-d30` sets the maximum *depth*; it tells the program to quit if it ever fails on a prism that has already been subdivided 30 times. Other command-line options include:

- b *filename* Maintain a backup file. This is essential for long computations; the backup file is updated frequently and contains enough information to continue a proof that has been interrupted by some computer disaster.
- g *filename* Make a graphics file. The program composes a PostScript program to draw figures like (3.16)-(3.18) and writes it on *filename*. If *filename* is the special name, *off*, then the graphics parts of the program are turned off.
- p *dp* Fix the precision used in the rigorous parts of the computation to *dp* decimal places; the example above uses the default, 35.
- s Be stubborn; keep on computing even if some prism cannot be successfully resolved at the maximum depth. This option is good for making pictures and for getting an idea of how hard a fully successful computation might be.
- t Change the *terseness*. Selecting this option makes the program more informative; it prints a message whenever it finds a successful prism. It also makes the output file much longer, and so I used it only during development of the program.
- r *filename* Restore an interrupted computation from a backup file.

The input file, `trig274.in`, looks like:

		<i>Parameters:</i>
0.3085	0.00125	<i>a_c and Δa</i>
0.3085	0.00125	<i>b_c and Δb</i>
0.617	0.0025	<i>c_c and Δc</i>
<i>Angles given in units of 2π.</i>		
1.0	1.0	<i>θ_{c,0} and Δθ₀</i>
1.0	1.0	<i>θ_{c,1} and Δθ₁</i>

0.0274 < epsilon < 0.0276

Run on kastor

May 2nd, 1989

The parts in the typewriter typeface are copied directly from the input file; the parts in italics are additional comments. The first three lines give the ranges for

parameters a , b and c . For example, the first line is the pair, $(a_c, \Delta a)$, which establishes that the initial prism will have $a_c - \Delta a \leq a \leq a_c + \Delta a$. The fifth and sixth lines specify that the prism will have $0 \leq \theta_j \leq 2\pi$, $j = 1, 2$. The last few lines are comments.

The computation above would yield an output file, trig.out, looking like:

```
apmValidate : null APM value in map.c at line 296.
```

```
Parameters :
```

```
a : 3.085000000000000e-01 1.250000000000000e-03
```

```
b : 3.085000000000000e-01 1.250000000000000e-03
```

```
c : 6.170000000000000e-01 2.500000000000000e-03
```

```
Initial region :
```

```
v[0] : 3.14159265358979e+00 3.14159265358979e+00
```

```
v[1] : 3.14159265358979e+00 3.14159265358979e+00
```

```
Comments :
```

```
0.0274 < epsilon < 0.0276
```

```
Run on kastor
```

```
May 2, 1989
```

```
+++++
```

```
I find no invariant tori for the range of parameters :
```

```
0.307250 < a < 0.309750
```

```
0.307250 < b < 0.309750
```

```
0.614500 < c < 0.619500
```

```
Did 322 quick checks, 318 semi-rigorous bounding tries,  
and 156 rigorous bounding tries.
```

```
The most deeply refined prism was cut 13 times.
```

```
The longest semi-rigorous orbit ran for 5 iterations,  
the longest successful orbit, 4 iterations.
```

```
Of the 156 successful prisms, 0 fell to the trace criterion,  
156 to the least eigenvalue test.
```

```
The best upper bound on the least eigenvalue came from  
the maxBlam criterion 0.0% of the time,  
the minBlam criterion 99.4% of the time,  
and from the trace criterion 0.6% of the time.
```

This investigation took 2697.53 seconds.

The first line is an error message from the initialization phase of the computation, saying that some variable was not properly allocated; the program automatically corrects this error. The next few lines are copied directly from the input and the lines after those give the result: no tori. The rest of the file reports details about the program's performance.

B.2 Representation of data

Here we explain how data are represented in the program. This section is fairly technical; it is partly intended as an introduction to the program and assumes some knowledge of C. Those wishing to avoid technical details should read only section B.2.1, in which numbers and arbitrary precision arithmetic are discussed. This leads into a description of *intervals* and *interval arithmetic*, which makes up the next section. Last, we explain how prisms are represented.

B.2.1 numbers and arithmetic

The computations in the rigorous parts of the program use an arbitrary precision arithmetic library written by Lloyd Zussman.¹ A description of his library and its constituent functions appears in appendix C; for now it is enough to know that it allows one to do arithmetic on numbers represented as finite strings of base 10000 "digits." We will call such strings *APMs*. Addition, subtraction and multiplication of two APMs, say, x and y , always yield another number representable as an APM, but

¹Mr. Zussman's library is licensed under a variant of the Free Software Foundation's *Gnu EMACS General Public License* and so I am obliged to provide a copy of the source code to anyone who asks. Complete source code for my program, *converse*, is also available on request.

division need not. The rational number $\frac{x}{y}$ may have an infinite repeating representation in base 10000. The division function, `apmDivide()`, deals with this problem by allowing the user to specify the number of decimal places (counting only those to the right of the decimal point) to which the result should be correct. The special functions, `apmSin()`, `apmCos()`, and `apmSqrt()`, which I have written, use the same strategy.

Fixed-precision calculations return a kind of implicit interval. An answer, \tilde{a} , that is accurate to dp decimal places, can be thought of as an interval guaranteed to contain the true answer, a ;

$$\tilde{a} - 10^{-dp} \leq a \leq \tilde{a} + 10^{-dp}.$$

The program also uses functions which do explicit interval arithmetic. An example is `Rbd_sin()`, which accepts as its argument an interval, $[\theta_-, \theta_+] \equiv I_\theta$, and returns an interval, $[s_-, s_+]$, certain to contain $\sin \theta$ for any $\theta \in I_\theta$. Most of the crucial estimates involve some fixed-precision calculation and so the program often uses the variables

$$\text{max_error} = 10^{-dp},$$

and

$$\text{precision} = dp + \text{SAFETY_DP}.$$

dp is the number of digits selected with the `-p` option and `SAFETY_DP` is a margin of safety. All the program's intermediate results are calculated to precision decimal places and then, for safety's sake, regarded as only accurate to $\pm \text{max_error}$. In the calculations summarized in table 3.1, $dp = 35$ and `SAFETY_DP = 5`.

B.2.2 intervals and expressions

The structure representing an interval is

```
typedef struct { APM          ub, lb ; } Bdd_apm ;,
```

called a *bounded APM*. The functions `Rbd_sin()` and `Rbd_cos()` each take one bounded APM as an argument and return another as the result. The only other operations on intervals used by the program are addition, subtraction, and multiplication. This is all handled through two other structures, the `Bapm_term`, and the `Bapm_expr`. The former is short for *bounded term*, the latter for *bounded expression*. Their full declarations are:

```
typedef struct { int          nfactores ;
                APM          coef ;
                Bdd_apm      **factores, bound ; } Bapm_term ;
```

and

```
typedef struct { int          nterms ;
                APM          const ;
                Bdd_apm      bound ;
                Bapm_term    *terms ; } Bapm_expr ;
```

To see the use of these structures, consider computing a bound on

$$2.0 - a \sin(\theta_0) - b \sin(\theta_1),$$

where a , b , and the θ_i all belong to intervals. One would set up a bounded expression composed of two bounded terms:

$$\underbrace{2.0}_{const.} - \underbrace{a \sin \theta_0}_{factors} - \underbrace{b \sin \theta_1}_{factors},$$

$\underbrace{\hspace{10em}}_{Bapm_term} \quad \underbrace{\hspace{10em}}_{Bapm_term}$

then use `Rbd_sin()` to bound the factors and, finally, use `Rbd_expr()` to get bounds on the whole thing.

B.2.3 prisms

The prisms introduced in section 3.2.2 are the fundamental objects of the program; they are stored in

```

typedef struct RPrsm { int          in_torus, n_cuts ;
                      APM          *matrix ;
                      char          *cuts[7] ;
                      Rxtnd_pt     *center ;
                      struct Rprsm *next ; } RPrism ;

```

The integer `in_torus` has one of the values `NO-TORI`, `UNTRIED`, `MAYBE`, `ACTIVE`, or `SYMMTRC` according to whether it definitely does not include points from a minimizing state, has not yet been tested, has been inconclusively tested, is under active consideration or may be disregarded on account of symmetry. The integer `n_cuts` tells how many subdivisions it took to make this prism and the character strings `cuts[]` explain how to produce this prism from the initial, big prism. `center` and `matrix` are the center point and defining matrix of the prism; `center` is an example of an *extended phase point*; it has seven components, three for the parameters and two for each of the delay coordinates. The pointer `next` gives the next Rprism on the list.

B.3 Algorithms

Here we explain and verify the crucial algorithms. In the first part of the section we will establish the correctness of `apmSin()`, `apmCos()`, which we approximate with truncated Taylor series, and of `apmSqrt()`, which uses Newton's method. Next we check the algorithms that set the bounds λ_{min} and Tr_{min} , then we turn to the computations used to compute l.b. $\lambda_-(d_j)$. In the last part of the section we examine the prism-bounding algorithms.

B.3.1 special functions

sine and cosine

The real computational work is done by two functions, `reducedSin()` and `reducedCos()`, which compute the sine and cosine of an angle from the interval $I_0 \equiv [0, \frac{\pi}{4}]$. These functions and the relations

$$\begin{aligned} \sin(\theta \pm \frac{\pi}{2}) &= \pm \cos(\theta), & \sin(-\theta) &= -\sin(\theta), \\ \cos(\theta \pm \frac{\pi}{2}) &= \mp \sin(\theta), & \cos(-\theta) &= \cos(\theta), \end{aligned}$$

allow us to calculate the sine and cosine of any angle. As mentioned in section B.2.1, we must set `dp`, the number of correct digits we want in the answer. `setTrigDp(dp)` does this; it also chooses the order of the Taylor approximation and picks the number of decimal places, `trig_dp`, to which intermediate results are calculated. To prove that all this works we will estimate the error made by `reducedSin()`,² leaving undetermined `trig_dp` and the number of terms in the polynomials, `trig_terms`. We will then show how to choose these two and how to reduce an arbitrary angle θ to one lying in $[0, \frac{\pi}{4}]$.

The form of the approximation is

$$\begin{aligned} \text{reducedSin}(\theta) \approx P_N(\theta) &\equiv \frac{1}{(2N+1)!} \sum_{j=0}^N \theta^{2j+1} (-1)^j \frac{(2N+1)!}{(2j+1)!} \\ &\approx \frac{1}{\text{sinFactr1}} \sum_{j=0}^N \text{sinCoef}[j] \theta^{2j+1} \end{aligned} \quad (\text{B.2})$$

where the second line substitutes names used in the code. Let us consider an angle, $\theta \in [0, \frac{\pi}{4}]$, which is approximately represented by an APM, $\tilde{\theta}$.

Proposition *If $\tilde{\theta}$ is such that $|\theta - \tilde{\theta}| \leq \epsilon < 1$, then*

$$|\sin \theta - P_N(\tilde{\theta})| \leq \epsilon + \frac{\theta^{2N+3}}{(2N+3)!}. \quad (\text{B.3})$$

²The analysis of `reducedCos()` is much the same.

Proof By straightforward computation,

$$\begin{aligned}
|\sin \theta - P_N(\tilde{\theta})| &\leq |\sin \theta - \sin \tilde{\theta}| + |\sin \tilde{\theta} - P_N(\tilde{\theta})|, \\
&\leq |\theta - \tilde{\theta}| + \left| \sum_{j=1}^N (-1)^j \frac{\theta^{2j+1}}{(2j+1)!} \right|, \\
&\leq \epsilon + \frac{\theta^{2N+3}}{(2N+3)!}.
\end{aligned}$$

Evaluating long power series like (B.2) can take immense amounts of computer time and memory; if the string of digits making up $\tilde{\theta}$ has length ℓ then the one representing $\tilde{\theta}^n$ will have length $\approx n\ell$. So, in the interest of computational speed, `reducedSin()` truncates some intermediate expressions. What it really calculates is a sequence of approximations to certain polynomials. In the equations below, $[x]_n$ is the number given by the truncating x after n places to the right of the decimal point, and *tdp* is short for `trig-dp`.

$$\begin{aligned}
\bar{S}_0 &= (-1)^N, \\
\bar{S}_1 &= \left[\tilde{\theta}^2 \bar{S}_0 + (2N+1)(2N)(-1)^{N-1} \right]_{tdp}, \\
&\approx \tilde{\theta}^2 (-1)^N + (2N+1)(2N)(-1)^{N-1}, \\
&\vdots \\
\bar{S}_N &= \left[\tilde{\theta}^2 \bar{S}_{N-1} + (2N+1)! \right]_{tdp}, \\
&\approx \sum_{j=0}^N \tilde{\theta}^{2j} (-1)^j \frac{(2N+1)!}{(2j+1)!}
\end{aligned}$$

and, finally,

$$\text{reducedSin}(\tilde{\theta}) \equiv \frac{\tilde{\theta} \bar{S}_N}{(2N+1)!} \approx P_N(\tilde{\theta}) \tag{B.4}$$

Let us consider the additional error introduced by truncation. Use S_j to denote the exact value of the polynomial approximated by \bar{S}_j . Then $\bar{S}_0 = S_0$ and so S_1 lies

in an interval,

$$\bar{S}_1 - \delta_1 < S_1 < \bar{S}_1 + \delta_1,$$

with $\delta_1 = 10^{-tdp}$. Since $S_2 = \tilde{\theta}^2 S_1 + C$, where C is a constant, we may be sure that S_2 is in the interval

$$[\tilde{\theta}^2(\bar{S}_1 - \delta_1) + C, \tilde{\theta}^2(\bar{S}_1 + \delta_1) + C] \subset [(\tilde{\theta}^2 \bar{S}_1 + C) - \delta_1, (\tilde{\theta}^2 \bar{S}_1 + C) + \delta_1].$$

After truncation we get

$$\bar{S}_2 - \delta_2 < S_2 < \bar{S}_2 + \delta_2$$

with $\delta_2 = 2\delta_1$ and after N such steps we are left with an error, $\delta_N = N 10^{-tdp}$. Combining this with equations (B.3) and (B.4) we get

$$|\text{reducedSin}(\tilde{\theta}) - \sin \theta| \leq |\tilde{\theta} - \theta| + \frac{N\delta_1}{(2N+1)!} + \frac{|\theta|^{2N+3}}{(2N+3)!} \quad (\text{B.5})$$

The only unknown quantity here is the difference between θ and its APM representation $\tilde{\theta}$. Suppose we can arrange for this to be at least as small as 10^{-tdp} . To ensure dp decimal places of accuracy in our answer we need only choose N large enough that $\frac{1}{(2N+3)!} < 10^{-(dp+2)}$ and then choose trig_dp so large that $N\delta_1 \leq 10^{-(dp+2)}$ too.

If we want the sine or cosine of an angle that lies outside the interval I_0 , we must relate it to some calculation that we can do with the reduced functions. The program contains a very accurate representation³ of π , so it can just subtract the appropriate number of multiples of $\frac{\pi}{2}$ and, perhaps, reflect about the origin. For very large angles, the reduction process may lose so much precision as to preclude a calculation to the specified accuracy. In that case the program writes an error message and calculates the best answer it can.

³The current implementation has one good to 45 decimal places, but it would be easy to add more.

square root

The square root function `apmSqrt()` is much simpler. It takes an argument, x , and uses Newton's method to solve the equation $y^2 - x = 0$. Suppose we want dp decimal places of accuracy in the answer; define $dp+ = dp + 2$. `apmSqrt()` recursively calculates a sequence $y_j \approx \sqrt{x}$ with

$$\begin{aligned} y_0 &= x \\ y_{j+1} &= \left[\frac{1}{2} \left(y_j + \left[\frac{x}{y_j} \right]_{dp+} \right) \right]_{dp+} \end{aligned} \quad (\text{B.6})$$

After the first few steps, the y_j decrease monotonically and so we may write $y_j = \sqrt{x} + r_j$; the error term, r_j , is a small, positive number. Equation (B.6) then yields the following extremely conservative estimate:

$$\begin{aligned} r_{j+1} &= y_{j+1} - \sqrt{x}, \\ &= \left[\frac{1}{2} \left(\sqrt{x} + r_j + \left[\frac{x}{\sqrt{x} + r_j} \right]_{dp+} \right) \right]_{dp+} - \sqrt{x}, \\ &\leq \left(\frac{r_j}{2} + \sqrt{x} + 2\epsilon_{dp+} \right) - \sqrt{x}, \\ &\leq \frac{r_j}{2} + 2\epsilon_{dp+} \end{aligned} \quad (\text{B.7})$$

where $\epsilon_{dp+} = 10^{-dp+}$ is the inevitable truncation error. If $r_j < \sqrt{x}$, Newton's method actually gives $r_{j+1} \sim \frac{r_j^2}{\sqrt{x}}$, but (B.7) will be good enough for us. It tells us that we must continue computing until the difference,

$$y_{j-1} - y_j = r_{j-1} - r_j > \frac{r_j}{2} - 2\epsilon_{dp+},$$

is less than $10^{-(dp+1)}$; the last y_j will be the answer.

B.3.2 uniform cones and the starting point

This section explains how the program evaluates the constants Tr_{min} , Tr_{max} , λ_{-min} and λ_{-max} ; it also explains how to get a good value for the starting point \mathbf{x}^* . The

main technical problem is the correct evaluation of the constants

$$B = \text{u.b. } \lambda_+(\boldsymbol{\beta}) \quad \text{and} \quad T = \text{u.b. } \text{Tr} [\boldsymbol{\beta}];$$

these, together with equations (3.39) and (3.40), determine everything else. Finding either B or T is a matter of maximizing a function on $[0, 1] \times [0, 1] \times \{\text{parameters}\}$, so it is enough to explain how to find one of them, say T .

When the program seeks T it sets a , b , and c to their values at the center of the initial prism, then uses Newton's method to find a zero of the gradient of $\text{Tr} [\boldsymbol{\beta}]$. For the computations presented in section 3.4.3, the search began at $(\frac{\pi}{2}, \frac{\pi}{2})$ and continued until it reached a point \boldsymbol{x}_T such that

$$\left| \frac{\partial \text{Tr} [\boldsymbol{\beta}(\boldsymbol{x}_T)]}{\partial \boldsymbol{x}} \right| < (|a_c| + |b_c| + |c_c|) \epsilon_{\text{newt}},$$

where ϵ_{newt} is a small constant. In the code, the search is done with ordinary double precision arithmetic and ϵ_{newt} is called `NEWT_TOL` and is equal to 10^{-9} . The \boldsymbol{x}_T it finds is very close to the true maximum, and so a suitable estimate is

$$T = \text{Tr} [\boldsymbol{\beta}(\boldsymbol{x}_T)] + (a_c + b_c + 2c_c)10^{-6} + (\Delta a + \Delta b + 2\Delta c)$$

where the last term is included to allow for the variation in a , b , and c over the prism. The point \boldsymbol{x}_T found by this technique is the natural starting point for an estimate based on Herman's trace condition, so I call it *Herman's starting point*.

The estimate for B works much the same way; a Newton's method search gives an approximate value for, \boldsymbol{x}_B , the position where $\max \lambda_+(\boldsymbol{\beta})$ is attained. B is then calculated according to

$$B = \lambda_+(\boldsymbol{\beta}(\boldsymbol{x}_B)) + (a_c + b_c + 2c_c)10^{-6} + (\Delta a + \Delta b + 2\Delta c)$$

After calculating B , the program sets up the starting point, \boldsymbol{x}^* , also called the *least-lambda starting point*. This point is essentially the same as \boldsymbol{x}_B , but is explicitly guaranteed to lie on the line $x_0 = x_1$ so that the calculation can exploit symmetry, as explained in section 3.4.4.

B.3.3 bounding traces and eigenvalues

This section explains how the program takes a prism, P , and evaluates the bounds

$$\begin{aligned} & \text{u.b.}_{(\boldsymbol{\varepsilon}, \mathbf{u}, \mathbf{v}) \in S} \lambda_-(\boldsymbol{\beta}), \\ & \text{u.b.}_{(\boldsymbol{\varepsilon}, \mathbf{u}, \mathbf{v}) \in S} \lambda_+(\boldsymbol{\beta}), \\ & \text{u.b.}_{(\boldsymbol{\varepsilon}, \mathbf{u}, \mathbf{v}) \in S} \text{Tr}[\boldsymbol{\beta}], \end{aligned}$$

where $\boldsymbol{\varepsilon} \in \mathbf{R}^3$ stands for the triple of parameters, (a, b, c) . These are the basic ingredients of the main suite of estimates, (3.45) – (3.47). Recall that the prism is determined by its center, $(\boldsymbol{\varepsilon}_c, \mathbf{u}_c, \mathbf{v}_c)$, and by the matrix that maps the hypercube, Q^7 , into the extended phase space. A point $\boldsymbol{\eta} \in Q^7$ has an image given by

$$\begin{bmatrix} a(\boldsymbol{\eta}) \\ b(\boldsymbol{\eta}) \\ c(\boldsymbol{\eta}) \\ u_0(\boldsymbol{\eta}) \\ u_1(\boldsymbol{\eta}) \\ v_0(\boldsymbol{\eta}) \\ v_1(\boldsymbol{\eta}) \end{bmatrix} = \begin{bmatrix} a_c \\ b_c \\ c_c \\ u_{c,0} \\ u_{c,1} \\ v_{c,0} \\ v_{c,1} \end{bmatrix} + \begin{bmatrix} \Delta a & 0 & 0 & \cdots & 0 \\ 0 & \Delta b & 0 & \cdots & 0 \\ 0 & 0 & \Delta c & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ p_{71} & p_{72} & p_{73} & \cdots & p_{77} \end{bmatrix} \begin{bmatrix} \eta_1 \\ \eta_2 \\ \eta_3 \\ \eta_4 \\ \eta_5 \\ \eta_6 \\ \eta_7 \end{bmatrix}. \quad (\text{B.8})$$

From this it is easy to show that any $(\boldsymbol{\varepsilon}, \mathbf{u}, \mathbf{v}) \in S$ has

$$|v_0 - v_{c,0}| \leq \sum_{j=1}^7 |p_{6j}| \quad \text{and} \quad |v_1 - v_{c,1}| \leq \sum_{j=1}^7 |p_{7j}|.$$

Once we have found bounds on the components of \mathbf{v} , we can invoke `Rbd.sin()` to get bounds on the functions $\sin(v_0)$, $\sin(v_1)$, and $\sin(v_0 + v_1)$, then combine those with Δa , Δb and Δc to obtain bounds on the expressions appearing in the trace and eigenvalues of $\boldsymbol{\beta}$.

In the program, all this is done with the `Bapm_expr` machinery described in section B.2.1. The expressions $a \sin(v_0)$, $b \sin(v_1)$, and $c \sin(v_0 + v_1)$ arise so often that

they are given their own names: `Ra_sin`, `Rb_sin` and `Rc_sin`; their values are set by `Rglobal_bounds(priz)`. In terms of these, the estimates we need are:

$$\begin{aligned} \text{u.b.}_S \text{Tr}[\beta] &= 4.0 + \text{Ra_sin.bound.ub} + \text{Rb_sin.bound.ub} + 2\text{Rc_sin.bound.ub} \\ \text{u.b.}_S \lambda_-(\beta) &= \frac{1}{2} \left\{ \text{u.b. Tr}[\beta] - \text{l.b.} \sqrt{\text{discrim.lb}} \right\}, \\ \text{u.b.}_S \lambda_+(\beta) &= \frac{1}{2} \left\{ \text{u.b. Tr}[\beta] + \text{l.b.} \sqrt{\text{discrim.ub}} \right\} \end{aligned}$$

where `discrim` is a bounded APM containing estimates over S of the quantity

$$(a \sin(v_0) + b \sin(v_1))^2 + 4c^2 \sin^2(v_0 + v_1). \quad (\text{B.9})$$

Note how, in every estimate described above, we allow each of the terms $a \sin(v_0) \dots$ to vary independently; the bounds we obtain are almost certainly too conservative.

B.3.4 bounding the images of prisms

The bulk of the computation is devoted to the kind of prism-bounding calculations described in section 3.2.2. In this section we will see how the program takes a prism in the extended phase space, $S = (\mathbf{x}_c, P)$, and constructs another, $S' = (\mathbf{x}'_c, P')$, guaranteed to contain $G(S)$. The computation of \mathbf{x}'_c is easy; $\mathbf{x}'_c \approx G(\mathbf{x}_c)$ where

$$\begin{aligned} G(a, b, c, \mathbf{u}, \mathbf{v}) &\equiv (a', b', c', \mathbf{u}', \mathbf{v}') = (a, b, c, \mathbf{u}', \mathbf{v}'), \\ \mathbf{u}' &= \mathbf{v}, \\ \mathbf{v}' &= 2\mathbf{v} - \mathbf{u} - \frac{\partial V_{abc}(\mathbf{v})}{\partial \mathbf{x}}. \end{aligned} \quad (\text{B.10})$$

Although only \mathbf{v}' involves any real computation, and so only it introduces any error, we will find it useful to assign a somewhat larger uncertainty, δ_c , to both \mathbf{u}' and \mathbf{v}' . The computation of P' is much more difficult; the work falls into two parts: setting up the matrix A and evaluating the numbers,

$$\begin{aligned} w_j &= \text{u.b.} |[A^{-1}(G(\mathbf{x}_c) - \mathbf{x}'_c)]_j| + \text{u.b.}_{\mathbf{x} \in S} \sum_{k=1}^7 \left| [A^{-1} \circ DG_{\mathbf{x}} \circ P]_{jk} \right|, \\ &\leq \sum_{k=1}^7 |A^{-1}|_j k \delta_c + \text{u.b.}_{\mathbf{x} \in S} \sum_{k=1}^7 \left| [A^{-1} \circ DG_{\mathbf{x}} \circ P]_{jk} \right|, \end{aligned} \quad (\text{B.11})$$

The second term, which involves bounds over $\mathbf{x} \in S$, will be the hard part. As was mentioned in section 3.2.3, the program uses two schemes to prepare A . The first, the fixed-form scheme, is specially suited to prisms with zero volume. Since all the prisms on the linked list are of the form

$$\{\text{parameters}\} \times \{\mathbf{x}^*\} \times \{\text{possible successors}\},$$

all are singular. Accordingly, the fixed-form scheme is always used on the first step of a round of prism-bounding. Since the first image is non-singular by construction, the second and subsequent iterates employ a different, more accurate scheme, the column-rotor. This section describes both schemes and verifies that they are correctly implemented.

Most of the work will come in showing that the w_j are calculated properly, a task simplified by the following definitions and proposition.

Definition For any real, $m \times n$, matrix A , define

$$[A]_{k*} \equiv \sum_{j=1}^n |a_{kj}|,$$

the k -th row sum of A , and

$$[A]_{**} \equiv \sum_{k=1}^m \sum_{j=1}^n |a_{kj}| = \sum_{k=1}^m [A]_{k*}$$

Proposition For any real, $m \times n$ matrix A and real, $n \times l$ matrix B , the product $C = AB$ satisfies

$$[C]_{k*} \leq [A]_{k*}[B]_{**} \quad \text{and} \quad [C]_{**} \leq [A]_{**}[B]_{**} \quad (\text{B.12})$$

Proof By direct calculation:

$$\begin{aligned} [C]_{k*} &= \sum_{j=1}^l |c_{kj}| = \sum_{j=1}^l \left| \sum_{i=1}^n a_{ki} b_{ij} \right|, \\ &\leq \sum_{j=1}^l \sum_{i=1}^n |a_{ki}| |b_{ij}|, \end{aligned}$$

$$\begin{aligned}
&\leq \sum_{i=1}^n |a_{ki}| [B]_{i*}, \\
&\leq \sum_{i=1}^n |a_{ki}| [B]_{**} = [A]_{k*} [B]_{**}.
\end{aligned}$$

Then, using the first part of (B.12), one finds

$$[C]_{**} = \sum_{k=1}^m [C]_{k*} \leq \sum_{k=1}^m [A]_{k*} [B]_{**} = [A]_{**} [B]_{**}.$$

It also follows from the definitions that

$$[(A + B)]_{k*} \leq [A]_{k*} + [B]_{k*}.$$

We will use a block-matrix representation for DG , the derivative of the map;

$$DG = \begin{bmatrix} \mathbf{I} & 0 & 0 \\ 0 & 0 & \mathbf{I} \\ \boldsymbol{\gamma} & -\mathbf{I} & \boldsymbol{\beta} \end{bmatrix}, \quad (\text{B.13})$$

where

$$\boldsymbol{\beta}(\mathbf{v}) = \begin{bmatrix} 2 - a \sin(v_0) - c \sin(v_0 + v_1) & -c \sin(v_0 + v_1) \\ -c \sin(v_0 + v_1) & 2 - b \sin(v_1) - c \sin(v_0 + v_1) \end{bmatrix}$$

and

$$\boldsymbol{\gamma}(\mathbf{v}) = \begin{bmatrix} \cos(v_0) & 0 & \cos(v_0 + v_1) \\ 0 & \cos(v_1) & \cos(v_0 + v_1) \end{bmatrix}.$$

It will also prove convenient to have block forms for the matrix P and to build a column vector, \mathbf{w} , out of the w_j .

$$P \equiv \begin{bmatrix} P_{pp} & 0 & 0 \\ P_{up} & P_{uu} & P_{uv} \\ P_{vp} & P_{vu} & P_{vv} \end{bmatrix} \quad \text{and} \quad \mathbf{w} \equiv \begin{bmatrix} \mathbf{w}_p \\ \mathbf{w}_u \\ \mathbf{w}_v \end{bmatrix}, \quad (\text{B.14})$$

where P_{pp} is 3×3 , P_{up} and P_{vp} are 3×2 , and the rest of the blocks are 2×2 . The elements of \mathbf{w} are:

$$w_p = \begin{bmatrix} w_1 \\ w_2 \\ w_3 \end{bmatrix}, \quad w_u = \begin{bmatrix} w_4 \\ w_5 \end{bmatrix} \quad \text{and} \quad w_v = \begin{bmatrix} w_6 \\ w_7 \end{bmatrix}.$$

the fixed-form fattener

When using this scheme we force the matrix A to be of the form

$$A = \begin{bmatrix} A_{pp} & 0 & 0 \\ A_{up} & 0 & A_{uv} \\ A_{vp} & A_{vu} & A_{vv} \end{bmatrix}. \quad (\text{B.15})$$

The explicit forms of the blocks will be chosen to simplify the calculation of the w_j .

Given (B.15), one can get a formula for A^{-1} in terms of the blocks and their inverses:

$$\begin{aligned} A^{-1} &= \begin{bmatrix} A_{pp}^{-1} & 0 & 0 \\ 0 & -A_{vu}^{-1}A_{vv}A_{uv}^{-1} & A_{vu}^{-1} \\ 0 & A_{uv}^{-1} & 0 \end{bmatrix} \begin{bmatrix} \mathbf{I} & 0 & 0 \\ -A_{up}A_{pp}^{-1} & \mathbf{I} & 0 \\ -A_{vp}A_{pp}^{-1} & 0 & \mathbf{I} \end{bmatrix} \\ &= \begin{bmatrix} A_{pp}^{-1} & 0 & 0 \\ \left\{ \begin{array}{l} A_{vu}^{-1}A_{vv}A_{uv}^{-1}A_{up}A_{pp}^{-1} \\ -A_{vu}^{-1}A_{vp}A_{pp}^{-1} \end{array} \right\} & -A_{vu}^{-1}A_{vv}A_{uv}^{-1} & A_{vu}^{-1} \\ -A_{uv}^{-1}A_{up}A_{pp}^{-1} & A_{uv}^{-1} & 0 \end{bmatrix} \quad (\text{B.16}) \end{aligned}$$

Taking $A_{pp} = P_{pp}$ and using (B.16), (B.14), and (B.13), we get $A^{-1} \circ DG \circ P =$

$$\begin{bmatrix} \mathbf{I} & 0 & 0 \\ \left\{ \begin{array}{l} A_{vu}^{-1}(\gamma P_{pp} - P_{up}) \\ + A_{vu}^{-1}(\beta P_{vp} - A_{vp}) \\ + A_{vu}^{-1}A_{vv}A_{uv}^{-1}(A_{vp} - P_{up}) \end{array} \right\} & \left\{ \begin{array}{l} A_{vu}^{-1}\beta P_{vu} - \\ A_{vu}^{-1}A_{vv}A_{uv}^{-1}P_{vu} \end{array} \right\} & \left\{ \begin{array}{l} A_{vu}^{-1}(\beta P_{vv} - P_{uv}) \\ -A_{vu}^{-1}A_{vv}A_{uv}^{-1}P_{vv} \end{array} \right\} \\ A_{uv}^{-1}(P_{vp} - A_{up}) & A_{uv}^{-1}P_{vu} & A_{uv}^{-1}P_{vv} \end{bmatrix}. \quad (\text{B.17})$$

When computing the w_j we must allow the matrices γ and β , which depend on a , b , c , and v to vary over S . All the other blocks, those in A and those in S , are constant. The form of (B.17) suggests the following choices for the blocks of A :

$$\begin{aligned}
A_{pp} &= P_{pp}, \\
A_{up} &= P_{vp}, \\
A_{vp} &= \gamma_c P_{pp} - P_{up} + \beta_c P_{vp}, \\
A_{uv} &= P_{vu} + P_{vv}, \\
A_{vu} &= \beta_c (P_{vu} + P_{vv}), \\
A_{vv} &= \beta_c P_{vv} - P_{uv},
\end{aligned} \tag{B.18}$$

where β_c and γ_c are the values of β and γ at the prism's center. Note that the entries in the blocks making up P are exactly represented as APMs; so are their sums, products, and differences. Thus A_{uv} , A_{up} and A_{pp} are exact; the other blocks of A , which involve the evaluation of special functions, are uncertain to the extent as the values of the special functions.

The choices (B.18) immediately determine most of the w_j ; the row sums contributing to \mathbf{w}_p are automatically equal to one and, unless A_{uv} is singular, $\mathbf{w}_v = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$. The program checks the invertibility of A_{uv} by evaluating its determinant, an exact calculation. If $\det[A_{uv}]$ were to be zero the program would write an error message and halt; this has never actually happened. The remaining row sums, those contributing to \mathbf{w}_u , are

$$\begin{aligned}
\text{u.b. } [A^{-1} \circ DG_{\mathbf{x}} \circ P]_{k\star} &= \text{u.b. } \left\{ \begin{array}{l} [A_{vu}^{-1}(\gamma - \gamma_c)P_{pp} + A_{vu}^{-1}(\beta - \beta_c)P_{vp}]_{j\star} + \\ [A_{vu}^{-1}\beta P_{vu} + A_{vu}^{-1}(\beta - \beta_c)P_{vv}]_{j\star} \end{array} \right\} \\
&\leq [A_{vu}^{-1}]_{j\star} \text{ u.b. } \left\{ \begin{array}{l} [(\gamma - \gamma_c)P_{pp} + (\beta - \beta_c)P_{vp}]_{\star\star} + \\ [\beta P_{vu} + (\beta - \beta_c)P_{vv}]_{\star\star} \end{array} \right\},
\end{aligned}$$

$$\leq [A_{vu}^{-1}]_{j*} \left\{ \begin{array}{l} \text{u.b.}([\gamma - \gamma_c]_{**})[P_{pp}]_{**} + \\ \text{u.b.}([\beta]_{**})[P_{vu}]_{**} + \\ \text{u.b.}([\beta - \beta_c]_{**})([P_{vp}]_{**} + [P_{vv}]_{**}) \end{array} \right\} \quad (\text{B.19})$$

where $k = j + 3$, $j = 1, 2$ and all upper bounds are taken over $\mathbf{x} \in S$. Out of all the numbers appearing in (B.19), only $[A_{vu}^{-1}]_{j*}$ and the upper bounds on $[\beta]_{**}$, $[\beta - \beta_c]_{**}$, and $[\gamma - \gamma_c]_{**}$ cannot be calculated exactly; the first can be estimated to any desired precision with the APM library, the rest are handled with the `Bapm_term`, `Bapm_expr` machinery.

the column-rotor scheme

This technique fattens matrices $A \approx DG_{\mathbf{x}_c} \circ P$, where DG and P are as in equations (B.13) and (B.14). Such A 's have almost the same form as (B.15), but they have non-vanishing A_{uu} blocks. The method's name comes from the way it tries to ensure that A is non-singular; it rotates parts of columns 4-7 with respect to each other so as to guarantee that they are not parallel. For example, the function `Rsubspace_rot()`, which performs the rotations, begins by finding the angle between the two, 2-d column vectors enclosed in braces in the matrix below.

$$\left[\begin{array}{cccccc} a_{11} & a_{12} & a_{13} & 0 & \cdots & \\ a_{21} & a_{22} & a_{23} & 0 & \cdots & \\ a_{31} & a_{32} & a_{33} & 0 & \cdots & \\ \vdots & \vdots & \vdots & \left[\begin{array}{c} a_{44} \\ a_{54} \end{array} \right] & \left[\begin{array}{c} a_{45} \\ a_{55} \end{array} \right] & a_{46} \quad a_{47} \\ & & & a_{64} & a_{65} & a_{66} \quad a_{67} \\ & & & a_{74} & a_{75} & a_{76} \quad a_{77} \end{array} \right]$$

If columns 4 and 5 are nearly parallel then so are these two vectors; `Rsubspace_rot()` would rotate the shorter of the two through some fixed angle, then go on to check and, perhaps rotate, other pairs until the matrix had no parallel columns. As we

noted in section 3.2.3, this technique is not at all optimal. Indeed, it is not even certain to produce a non-singular matrix, though, in practice, it always does. The column-rotor scheme produces smaller, more snugly fitting bounding prisms than the fixed-form fattener and so improves the program's performance.

The main computational work in this scheme is in inverting the matrix A and in calculating the w_j . Since, after column-rotation, A bears no direct relation to $DG_{x_c} \circ P$, we cannot expect any special form for $A^{-1} \circ DG_x \circ P$. Instead, we must use the APM library to compute some $\tilde{A} \approx A^{-1}$ directly. Define⁴ a 4×4 matrix B such that

$$\begin{bmatrix} B_{uu} & B_{uv} \\ B_{vu} & B_{vv} \end{bmatrix} \begin{bmatrix} A_{uu} & A_{uv} \\ A_{vu} & A_{vv} \end{bmatrix} = \mathbf{I}.$$

Then

$$\begin{aligned} A^{-1} &= \begin{bmatrix} \mathbf{I} & 0 & 0 \\ 0 & B_{uu} & B_{uv} \\ 0 & B_{vu} & B_{vv} \end{bmatrix} \begin{bmatrix} A_{pp}^{-1} & 0 & 0 \\ -A_{up}A_{pp}^{-1} & \mathbf{I} & 0 \\ -A_{vp}A_{pp}^{-1} & 0 & \mathbf{I} \end{bmatrix}, \\ &= \begin{bmatrix} A_{pp}^{-1} & 0 & 0 \\ \left\{ \begin{array}{l} -B_{uu}A_{up}A_{pp}^{-1} \\ -B_{uv}A_{vp}A_{pp}^{-1} \end{array} \right\} & B_{uu} & B_{uv} \\ \left\{ \begin{array}{l} -B_{vu}A_{up}A_{pp}^{-1} \\ -B_{vv}A_{vp}A_{pp}^{-1} \end{array} \right\} & B_{vu} & B_{vv} \end{bmatrix} \approx \begin{bmatrix} \tilde{A}_{pp} & 0 & 0 \\ \tilde{A}_{up} & \tilde{A}_{uu} & \tilde{A}_{uv} \\ \tilde{A}_{vp} & \tilde{A}_{vu} & \tilde{A}_{vv} \end{bmatrix}. \quad (\text{B.20}) \end{aligned}$$

Note that the lower-left, 4×4 block of \tilde{A} is just B . Then, again taking $A_{pp} = P_{pp}$,

⁴Some of the notation in this section, like B here, is introduced as a guide to the names of variables used in the code.

the product $A^{-1} \circ DG_{\mathbf{x}} \circ P$ is

$$\left[\begin{array}{ccc} \mathbf{I} & 0 & 0 \\ \left\{ \begin{array}{l} \tilde{A}_{up}P_{pp} + \tilde{A}_{uu}P_{vp} + \\ \tilde{A}_{uv}(\gamma P_{pp} - P_{up} + \beta P_{vp}) \end{array} \right\} & \left\{ \begin{array}{l} \tilde{A}_{uu}P_{vu} + \\ \tilde{A}_{uv}(\beta P_{vu} - P_{uu}) \end{array} \right\} & \left\{ \begin{array}{l} \tilde{A}_{uu}P_{vv} + \\ \tilde{A}_{uv}(\beta P_{vv} - P_{uv}) \end{array} \right\} \\ \left\{ \begin{array}{l} \tilde{A}_{vp}P_{pp} + \tilde{A}_{vu}P_{vp} + \\ \tilde{A}_{vv}(\gamma P_{pp} - P_{up} + \beta P_{vp}) \end{array} \right\} & \left\{ \begin{array}{l} \tilde{A}_{vu}P_{vu} + \\ \tilde{A}_{vv}(\beta P_{vu} - P_{uu}) \end{array} \right\} & \left\{ \begin{array}{l} \tilde{A}_{vu}P_{vv} + \\ \tilde{A}_{vv}(\beta P_{vv} - P_{uv}) \end{array} \right\} \end{array} \right]. \quad (\text{B.21})$$

Since the fattening scheme does not alter the first three columns, the blocks A_{up} and A_{vp} have the forms dictated by $A = DG_{\mathbf{x}_c} \circ P$; these are the same as the forms used in equation (B.18) for the fixed-form scheme. Equation (B.21) then simplifies to

$$\left[\begin{array}{ccc} \mathbf{I} & 0 & 0 \\ \left\{ \begin{array}{l} \tilde{A}_{uv}(\gamma - \gamma_c)P_{pp} + \\ \tilde{A}_{uv}(\beta - \beta_c)P_{vp} \end{array} \right\} & \left\{ \begin{array}{l} \tilde{A}_{uu}P_{vu} + \\ \tilde{A}_{uv}(\beta P_{vu} - P_{uu}) \end{array} \right\} & \left\{ \begin{array}{l} \tilde{A}_{uu}P_{vv} + \\ \tilde{A}_{uv}(\beta P_{vv} - P_{uv}) \end{array} \right\} \\ \left\{ \begin{array}{l} \tilde{A}_{uv}(\gamma - \gamma_c)P_{pp} + \\ \tilde{A}_{uv}(\beta - \beta_c)P_{vp} \end{array} \right\} & \left\{ \begin{array}{l} \tilde{A}_{vu}P_{vu} + \\ \tilde{A}_{vv}(\beta P_{vu} - P_{uu}) \end{array} \right\} & \left\{ \begin{array}{l} \tilde{A}_{vu}P_{vv} + \\ \tilde{A}_{vv}(\beta P_{vv} - P_{uv}) \end{array} \right\} \end{array} \right]$$

and the row sums contributing to \mathbf{w}_u are

$$\begin{aligned} & \text{u.b.} \left\{ \begin{array}{l} [\tilde{A}_{uv}(\gamma - \gamma_c)P_{pp} + \tilde{A}_{uv}(\beta - \beta_c)P_{vp}]_{j\star} + \\ [\tilde{A}_{uu}P_{vu} + \tilde{A}_{uv}(\beta P_{vu} - P_{uu})]_{j\star} + \\ [\tilde{A}_{uu}P_{vv} + \tilde{A}_{uv}(\beta P_{vv} - P_{uv})]_{j\star} \end{array} \right\}, \\ & \leq \text{u.b.} [\tilde{A}_{vu}]_{j\star} \{ \text{u.b.}([\gamma - \gamma_c]_{\star\star})[P_{pp}]_{\star\star} + \text{u.b.}([\beta - \beta_c]_{\star\star})[P_{vp}]_{\star\star} \} + \\ & \quad \text{u.b.} [\tilde{A}_{uu}P_{vu} + \tilde{A}_{uv}(\beta P_{vu} - P_{uu})]_{\star\star} + \\ & \quad \text{u.b.} [\tilde{A}_{uu}P_{vv} + \tilde{A}_{uv}(\beta P_{vv} - P_{uv})]_{\star\star}. \end{aligned} \quad (\text{B.22})$$

All the upper bounds are taken over $\mathbf{x} \in S$; the formulae for \mathbf{w}_v are similar. The program calculates the entries in \tilde{A} to at least precision decimal places, then treats them as exact in the evaluation of $[\tilde{A}_{vu}]_{j\star}$ and in expressions like

$$\text{u.b.} [\tilde{A}_{uu}P_{vv} + \tilde{A}_{uv}(\beta P_{vv} - P_{uv})]_{\star\star}. \quad (\text{B.23})$$

Upper bounds like (B.23) are so important that the program includes a special function, `Rbound_rows()`, to evaluate them. To account for the small errors ($\leq 10^{-\text{precision}}$) in \tilde{A} , the program adds `max_error` to the value of w_j as computed according to (B.22). Since the entries of β and P are all less in absolute value than 10, and since `max_error` is at least five orders of magnitude bigger than the largest error in \tilde{A} , this is a very conservative estimate.

matrix inversion

Notice that only blocks from the lower-left corner of \tilde{A} appear in equation (B.22); it will be enough to calculate just these blocks to `precision` decimal places. The function, `Rgauss()`, which does the calculation, takes a matrix M and uses the Gauss-Jordan algorithm with full pivoting to produce a result $\tilde{M} \approx M^{-1}$ such that $M\tilde{M} = \mathbf{I} + O(\epsilon)$, that is

$$|[M\tilde{M}]_{ij} - \delta_{ij}| \leq \epsilon$$

where δ_{ij} is the Kroneker delta function and ϵ is, as usual, $10^{-\text{precision}}$.

To apply the Gauss-Jordan algorithm to an $n \times n$ matrix M one constructs the $n \times 2n$ matrix

$$G = \left[\begin{array}{cccc|cccc} M_{11} & M_{12} & \cdots & M_{1n} & 1 & 0 & \cdots & 0 \\ M_{21} & M_{22} & \cdots & M_{2n} & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & & \vdots & \vdots & \ddots & \vdots \\ M_{n1} & M_{n2} & & M_{nn} & 0 & 0 & & 1 \end{array} \right]$$

made by appending a copy of the identity to the right side of M . The algorithm transforms the left side of G into the identity through a sequence of row operations that simultaneously transform the right side into A^{-1} . The first step is to multiply the top row by a constant so that the (1,1) entry is equal to one, then subtract suitably scaled multiples of the first row from each of the others in such a way as to eliminate

the entries in the first column. After this step the system looks like

$$G' = \left[\begin{array}{cccc|cccc} 1 & \frac{M_{12}}{M_{11}} & \dots & \frac{M_{1n}}{M_{11}} & \frac{1}{M_{11}} & 0 & \dots & 0 \\ 0 & M_{22} - \frac{M_{21}M_{12}}{M_{11}} & & & -\frac{M_{21}}{M_{11}} & 1 & & \\ \vdots & & \ddots & & \vdots & \vdots & \ddots & \\ 0 & M_{n2} - \frac{M_{n1}M_{12}}{M_{11}} & & & -\frac{M_{n1}}{M_{11}} & & & 1 \end{array} \right]. \quad (\text{B.24})$$

In the second step one uses multiples of the second row to eliminate all but the (2,2) entry from the second column ... and so on. The true Gauss-Jordan algorithm with full pivoting may rearrange some of the rows and columns so as to place large entries on the diagonal of the left-hand block; also, real implementations use only a single $n \times n$ array, gradually replacing the matrix M by its approximate inverse, \tilde{M} . The reader interested in the details of the algorithm should consult either the code, which is in appendix C, or the excellent book [PFTV86]. Here, we will mostly ignore the rearrangements, because they do not affect the error estimates we need.

The divisions needed to calculate intermediate results like (B.24) can only be done approximately so we must calculate bounds on the errors they introduce. Suppose all the calculations are done to some fixed precision, `inv_dp` and define $\epsilon_{inv} = 10^{inv_dp}$. We will need a new symbol, \tilde{G}' , to denote the approximate value of the matrix G' and will also need to define δ_1 , the largest error made in calculating an entry of \tilde{G}' ;

$$\delta_1 = \text{u.b.}_{j,k} |[\tilde{G}' - G']_{jk}|.$$

The second step produces

$$G'' = \left[\begin{array}{cccc|cccc} 1 & 0 & \star & \dots & \frac{1}{M_{11}} & 0 & 0 & \dots \\ 0 & 1 & \star & \dots & \star & \frac{M_{11}}{M_{11}M_{22} - M_{21}M_{12}} & 0 & \dots \\ 0 & 0 & \star & \dots & \star & \star & 1 & \dots \\ \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots & \end{array} \right]. \quad (\text{B.25})$$

Ideally, we would use G' to calculate G'' according to

$$G''_{ij} = \begin{cases} \frac{G'_{ij}}{G'_{22}} & \text{if } i = 2 \\ G'_{ij} - \frac{G'_{i2}G'_{2j}}{G'_{22}} & \text{if } i \neq 2. \end{cases},$$

but instead, `Rgauss()` actually calculates

$$\tilde{G}''_{ij} = \begin{cases} \left[\frac{\tilde{G}'_{ij}}{\tilde{G}'_{22}} \right]_{inv_dp} & \text{if } i = 2 \\ \left[\tilde{G}'_{ij} - \left[\frac{\tilde{G}'_{i2}\tilde{G}'_{2j}}{\tilde{G}'_{22}} \right]_{inv_dp} \right]_{inv_dp} & \text{if } i \neq 2 \end{cases} \quad (\text{B.26})$$

From this we must estimate δ_2 , an upper bound on the difference between \tilde{G}'' and G'' . `Rgauss()` finds δ_2 in stages, as follows:

(i) Compute

$$\begin{aligned} \delta_{piv} &= \frac{\delta_1}{|\tilde{G}'_{22}| - \delta_1} + \epsilon_{inv} \\ &\leq \left[\frac{\delta_1}{|\tilde{G}'_{22}| - \delta_1} \right]_{inv_dp} + 2\epsilon_{inv}. \end{aligned}$$

This is a bound on the error made by taking

$$\frac{1}{G'_{22}} = \left[\frac{1}{\tilde{G}'_{22}} \right]_{inv_dp} \equiv \text{piv_inv};$$

`piv_inv` is the name used in the code.

(ii)

$$\delta_r = \delta_1 |\text{piv_inv}| + \delta_p (\text{u.b.}_{k \neq 2} |\tilde{G}'_{2k}|) + \delta_1 \delta_p.$$

This is a bound on the error introduced by normalizing the second row so that its (2,2) entry is equal to one.

(iii)

$$\begin{aligned}\delta_m &= 2\delta_1 + \delta_r \text{ u.b.}_{l \neq 2} |\tilde{G}'_{l2}| + \delta_1 \delta_r, \\ &\geq \delta_1 + \delta_1 \text{ u.b.}_{k \neq 2} |\text{piv_inv } \tilde{G}'_{2k}| + \delta_r \text{ u.b.}_{l \neq 2} |\tilde{G}'_{l2}| + \delta_1 \delta_r.\end{aligned}$$

This is a matrix-wide bound on the errors made in computations like those in (B.26). The inequality is a consequence of the pivoting part of the algorithm, which ensures that $|\text{piv_inv } \tilde{G}'_{2k}| \leq 1$.

(iv) Finally,

$$\delta_2 = [\delta_m]_{\text{inv_dp}} + \epsilon_{\text{inv}}.$$

Similar estimates eventually give δ_n , a matrix-wide estimate on the difference between entries of \tilde{M} and the true inverse, M^{-1} . From this we can conclude

$$|[M\tilde{M}]_{ij} - \delta_{ij}| \leq n\delta_n \text{ u.b.}_{l,m} |M_{lm}|. \quad (\text{B.27})$$

Unless M is singular, we can choose `inv_dp` to make the error (B.27) as small as we like. `Rgauss()` guarantees both δ_n and the error given by (B.27) to be less than $10^{-\text{precision}}$.

about truncation

Both the schemes described above produce matrices, P' , whose entries are long strings of digits, longer than those of the original matrix, P . To avoid the computational cost of storing and manipulating long strings, the program truncates the entries in P' to `precision` decimal places; this introduces a small, readily manageable error.

Call the truncated prism P'_{trunc} ; its entries differ from those of P' by, at most, $\epsilon = 10^{-\text{precision}}$, so that $\mathbf{x} \in S'$

$$\mathbf{x} = \mathbf{x}'_c + P'\boldsymbol{\eta} \quad \text{for some } \boldsymbol{\eta} \in Q^7$$

differs from

$$\tilde{\mathbf{x}} = \mathbf{x}'_c + P'_{trunc}\boldsymbol{\eta}$$

by, at most, 7ϵ in each coordinate. The simplest way to handle this error is to incorporate it into δ_c , the upper bound on the difference $|(G_{abc}(\mathbf{x}_c) - \mathbf{x}_c)'_j|$. The coordinates of $G_{abc}(\mathbf{x}_c)$ are calculated out to precision decimal places, so we must have

$$\delta_c \geq 8\epsilon.$$

Since the program uses $\delta_c = \text{max_error} = 10^{\text{safety_dp}}\epsilon = 10^5\epsilon$, this condition is abundantly satisfied.

Appendix C

Computer Programs

This appendix contains the most important parts of the C programs used to prove the results described in chapter 3. In the interest of economy, we have deleted most of the non-rigorous and semi-rigorous parts of the code, leaving only those parts bear on that the correctness of our converse KAM results. The first section contains Lloyd Zussman's own description of his arbitrary precision library, the rest of the appendix has been copied directly from the source files used to compile the program.

C.1 Arbitrary precision library

```

APM
apmInit(init, scale_factor, base)
long init;
int scale_factor;
short base;
{}

```

This routine initializes a new APM value. The 'init' parameter is a long integer that represents its initial value, the 'scale_factor' variable indicates how this initial value should be scaled, and 'base' is the base of the initial value. Note that the APM value returned by this routine is normally a reclaimed APM value that has been previously disposed of via `apmDispose()`; only if there are no previous values to be reclaimed will this routine allocate a fresh APM value (see also the `apmGarbageCollect()` routine).

Bases can be 2 - 36, 10000, or 0, where 0 defaults to base 10000.

If the call fails, it will return `(APM)NULL` and 'apm_errno' will contain a

meaningful result. Otherwise, a new APM value will be initialized.

For example, assume that we want to initialize two APM values in base 10000, the first to 1.23456 and the second to 1 E20 ("one times 10 to the 20th power"):

```
APM apm_1 = apmInit(123456L, -5, 0);
APM apm_2 = apmInit(1L, 20, 0);
```

As a convenience, the following macro is defined in apm.h:

```
#define apmNew(BASE)    apmInit(OL, 0, (BASE))
```

```
int
```

```
apmDispose(apm)
```

```
APM apm;
```

```
{}
```

This routine disposes of a APM value 'apm' by returning it to the list of unused APM values (see also the apmGarbageCollect() routine). It returns an appropriate status which is also put into 'apm_errno'.

```
int
```

```
apmGarbageCollect()
```

```
{}
```

When APM values are disposed of, they remain allocated. Subsequent calls to apmInit() may then return a previously allocated but disposed APM value. This is done for speed considerations, but after a while there may be lots of these unused APM values lying around. This routine reclaims the space taken up by these unused APM values (it frees them). It returns an appropriate status which is also put into 'apm_errno'.

```
int
```

```
apmAdd(result, apm1, apm2)
```

```
APM result;
```

```
APM apm1;
```

```
APM apm2;
```

```
{}
```

This routine adds 'apm1' and 'apm2', putting the sum into 'result', whose previous value is destroyed. Note that all three parameters must have been previously initialized via apmInit().

The 'result' parameter cannot be one of the other APM parameters.

The return code and the 'apm_error' variable reflect the status of this function.

```
int
```

```
apmSubtract(result, apm1, apm2)
```

```
APM result;
```

```
APM apm1;
```

```
APM apm2;
```

```
{}
```

This routine subtracts 'apm2' from 'apm1', putting the difference into 'result', whose previous value is destroyed. Note that all three parameters must have been previously initialized via apmInit().

The 'result' parameter cannot be one of the other APM parameters.

The return code and the 'apm_errno' variable reflect the status of this function.

```
int
```

```

apmMultiply(result, apm1, apm2)
APM result;
APM apm1;
APM apm2;
{}

```

This routine multiplies 'apm1' and 'apm2', putting the product into 'result', whose previous value is destroyed. Note that all three parameters must have been previously initialized via apmInit().

The 'result' parameter cannot be one of the other APM parameters.

The return code and the 'apm_errno' variable reflect the status of this function.

```

int
apmDivide(quotient, radix_places, remainder, apm1, apm2)
APM quotient;
int radix_places;
APM remainder;
APM apm1;
APM apm2;
{}

```

This routine divides 'apm1' by 'apm2', producing the 'quotient' and 'remainder' variables. Unlike the other three basic operations, division cannot be counted on to produce non-repeating decimals, so the 'radix_places' variable exists to tell this routine how many digits to the right of the radix point are to be calculated before stopping. If the 'remainder' variable is set to (APM)NULL, no remainder is calculated ... this saves quite a bit of computation time and hence is recommended whenever possible.

All APM values must have been previously initialized via apmInit() (except, of course the 'remainder' value if it is to be set to NULL).

Division by zero creates a zero result and a warning.

The 'quotient' and 'remainder' variables can't be one of the other APM parameters.

The return code and the 'apm_errno' variable reflect the status of this function.

```

int
apmCompare(apm1, apm2)
APM apm1;
APM apm2;
{}

```

This routine compares 'apm1' and 'apm2', returning -1 if 'apm1' is less than 'apm2', 1 if 'apm1' is greater than 'apm2', and 0 if they are equal.

It is not an error if 'apm1' and 'apm2' are identical, and in this case the return value is 0.

The 'apm_errno' variable contains the error code. You must check this value: if it is set to an error indication, the comparison failed and the return value is therefore meaningless.

```

int
apmCompareLong(apm, longval, scale_factor, base)
APM apm;
long longval;
int scale_factor;

```

```
short base;
```

```
{}
```

This routine works just like `apmCompare()`, but it compares the 'apm' value to 'longval', scaled by 'scale_factor' in 'base'. The 'apm_errno' variable contains the error code.

```
int
```

```
apmSign(apm)
```

```
APM apm;
```

```
{}
```

This routine returns the sign of the 'apm' value: -1 for negative, 1 for positive. The 'apm_errno' variable contains the error code. You must check 'apm_errno': if it's non-zero, the function return value is meaningless.

```
int
```

```
apmAbsoluteValue(result, apm)
```

```
APM result;
```

```
APM apm;
```

```
{}
```

This routine puts the absolute value of 'apm' into 'result', whose previous value is destroyed. Note that the two parameters must have been previously initialized via `apmInit()`.

The 'result' parameter cannot be the other APM parameter.

The return code and the 'apm_errno' variable reflect the status of this function.

```
int
```

```
apmNegate(result, apm)
```

```
APM result;
```

```
APM num;
```

```
{}
```

This routine puts the additive inverse of 'apm' into 'result', whose previous value is destroyed. Note that the two parameters must have been previously initialized via `apmInit()`.

The 'result' parameter cannot be the other APM parameter.

The return code and the 'apm_errno' variable reflect the status of this function.

```
int
```

```
apmReciprocal(result, radix_places, apm)
```

```
APM result;
```

```
int radix_places;
```

```
APM num;
```

```
{}
```

This routine puts the multiplicative inverse of 'apm' into 'result', whose previous value is destroyed. Note that the two APM parameters must have been previously initialized via `apmInit()`. Since taking the reciprocal involves doing a division, the 'radix_places' parameter is needed here for the same reason it's needed in the `apmDivide()` routine.

Taking the reciprocal of zero yields zero with a warning status.

The 'result' parameter cannot be the other APM parameter.

The return code and the 'apm_errno' variable reflect the status of this function.

```
int
```

```
apmScale(result, apm, scale_factor)
```

```
APM result;
APM apm;
int scale_factor;
{}
```

This routine assigns to 'result' the value of 'apm' with its radix point shifted by 'scale_factor' (positive 'scale_factor' means shift left). The 'scale_factor' represents how many places the radix is shifted in the base of 'apm' unless 'apm' is in base 10000 ... in this special case, 'scale_factor' is treated as if the base were 10.

This is a very quick and accurate way to multiply or divide by a power of 10 (or the number's base).

The 'result' parameter cannot be the other APM parameter.

The return code and the 'apm_errno' variable reflect the status of this function.

```
int
apmValidate(apm)
APM apm;
{}
```

This routine sets 'apm_errno' and its return status to some non-zero value if 'apm' is not a valid APM value.

```
int
apmAssign(result, apm)
APM result;
APM num;
{}
```

This routine assigns the value of 'apm' to 'result', whose previous value is destroyed. Note that the two parameters must have been previously initialized via apmInit().

It is not considered an error if 'result' and 'apm' are identical; this case is a virtual no-op.

The return code and the 'apm_errno' variable reflect the status of this function.

```
int
apmAssignLong(result, long_value, scale_factor, base)
APM result;
long long_value;
int scale_factor;
short base;
{}
```

This routine assigns a long int to 'result'. Its second through fourth parameters correspond exactly to the parameters of apmInit(). The only difference between the two routines is that this one requires that its result be previously initialized. The 'long_value' parameter is a long that represents the value to assign to 'result', the 'scale_factor' variable indicates how this value should be scaled, and 'base' is the base of the value.

Bases can be 2 - 36, 10000, or 0, where 0 defaults to base 10000.

For example, assume that we want to assign values to two previously initialized APM entities, apm_1 and apm_2. The base will be base 10000, the first value will be set to 1.23456 and the second will be set to 1 E20 ("one times 10 to the 20th power"):


```

int  ercode;

ercode = apmAssignLong(apm_1, 123456L, -5, 0);
...

ercode = apmAssignLong(apm_2, 1L, 20, 0);
...

```

The return code and the 'apm_errno' variable reflect the status of this function.

```

int
apmAssignString(apm, string, base)
APM apm;
char *string;
short base;
{}

```

This routine takes a character string containing the ASCII representation of a numeric value and converts it into a APM value in the base specified. The 'apm' parameter must have been previously initialized, 'string' must be non-NULL and valid in the specified base, and 'base' must be a valid base.

The return code and the 'apm_errno' variable reflect the status of this function.

```

int
apmConvert(string, length, decimals, round, leftjustify, apm)
char *string;
int length;
int decimals;
int round;
int leftjustify;
APM apm;
{}

```

This routine converts a APM value 'apm' into its ASCII representation 'string'. The 'length' parameter is the maximum size of the string (including the trailing null), the 'decimals' parameter is the number of decimal places to display, the 'round' parameter is a true-false value which determines whether rounding is to take place (0 = false = no rounding), the 'leftjustify' parameter is a true-false value which determines whether the result is to be left justified (0 = false = right justify; non-zero = true = left justify), and the 'apm' parameter is the APM value to be converted.

The 'string' parameter must point to an area that can hold at least 'length' bytes.

If the 'decimals' parameter is < 0, the string will contain the number of decimal places that are inherent in the APM value passed in.

The return code and the 'apm_errno' variable reflect the status of this function.

```

int
(*apmErrorFunc(newfunc))()
int (*newfunc)();
{}

```

This routine registers an error handler for errors and warnings. Before any of the other APM routines return to the caller, an optional error handler specified in 'newfunc' can be called to intercept the result of the operation. With a registered error handler, the caller can dispense with the repetitious code for checking 'apm_errno' or the function return status after

each call to a APM routine.

If no error handler is registered or if 'newfunc' is set to NULL, no action will be taken on errors and warnings except to set the 'apm_errno' variable. If there is an error handler, it is called as follows when there is an error or a warning:

```
retcode = (*newfunc)(rcode, message, file, line, function)
```

where ...

```
int retcode;          /* returned by 'newfunc': should be 'rcode' */
int rcode;           /* error code */
char *message;       /* a short string describing the error */
char *file;          /* the file in which the error occurred */
int line;            /* the line on which the error occurred */
char *function;      /* the name of the function in error */
```

Note that your error handler should normally return 'rcode' unless it does a longjmp, calls exit(), or in some other way interrupts the normal processing flow. The value returned from your error handler is the value that the apm routine in error will return to its caller.

The error handler is called after 'apm_errno' is set.

This routine returns a pointer to the previously registered error handler or NULL if one isn't registered.

```
int
apmCalc(result, operand, ..., NULL)
APM result;
APM operand, ...;
{}
```

This routine performs a series of calculations in an RPN ("Reverse Polish Notation") fashion, returning the final result in the 'result' variable. It takes a variable number of arguments and hence the rightmost argument must be a NULL.

Each 'operand' is either a APM value or a special constant indicating the operation that is to be performed (see below). This routine makes use of a stack (16 levels deep) similar to that in many pocket calculators. It also is able to access a set of 16 auxiliary registers (numbered 0 through 15) for holding intermediate values.

The stack gets reinitialized at the start of this routine, so values that have been left on the stack from a previous call will disappear. However, the auxiliary registers are static and values remain in these registers for the duration of your program. They may also be retrieved outside of this routine (see the apmGetRegister() and apmSetRegister() routines, below).

An operand that is an APM value is automatically pushed onto the stack simply by naming it in the function call. If the stack is full when a value is being pushed onto it, the bottommost value drops off the stack and the push succeeds; this is similar to how many pocket calculators work. Also, if the stack is empty, a pop will succeed, yielding a zero value and keeping the stack empty. The topmost value on the stack is automatically popped into the 'result' parameter after all the operations have been performed.

An operand that is one of the following special values will cause an operation to be performed. These operations are described in the

following list. Note that the values "V", "V1", and "V2" are used in the following list to stand for temporary values:

```

APM_ABS           pop V, push absolute value of V
APM_NEG           pop V, push -V
APM_CLEAR         empty the stack
APM_DUP           pop V, push V, push V
APM_SWAP          pop V1, pop V2, push V1, push V2
APM_SCALE(N)      pop V, push V scaled by N [ as in apmScale() ]
APM_PUSH(N)       V = value in register N, push V
APM_POP(N)        pop V, store it in register N
APM_ADD           pop V1, pop V2, push (V2 + V1)
APM_SUB           pop V1, pop V2, push (V2 - V1)
APM_MUL           pop V1, pop V2, push (V2 * V1)
APM_DIV(N)        pop V1, pop V2, push (V2 / V1) with N radix places
                  [ as in apmDivide() ], remainder goes into register 0
APM_RECIP(N)      pop V, push 1/V with N radix places
                  [ as in apmReciprocal() ]

```

Since register 0 is used to hold the remainder in a division, it is recommended that this register not be used to hold other values.

As an example, assume that APM values "foo", "bar", and "baz" have been initialized via `apmInit()` and that "foo" and "bar" are to be used to calculate "baz" as follows (assume that divisions stop after 16 decimal places have been calculated):

```
baz = 1 / (((foo * bar) + foo) / bar) - foo
```

The function call will be:

```

bcdCalc(baz, foo, APM_DUP, APM_POP(1), bar, APM_DUP, APM_POP(2),
        APM_MUL, APM_PUSH(1), APM_ADD, APM_PUSH(2), APM_DIV(16),
        APM_PUSH(1), APM_SUB, APM_RECIP(16), NULL);

```

Note that the value of "foo" is stored in register 1 and the value of "bar" is stored in register 2. After this call, these registers will still contain those values.

```

int
apmGetRegister(regvalue, regnumber)
APM regvalue;
int regnumber;
{}

```

The value in auxiliary register number 'regnumber' is assigned to APM value 'regvalue'. The 'regnumber' parameter must be between 0 and 15, inclusive. The 'regvalue' parameter must have been previously initialized via `apmInit()`.

```

int
apmSetRegister(regvalue, regnumber, newvalue)
APM regvalue;
int regnumber;
APM newvalue;
{}

```

The value in auxiliary register number 'regnumber' is assigned to APM value 'regvalue', and then the APM value 'newvalue' is stored in that same register. The 'regnumber' parameter must be between 0 and 15, inclusive. The 'regvalue' and 'newvalue' parameters must have been previously initialized via `apmInit()`.

C.2 Source code

The listings below contain only those functions crucial to the correct execution of a converse KAM calculation. Some references to inessential or semi-rigorous parts of the code have been left in place because we wished to present the important functions exactly as they appear in the original source files.

C.2.1 special functions

the header files `apmSpecial.h` and `apmPrint.h`

```
# define MAX_TRIG_TERMS 100
# define DFLT_TRIG_DP 20

# define PI_DP      (sizeof(pi_str) / sizeof(char) - 3)

# ifndef YES
# define YES 1
# define NO 0
# endif

# ifndef m_swap
# define m_swap(x,y,t) (t=x, x=y, y=t)
# endif

extern APM  zero, one, two ;
extern APM  pi, two_pi, half_pi, threeHalf_pi, eighths_2pi[8] ;
extern APM  Theta, scratch, xMod2pi, Theta_sq, Answer ;
extern APM  Factrl, coef, apmOrder ;
extern APM  approx[2], diff, ub_diff ;
extern int  trig_dp, specialsInit ;
extern int  trig_terms, dp_lost ;
extern char pi_str[] ;
```

`apmCos()`, etc.

```
# include <stdio.h>
# include <math.h>
# include "apm.h"
# include "apmPrint.h"
# include "apmSpecial.h"

# define BUF_SZ 256

APM  *sinCoef, *cosCoef ;
APM  zero, one, two ;
APM  pi, two_pi, half_pi, threeHalf_pi, eighths_2pi[8] ;
APM  Theta, scratch, xMod2pi, Theta_sq, Answer ;
APM  sinFactrl, cosFactrl, apmOrder ;
APM  approx[2], diff, ub_diff ;
int  trig_dp, specialsInit = NO ;
```

```

int    trig_terms, dp_lost ;
char   pi_str[] = "3.14159265358979323846243383279502884197169399375" ;
char   log_buf[BUF_SZ] ;

/* ++++++ */

initApmSpecials()
{
    int    k ;

    /* Initialize a bunch of APMs.  Theta will be the reduced argument
       of a trig function; it will be between zero and pi / 4.  */

    pi = apmNew( 0 ) ;
    one = apmInit( 1L, 0, 0 ) ;
    two = apmInit( 2L, 0, 0 ) ;
    zero = apmInit( 0L, 0, 0 ) ;
    diff = apmNew( 0 ) ;
    Theta = apmNew( 0 ) ;
    Answer = apmNew( 0 ) ;
    two_pi = apmNew( 0 ) ;
    half_pi = apmNew( 0 ) ;
    scratch = apmNew( 0 ) ;
    ub_diff = apmNew( 0 ) ;
    xMod2pi = apmNew( 0 ) ;
    apmOrder = apmNew( 0 ) ;
    Theta_sq = apmNew( 0 ) ;
    sinFactrl = apmNew( 0 ) ;
    cosFactrl = apmNew( 0 ) ;
    approx[0] = apmNew( 0 ) ;
    approx[1] = apmNew( 0 ) ;
    threeHalf_pi = apmNew( 0 ) ;
    for( k=0 ; k < 8 ; k++ )
        eighths_2pi[k] = apmNew( 0 ) ;

    /* Obtain some rational multiples of pi.  These will be helpful
       when we go to restrict the domain of the trig functions to
       between zero and pi / 4 .  */

    apmAssignString( pi, pi_str, 0 ) ;

    apmMultiply( scratch, two, two ) ;
    apmDivide( eighths_2pi[0], (PI_DP+2), (APM)NULL, pi, scratch ) ;

    for( k=1 ; k < 8 ; k++ )
        apmAdd( eighths_2pi[k], eighths_2pi[0], eighths_2pi[k-1] ) ;

    apmMultiply( two_pi, pi, two ) ;
    apmAssign( half_pi, eighths_2pi[1] ) ;
    apmAssign( threeHalf_pi, eighths_2pi[5] ) ;

    setTrigDp( DFLT_TRIG_DP ) ;

    dp_lost = 0 ;
    specialsInit = YES ;

    return( 1 ) ;
}
/* ++++++ */

setTrigDp( dp )

```

```

int dp ;
{
    double j, j_fact, ten_to_dp ;

    /* Check to see that the desired accuracy is compatible
       with our knowledge of pi. */

    if( (dp+2) > PI_DP ) {
        fprintf( stderr,
            "We don't know pi well enough to achieve the desired accuracy. \n" ) ;
        return( 0 ) ;
    }
    else
        trig_dp = dp+2 ;

    /* Assume the argument is between zero and pi / 4. How many
       terms from the Taylor series do we need to include ? */

    trig_terms = 1 ;
    ten_to_dp = pow( 10.0, (double)dp ) ;
    for( j = 1.0, j_fact = 1.0 ; j_fact < ten_to_dp ; j += 2.0 ) {
        j_fact *= j * (j + 1) ;
        trig_terms++ ;
        if( trig_terms > MAX_TRIG_TERMS ) {
            fprintf( stderr, "Too many terms required. \n" ) ;
            return(0) ;
        }
    }

    trig_dp += (int)( ceil( log10((double) trig_terms) ) ) ;
    setTrigCoef() ;
    return( dp ) ;
}
/* ++++++ */

reduceArg( x )
/*
    Takes x, chops off enough multiples of two_pi to get it
    into the interval between zero and two_pi. Checks that we
    haven't lost an unacceptable amount of precision in doing
    this stage of the reduction. Then chops off multiples
    of pi/4 to get the argument into the interval between zero and
    pi/4. Sets Theta equal to the reduced argument and returns
    an integer indicating in which of eight equally spaced intervals
    x (mod two_pi) lay. If any precision is lost, dp_lost is set
    to the number of decimal places lost.
*/

APM x ;
{
    int octant ;
    char qtnt_str[BUF_SZ] ;

    /* Note that we haven't lost any decimal places yet. */
    dp_lost = 0 ;

    /* Whack out many multiples of two_pi. */
    apmDivide( scratch, 3, (APM)NULL, x, two_pi ) ;
    apmFloorString( qtnt_str, BUF_SZ, scratch ) ;
    apmAssignString( scratch, qtnt_str, 0 ) ;
    apmMultiply( Answer, scratch, two_pi ) ;
    apmSubtract( xMod2pi, x, Answer ) ;
    if( apmSign( xMod2pi ) == -1 )

```

```

    apmCalc( xMod2pi, xMod2pi, two_pi, APM_ADD, NULL ) ;

for( octant=0 ; (octant < 8) ; octant++ ) {
    if( apmCompare(xMod2pi, eighths_2pi[octant]) < 0 )
        break ;
}

switch( octant ) {
    case 0 :
        apmAssign( Theta, xMod2pi ) ;
        break ;

    case 1 :
        apmSubtract( Theta, half_pi, xMod2pi ) ;
        break ;

    case 2 :
        apmSubtract( Theta, xMod2pi, half_pi ) ;
        break ;

    case 3 :
        apmSubtract( Theta, pi, xMod2pi ) ;
        break ;

    case 4 :
        apmSubtract( Theta, xMod2pi, pi ) ;
        break ;

    case 5 :
        apmSubtract( Theta, threeHalf_pi, xMod2pi ) ;
        break ;

    case 6 :
        apmSubtract( Theta, xMod2pi, threeHalf_pi ) ;
        break ;

    case 7 :
        apmSubtract( Theta, two_pi, xMod2pi ) ;
        break ;

    default :
        break ;
}

    /* Check for loss of precision */
if( (PI_DP - strlen(qtnt_str)) < trig_dp )
    dp_lost = trig_dp - PI_DP + strlen(qtnt_str) ;
else
    dp_lost = 0 ;

return( octant ) ;
}
/* ++++++ */

reducedSin()
/*
    Takes the sine of Theta, puts the result in Answer.
*/
{
    int order, dp_to_find, term_num ;

    apmAssign( Answer, zero ) ;
}

```

```

apmMultiply( Theta_sq, Theta, Theta ) ;

term_num = trig_terms - 1 ;
for( order = ( 2 * trig_terms - 1 ) ; order > 0 ; order -= 2 ) {

    /* Multiply the old partial sum by Theta squared
       and add in a new coefficient */
    apmMultiply( scratch, Answer, Theta_sq ) ;
    apmAdd( Answer, sinCoef[term_num--], scratch ) ;
    apmTruncate( Answer, trig_dp ) ;
}

/* Multiply by the final factor of Theta,
   divide by the factorial, and return */

if( dp_lost > 0 )
    dp_to_find = trig_dp + 1 - dp_lost ;
else
    dp_to_find = trig_dp + 1 ;

apmMultiply( scratch, Answer, Theta ) ;
apmDivide( Answer, dp_to_find, (APM)NULL, scratch, sinFactrl ) ;
return ;
}
/* ++++++ */

reducedCos()
/*
   Takes the cosine of Theta, puts the result in Answer.
*/
{
    int order, dp_to_find, term_num ;

    apmAssign( Answer, zero ) ;
    apmMultiply( Theta_sq, Theta, Theta ) ;

    term_num = trig_terms - 1 ;
    for( order = ( 2 * trig_terms - 2 ) ; order >= 0 ; order -= 2 ) {

        /* Multiply the old partial sum by Theta squared
           and add in a new coefficient */
        apmMultiply( scratch, Answer, Theta_sq ) ;
        apmAdd( Answer, cosCoef[term_num--], scratch ) ;

        apmTruncate( Answer, trig_dp ) ;
    }

    /* Divide by the factorial,
       Put the result into Answer, and return */

    if( dp_lost > 0 )
        dp_to_find = trig_dp + 1 - dp_lost ;
    else
        dp_to_find = trig_dp + 1 ;

    apmDivide( scratch, dp_to_find, (APM)NULL, Answer, cosFactrl ) ;
    apmAssign( Answer, scratch ) ;
    return ;
}
/* ++++++ */

apmSin( result, x )

```



```

APM result, x ;
{
    int octant ;

    if( specialsInit == NO ) {
        fprintf( stderr,
            "apmSin() : Please call initApmSpecials(). \n" ) ;
        apmAssignLong( result, OL, 0, 0 ) ;
        apm_errno = APM_EPARM ;
        return ;
    }
    else
        apm_errno = APM_OK ;

    /* Reduce the argument, report any loss of precision, and
       note in which octant x (mod two_pi) lay. */

    octant = reduceArg( x ) ;
    if( dp_lost > 0 ) {
        fprintf( stderr,
            "apmSin : Big argument, lost %d decimal places from the answer. \n",
            dp_lost ) ;
        apm_errno = APM_WTRUNC ;
    }
    else
        apm_errno = APM_OK ;

    /* Evaluate the sine. Which of the two reduced functions
       one uses depends on the octant. */

    switch( octant ) {
        case 0 :
            reducedSin() ;
            break ;

        case 1 :
            reducedCos() ;
            break ;

        case 2 :
            reducedCos() ;
            break ;

        case 3 :
            reducedSin() ;
            break ;

        case 4 :
            reducedSin() ;
            apmNegate( scratch, Answer ) ;
            apmAssign( Answer, scratch ) ;
            break ;

        case 5 :
            reducedCos() ;
            apmNegate( scratch, Answer ) ;
            apmAssign( Answer, scratch ) ;
            break ;

        case 6 :
            reducedCos() ;

```

```

    apmNegate( scratch, Answer ) ;
    apmAssign( Answer, scratch ) ;
    break ;

case 7 :
    reducedSin() ;
    apmNegate( scratch, Answer ) ;
    apmAssign( Answer, scratch ) ;
    break ;

default :
    break ;
}

apmAssign( result, Answer ) ;

return ;
}
/* ++++++ */

apmCos( result, x )

APM result, x ;
{
    int octant ;

    if( specialsInit == NO ) {
        fprintf( stderr,
            "apmCos() : Please call initApmSpecials() first. \n" ) ;
        apmAssignLong( result, OL, 0, 0 ) ;
        apm_errno = APM_EPARM ;
        return ;
    }
    else
        apm_errno = APM_OK ;

    /* Reduce the argument, report any loss of precision, and
       note in which octant x (mod two_pi) lay. */

    octant = reduceArg( x ) ;
    if( dp_lost > 0 ) {
        fprintf( stderr,
            "apmCos : Big argument, lost %d decimal places from the answer. \n",
                                                    dp_lost ) ;
        apm_errno = APM_WTRUNC ;
    }
    else
        apm_errno = APM_OK ;

    /* Evaluate the cosine. Which of the two reduced functions
       one uses depends on the octant. */

    switch( octant ) {
        case 0 :
            reducedCos() ;
            break ;

        case 1 :
            reducedSin() ;
            break ;
    }
}

```

```

    case 2 :
        reducedSin() ;
        apmNegate( scratch, Answer ) ;
        apmAssign( Answer, scratch ) ;
        break ;

    case 3 :
        reducedCos() ;
        apmNegate( scratch, Answer ) ;
        apmAssign( Answer, scratch ) ;
        break ;

    case 4 :
        reducedCos() ;
        apmNegate( scratch, Answer ) ;
        apmAssign( Answer, scratch ) ;
        break ;

    case 5 :
        reducedSin() ;
        apmNegate( scratch, Answer ) ;
        apmAssign( Answer, scratch ) ;
        break ;

    case 6 :
        reducedSin() ;
        break ;

    case 7 :
        reducedCos() ;
        break ;

    default :
        break ;
}

apmAssign( result, Answer ) ;
return ;
}
/* ++++++ */

apmSqrt( result, dp, x )
/*
    Find square roots using Newton's method.
*/
int    dp ;
APM    x, result ;
{
    int    comp, dp_plus ;
    APM    *this_approx, *next_approx, *temp ;

/*
    Check that all the scratch variables are ready.
*/

    if( specialsInit == NO ) {
        fprintf( stderr,
            "apmSqrt() : Please call initApmSpecials() first. \n" ) ;
        apmAssignLong( result, OL, 0, 0 ) ;
        apm_errno = APM_EPARM ;
        return ;
    }

```

```

    }
    else
        apm_errno = APM_OK ;

/*
    If the argument is zero, just return zero.
    If the argument is negative, whine.
*/
if( (comp = apmCompare( x, zero )) == 0 ) {
    apmAssign( result, zero ) ;
    return ;
}
else if( comp == -1 ) {
    fprintf( stderr, "apmSqrt() : Can't handle negative arguments.\n" ) ;
    apm_errno = APM_EPARM ;
    return ;
}
else
    apm_errno = APM_OK ;

/*
    Do up Newton. The rule is

        y[n+1] = (y[n] + x/y[n]) / 2.0
*/
dp_plus = dp + 2 ;
apmAssignLong( ub_diff, 1L, -dp_plus, 0 ) ;

this_approx = &approx[0] ;
next_approx = &approx[1] ;

apmAssign( *this_approx, x ) ;
apmAssign( *next_approx, zero ) ;
apmSubtract( diff, *this_approx, *next_approx ) ;
while( apmCompare( diff, ub_diff ) > 0 ) {
    apmDivide( scratch, dp_plus, (APM) NULL, x, *this_approx ) ;
    apmCalc( scratch, scratch, *this_approx, APM_ADD, NULL ) ;
    apmDivide( *next_approx, dp_plus, (APM) NULL, scratch, two ) ;
    apmTruncate( *next_approx, dp_plus ) ;

    apmCalc( diff, *this_approx, *next_approx, APM_SUB, APM_ABS, NULL ) ;
    m_swap( this_approx, next_approx, temp ) ;
}

apmAssign( result, *this_approx ) ;
return ;
}
/* ++++++ */

apmFloor( result, arg, base )

int base ;
APM result, arg ;
{
    char buf[BUF_SZ], *cpt ;

    apmConvert( buf, BUF_SZ, 2, NO_ROUND, LEFT_JUST, arg ) ;
    for( cpt = buf ; *cpt != '\0' ; cpt++ )
        if( *cpt == '.' )
            *cpt = '\0' ;

    apmAssignString( result, buf, base ) ;
}

```

```

}
/* ++++++ */

setTrigCoef()
{
    int j, order, coef_num ;
    char *malloc() ;

    sinCoef = (APM *) malloc( trig_terms * sizeof( APM ) ) ;
    cosCoef = (APM *) malloc( trig_terms * sizeof( APM ) ) ;
    if( (sinCoef == NULL) || (cosCoef == NULL) ) {
        fprintf( stderr, "Trouble allocating %d APMs for coefficients.\n" ) ;
        exit(0) ;
    }

    for( j=0 ; j < trig_terms ; j++ ) {
        sinCoef[j] = apmNew( 0 ) ;
        cosCoef[j] = apmNew( 0 ) ;
    }

    if( (trig_terms % 2) != 0 ) {
        apmAssignLong( sinCoef[trig_terms-1], -1L, 0, 0 ) ;
        apmAssignLong( cosCoef[trig_terms-1], -1L, 0, 0 ) ;
    }
    else {
        apmAssignLong( sinCoef[trig_terms-1], 1L, 0, 0 ) ;
        apmAssignLong( cosCoef[trig_terms-1], 1L, 0, 0 ) ;
    }

    coef_num = trig_terms - 2 ;
    for( order = (2 * trig_terms - 1) ; order > 1 ; order -= 2 ) {
        /* coefficients for the sine */

        apmAssignLong( apmOrder, -(long) order, 0, 0 ) ;
        apmMultiply( scratch, sinCoef[coef_num+1], apmOrder ) ;
        apmAssignLong( apmOrder, (long)(order-1), 0, 0 ) ;
        apmMultiply( sinCoef[coef_num], scratch, apmOrder ) ;

        /* coefficients for the cosine */
        apmMultiply( scratch, cosCoef[coef_num+1], apmOrder ) ;
        apmAssignLong( apmOrder, -(long)(order-2), 0, 0 ) ;
        apmMultiply( cosCoef[coef_num], scratch, apmOrder ) ;

        coef_num-- ;
    }

    apmAssign( sinFactr1, sinCoef[0] ) ;
    apmAssign( cosFactr1, cosCoef[0] ) ;
}
/* ++++++ */

apmFloorString( s, n, x )

APM x ;
int n ;
char *s ;
{
    apmConvert( s, n, 1, NO_ROUND, LEFT_JUST, x ) ;
    strip_frac( s ) ;
}
/* ++++++ */

```

```

strip_frac( str )

char *str ;
{
    char *cpt ;

    for( cpt = str ; cpt != '\0' ; cpt++ )
        if( *cpt == '.' ) {
            *cpt = '\0' ;
            break ;
        }
}
/* ++++++ */

apmLogBd( x )

APM x ;
/*
    Returns an upper bound on the base-10 log of an apm.
*/
{
    int order ;
    char *bpt ;

    if( apmCompare( one, x ) <= 0 ) {
        apmFloorString( log_buf, BUF_SZ, x ) ;
        return( strlen( log_buf ) ) ;
    }
    else {
        apmConvert( log_buf, BUF_SZ, (BUF_SZ-4), NO_ROUND, LEFT_JUST, x ) ;
        /*
            Skip to the digits beyond the decimal point
        */
        for( bpt=log_buf ; *bpt != '.' ; bpt++ ) ;
        bpt++ ;
        /*
            Count the number of zeroes to the right of the decimal point.
        */
        for( order=0 ; (*bpt == '0') ; bpt++, order-- ) ;
        return( order ) ;
    }
}

```

C.2.2 interval arithmetic

the header file bounding.h

```

/*
    Data structures for calculating semi-rigorous bounds
    on expressions.
*/

typedef struct { double ub, lb ; } Bdd_dbl ;

typedef struct { int nfactores ;
                double coef ;
                Bdd_dbl **factores, bound ; } Bdd_term ;

typedef struct { int nterms ;

```

```

        double      const ;
        Bdd_dbl     bound ;
        Bdd_term    *terms ; } Bdd_expr ;

/*
   APM partners to the structures above
*/

typedef struct { APM  ub, lb ; } Bdd_apm ;

typedef struct { int      nfactores ;
                APM      coef ;
                Bdd_apm   **factores, bound ; } Bapm_term ;

typedef struct { int      nterms ;
                APM      const ;
                Bdd_apm   bound ;
                Bapm_term *terms ; } Bapm_expr ;

/* ++++++ */

# define  assignBapm( empty, full )    (apmAssign( empty->ub, full->ub), \
                                       apmAssign( empty->lb, full->lb) )
# define  assignBdbl( empty, full )    (empty->ub = full->ub, \
                                       empty->lb = full->lb )
# define  newBapm( new, base )         (new.ub = apmNew( base ), \
                                       new.lb = apmNew( base ) )

# define  maxAbs( x, y )               ( (fabs(x) > fabs(y)) ? fabs(x) : fabs(y) )

extern int RmaxAbs() ;

```

expressions

```

# include <stdio.h>
# include <math.h>
# include "apm.h"
# include "converse.h"
# include "bounding.h"

APM  Rextrema, Rextremb, Rub, Rlb ;
APM  Rprod[4], *Rlastp = (Rprod + 4) ;
double prod[4], *lastp = (prod + 4) ;
/* ++++++ */
initBounding()
{
    int  j ;

    Rub = apmNew( BASE ) ;
    Rlb = apmNew( BASE ) ;

    Rextrema = apmNew( BASE ) ;
    Rextremb = apmNew( BASE ) ;

    for( j=0 ; j < 4 ; j++ )
        Rprod[j] = apmNew( BASE ) ;
}
/* ++++++ */

Rbound_term( tpt )
/*
   Take a list of bounded factors and obtain a bound on their

```

```

    product.
*/
Bapm_term *tpt ;
{
    APM      *ppt ;
    Bdd_apm  *facptr, **lastf, **fpt ;

/*
    If there is only one factor, deal with it directly.
*/
    if( tpt->nfactors == 1 ) {
        apmAssign( Rextrema, tpt->factors[0]->ub ) ;
        apmAssign( Rextremb, tpt->factors[0]->lb ) ;
    }
/*
    Handle expressions with more than one factor.
    Since some of the factors may be negative we
    can't just multiply to gether all the upper
    and lower bounds.
*/
    else {
        apmAssign( Rextrema, tpt->factors[0]->ub ) ;
        apmAssign( Rextremb, tpt->factors[0]->lb ) ;

        fpt = &tpt->factors[1] ;
        for( lastf = tpt->factors + tpt->nfactors ; fpt < lastf ; fpt++ ) {
            facptr = *fpt ;

            apmMultiply( Rprod[0], facptr->ub, Rextrema ) ;
            apmMultiply( Rprod[1], facptr->ub, Rextremb ) ;
            apmMultiply( Rprod[2], facptr->lb, Rextrema ) ;
            apmMultiply( Rprod[3], facptr->lb, Rextremb ) ;

            apmAssign( Rextrema, Rprod[0] ) ;
            apmAssign( Rextremb, Rprod[0] ) ;
            for( ppt = (Rprod+1) ; ppt < Rlastp ; ppt++ ) {
                if( apmCompare( *ppt, Rextrema ) == 1 )
                    apmAssign( Rextrema, *ppt ) ;
                else if( apmCompare( *ppt, Rextremb ) == -1 )
                    apmAssign( Rextremb, *ppt ) ;
            }
        }
    }

    apmCalc( Rextrema, Rextrema, tpt->coef, APM_MUL, NULL ) ;
    apmCalc( Rextremb, Rextremb, tpt->coef, APM_MUL, NULL ) ;
    if( apmCompare( Rextrema, Rextremb ) == -1 ) {
        apmAssign( tpt->bound.ub, Rextremb ) ;
        apmAssign( tpt->bound.lb, Rextrema ) ;
    }
    else {
        apmAssign( tpt->bound.ub, Rextrema ) ;
        apmAssign( tpt->bound.lb, Rextremb ) ;
    }
}
/* ++++++ */

Rbound_expr( ept )
/*
    Obtain bounds on the terms in a bounded expression, add them up,
    and so obtain a bound on the whole.

```



```

*/
Bapm_expr  *ept ;
{
    Bapm_term *tpt, *last_term ;

    apmAssign( Rub, ept->const ) ;
    apmAssign( Rlb, ept->const ) ;

    tpt = ept->terms ;
    for( last_term = tpt + ept->nterms ; tpt < last_term ; tpt++ ) {
        Rbound_term( tpt ) ;
        apmCalc( Rub, Rub, tpt->bound.ub, APM_ADD, NULL ) ;
        apmCalc( Rlb, Rlb, tpt->bound.lb, APM_ADD, NULL ) ;
    }

    apmAssign( ept->bound.ub, Rub ) ;
    apmAssign( ept->bound.lb, Rlb ) ;
}
/* ++++++ */

RmaxAbs( result, x, y )

APM  result, x, y ;
{
    apmAbsoluteValue( Rub, x ) ;
    apmAbsoluteValue( Rlb, y ) ;

    if( apmCompare( Rub, Rlb ) == 1 )
        apmAssign( result, Rub ) ;
    else
        apmAssign( result, Rlb ) ;
}

```

bounding trig. functions

```

# include <stdio.h>
# include <math.h>
# include "apm.h"
# include "apmSpecial.h"
# include "converse.h"
# include "bounding.h"
# include "pi.h"

APM  half, three_halves ;
APM  Rdelta, Rmax_cos, Rmin_cos ;
APM  Rmax_x, Rmin_x, Rfloor_x, Rlft_val, Rrght_val ;

Bdd_apm Rnew_theta ;
/* ----- */

initTrigBd()
/*
    Set up the APM's defined above.
*/
{
    Rdelta = apmNew( BASE ) ;
    Rmin_x = apmNew( BASE ) ;
    Rmax_x = apmNew( BASE ) ;
    Rfloor_x = apmNew( BASE ) ;
}

```

```

Rmax_cos = apmNew( BASE ) ;
Rmin_cos = apmNew( BASE ) ;
Rlft_val = apmNew( BASE ) ;
Rrght_val = apmNew( BASE ) ;

Rnew_theta.ub = apmNew( BASE ) ;
Rnew_theta.lb = apmNew( BASE ) ;

half = apmInit( 2L, 0, BASE ) ;
three_halfs = apmInit( 3L, 0, BASE ) ;
apmCalc( half, half, APM_RECIP( precision ), NULL ) ;
apmCalc( three_halfs, half, three_halfs, APM_MUL, NULL ) ;
}
/* ++++++ */

Rbd_cos( bound, theta )
/*
    Obtain bounds for the cosine function over
    a certain given range of angles.
*/

Bdd_apm *theta, *bound ;
{
/*
    An APM partner to the function above. The variables
    used here are static, and are defined at the top
    of the file.
*/
/*
    Get some variables equal to theta / TWO_PI. These will
    help decide whether the interval under consideration
    contains any extrema.
*/
    apmDivide( Rmin_x, precision, (APM)NULL, theta->lb, two_pi ) ;
    apmDivide( Rmax_x, precision, (APM)NULL, theta->ub, two_pi ) ;

    apmFloor( Rfloor_x, Rmin_x, BASE ) ;
    apmCalc( Rmin_x, Rmin_x, Rfloor_x, APM_SUB, NULL ) ;
    apmCalc( Rmax_x, Rmax_x, Rfloor_x, APM_SUB, NULL ) ;
    apmSubtract( Rdelta, Rmax_x, Rmin_x ) ;
    if( apmCompare( Rdelta, one ) == 1 ) {
        apmAssign( bound->ub, one ) ;
        apmNegate( bound->lb, one ) ;
    }

    else {
        apmCos( Rlft_val, theta->lb ) ;
        apmCos( Rrght_val, theta->ub ) ;
        if( apmCompare( Rlft_val, Rrght_val ) == 1 ) {
            apmAssign( Rmax_cos, Rlft_val ) ;
            apmAssign( Rmin_cos, Rrght_val ) ;
        }
        else {
            apmAssign( Rmax_cos, Rrght_val ) ;
            apmAssign( Rmin_cos, Rlft_val ) ;
        }
    }
/*
    Check for extrema.
*/
    if( apmCompare( Rmax_x, one ) == 1 )
        apmAssign( Rmax_cos, one ) ;

```

```

    if (apmCompare( Rmax_x, three_halfs) == 1) ||
        ((apmCompare( Rmin_x, half) == -1) &&
         (apmCompare( Rmax_x, half) == 1)) ) apmNegate( Rmin_cos, one ) ;

    apmAdd( bound->ub, Rmax_cos, max_error ) ;
    apmSubtract( bound->lb, Rmin_cos, max_error ) ;
}

return ;
}
/* ++++++ */

Rbd_sin( bound, theta )
/*
   Use the relation  $\sin(x - \text{HALF\_PI}) = \cos(x)$ 
   and the function bd_cos() to obtain a bound on
   the sines of angles lying in a given range.
*/

Bdd_apm *theta, *bound ;
{
/*
   Rnew_theta is used here but is declared at the top of
   the file
*/
    apmSubtract( Rnew_theta.ub, theta->ub, half_pi ) ;
    apmSubtract( Rnew_theta.lb, theta->lb, half_pi ) ;

    Rbd_cos( bound, &Rnew_theta ) ;
    return ;
}

```

C.2.3 starting points and global bounds

```

# include <stdio.h>
# include <math.h>
# include "apm.h"
# include "converse.h"
# include "pi.h"

# define DELTA      0.01
# define MAX_JUMP   0.1

APM Rstart_size ;
/* ++++++ */
setHermStart( priz )

RPrism *priz ;
{
    double a, b, c, two_c, x, y ;
    double jump_sz, jump_scl, dx, dy ;
    double gx, gy, hxx, hxy, hyy, hdet, tolerance ;

    a = apmtodbl( priz->center->p[0] ) ;
    b = apmtodbl( priz->center->p[1] ) ;
    c = apmtodbl( priz->center->p[2] ) ;
    two_c = 2.0 * c ;

    tolerance = NEWT_TOL * (fabs(a) + fabs(b) + fabs(c)) ;
}

```

```

/*
    Use Newton's method to try to find a minimum for the
    trace of the matrix beta.
*/

x = HALF_PI ;
y = HALF_PI ;

do {
    /*      components of the gradient.      */

    gx = -a * cos( x ) - two_c * cos( x + y ) ;
    gy = -b * cos( y ) - two_c * cos( x + y ) ;

    /*      components of the Hessian      */

    hxx = a * sin( x ) + two_c * sin( x + y ) ;
    hxy = two_c * sin( x + y ) ;
    hyy = b * sin( y ) + two_c * sin( x + y ) ;
    hdet = hxx * hyy - hxy * hxy ;

    /*      A Newton's method step      */
    if( hdet != 0.0 ) {
        dx = ( gx * hyy - gy * hxy ) / hdet ;
        dy = ( -gx * hxy + gy * hxx ) / hdet ;

        if( ( jump_sz = fabs(dx) + fabs(dy) ) > MAX_JUMP ) {
            jump_scl = MAX_JUMP / jump_sz ;
            dx *= jump_scl ;
            dy *= jump_scl ;
        }

        x -= dx ;
        y -= dy ;

    }
    else {
        fprintf( stderr, "Death during Newton's method. \n" ) ;
        cease() ;
    }
} while( ( fabs(gx) + fabs(gy) ) > tolerance ) ;

/*
    Force the starting point to lie on the line x=y.
*/
dbltoapm( priz->center->z.u[0], BASE, x ) ;
dbltoapm( priz->center->z.u[1], BASE, x ) ;

#ifdef DEBUG
    printf( "Herman's starting point : x = %.6e, y = %.6e \n", x, x ) ;
    fflush( stdout ) ;
#endif
}
/* ++++++ */

setLLStart( priz )

RPrism *priz ;
{
/*
    Beware : this function expects to be called AFTER

```

```

setHermStart(), no matter which criterion is in force.
*/
double discrim, sqrt_disc, sqrt();
double a_sin, a_cos, b_sin, b_cos, c_sin, c_cos;
double a, b, c, two_c, x, y;
double jump_sz, jump_scl, dx, dy;
double gx, gy, hxx, hxy, hyy, hdet, tolerance;
double dDisc_dx, dDisc_dy;

a = apmtodbl( priz->center->p[0] );
b = apmtodbl( priz->center->p[1] );
c = apmtodbl( priz->center->p[2] );
two_c = 2.0 * c;

x = apmtodbl( priz->center->z.u[0] );
y = apmtodbl( priz->center->z.u[1] );

tolerance = HEWT_TOL * ( a + b + c );

do {
    /* preliminaries */

    a_sin = a * sin( x );
    b_sin = b * sin( y );
    c_sin = two_c * sin( x + y );

    a_cos = a * cos( x );
    b_cos = b * cos( y );
    c_cos = two_c * cos( x + y );

    discrim = ( a_sin - b_sin ) * ( a_sin - b_sin ) +
               c_sin * c_sin;
    sqrt_disc = sqrt( discrim );
    dDisc_dx = a_cos * ( a_sin - b_sin ) + c_cos * c_sin;
    dDisc_dy = b_cos * ( b_sin - a_sin ) + c_cos * c_sin;

    /* components of the gradient. */

    gx = -a_cos - c_cos - dDisc_dx / sqrt_disc;
    gy = -b_cos - c_cos - dDisc_dy / sqrt_disc;

    /* components of the Hessian */

    hxx = a_sin + c_sin +
          ( a_sin * ( a_sin - b_sin ) -
            a_cos * a_cos - c_cos * c_cos +
            c_sin * c_sin ) / sqrt_disc
          + dDisc_dx * dDisc_dx / ( discrim * sqrt_disc );

    hxy = c_sin +
          ( a_cos * b_cos + c_sin * c_sin -
            c_cos * c_cos ) / sqrt_disc
          + dDisc_dx * dDisc_dy / ( discrim * sqrt_disc );

    hyy = b_sin + c_sin +
          ( b_sin * ( b_sin - a_sin ) -
            b_cos * b_cos - c_cos * c_cos +
            c_sin * c_sin ) / sqrt_disc
          + dDisc_dy * dDisc_dy / ( discrim * sqrt_disc );
}

```

```

hdet = hxx * hyy - hxy * hxy ;

/*      A Newton's method step      */
if( hdet != 0.0 ) {
    dx = ( gx * hyy - gy * hxy ) / hdet ;
    dy = ( -gx * hxy + gy * hxx ) / hdet ;

    if( (jump_sz = fabs(dx) + fabs(dy)) > MAX_JUMP ) {
        jump_scl = MAX_JUMP / jump_sz ;
        dx *= jump_scl ;
        dy *= jump_scl ;
    }

    x -= dx ;
    y -= dy ;

}
else {
    fprintf( stderr, "Death during Newton's method. \n" ) ;
    cease() ;
}
} while( (fabs(gx) + fabs(gy)) > tolerance ) ;

/*
Force the starting point to lie on the line x=y.
*/
dbltoapm( priz->center->z.u[0], BASE, x ) ;
dbltoapm( priz->center->z.u[1], BASE, x ) ;

#if DEBUG
printf( "Least eigenvalue starting point : x = %.6e, y= %.6e \n", x, x ) ;
fflush( stdout ) ;
#endif
}

# include <stdio.h>
# include <math.h>
# include "apm.h"
# include "apmSpecial.h"
# include "converse.h"
# include "bounding.h"
# include "pi.h"

APM    Rdf_sq, Rdf ;
APM    lip_scratch ;
APM    sixteen, eight, four ;
APM    Rdscrm, Rsqrt_disc ;
APM    Rmax_slope, Rmin_slope, Rfirst_slope ;
double max_slope, min_slope, first_slope ;
RPrism *earliest ;
Bdd_apm Rmax_btrace, Rmin_btrace, Rfirst_btrace ;
/* ++++++ */

initLip()
{
/*
This function depends in detail on the choice of map.
*/

/*

```

```

        APM stuff
*/
four = apmInit( 4L, 0, BASE );
eight = apmInit( 8L, 0, BASE );
sixteen = apmInit( 16L, 0, BASE );

Rmin_slope = apmNew( BASE );          /* The external APMs */
Rmax_slope = apmNew( BASE );
Rfirst_slope = apmNew( BASE );
Rdf = apmInit( (long)(DEG_FREE), 0, BASE );
Rdf_sq = apmInit( (long)(DF_SQ), 0, BASE );
Rstart_size = apmInit( 1L, -START_SZ, BASE );

Rdscrm = apmNew( BASE );
Rsqrt_disc = apmNew( BASE );
lip_scratch = apmNew( BASE );

newBapm( Rmax_btrace, BASE );
newBapm( Rmin_btrace, BASE );
newBapm( Rfirst_btrace, BASE );

earliest = conjureRPrism();
}
/* ++++++ */

setCone( priz )

RPrism *priz ;
/*
    Get the minimum and maximum values for the
    trace of the slope object. Note that we
    exploit the symmetry of the potential; the minimum
    and maximum values of the trace of (beta - 2I) have
    the same absolute value.
*/
{
    int j ;
    APM *mat_pos ;

    for( j=0 ; j < N_PARMS ; j++ )
        apmAssign( earliest->center->p[j], priz->center->p[j] ) ;

    for( j=0 ; j < DEG_FREE ; j++ ) {
        apmAssign( earliest->center->z.v[j], priz->center->z.u[j] ) ;
    }

    Rglobal_bounds( earliest ) ;
    Rbound_btrace( &Rmin_btrace, earliest ) ;
/*
    Account for the imprecision of the starting point
    and the variation of the parameters.
*/
    apmAssignLong( lip_scratch, 0L, 0, BASE ) ;
    mat_pos = priz->matrix ;

    for( j=0 ; j < N_PARMS ; j++ ) {
        apmCalc( lip_scratch, lip_scratch,
                priz->center->p[j] , Rstart_size,
                APM_MUL, APM_ADD,
                *mat_pos,
                APM_ABS, APM_ADD, NULL ) ;
    }
}

```

```

    mat_pos += 1 + MAT_DIM ;
}

apmCalc( Rmin_btrace.lb, Rmin_btrace.lb, lip_scratch,
         APM_SUB, NULL ) ;
apmCalc( Rmin_btrace.ub, Rmin_btrace.ub, lip_scratch,
         APM_ADD, NULL ) ;

/* exploit the symmetry */
apmSubtract( Rmax_btrace.ub, eight, Rmin_btrace.lb ) ;
apmSubtract( Rmax_btrace.lb, eight, Rmin_btrace.ub ) ;

apmCalc( Rdscrm, Rmax_btrace.lb, APM_DUP, APM_MUL,
         four, Rdf_sq, APM_MUL, APM_SUB, NULL ) ;

apmSqrt( Rsqrt_disc, precision, Rdscrm ) ;
apmAdd( lip_scratch, Rmax_btrace.lb, Rsqrt_disc ) ;
apmDivide( Rmax_slope, precision, (APM)NULL, lip_scratch, two ) ;

apmSubtract( lip_scratch, Rmax_btrace.lb, Rsqrt_disc ) ;
apmDivide( Rmin_slope, precision, (APM)NULL, lip_scratch, two ) ;

min_slope = apmtodbl( Rmin_slope ) ;
max_slope = apmtodbl( Rmax_slope ) ;

}
/* ++++++ */

setSlopes( priz )

RPrism *priz ;
/*
    Recall that our orbit will, at the beginning of
    a round of orbit-following, have just passed through a
    point on the torus whose beta will diminish the
    slope. This implies that the slope is already smaller
    than the value of max_slope found above. Calculate
    a better upper bound on what the slope could be and
    store it in first_slope and Rfirst_slope.
*/
{
    int j, mat_pos ;

    for( j=0 ; j < N_PARMS ; j++ ) {
        apmAssign( earliest->center->p[j], priz->center->p[j] ) ;

        mat_pos = j * (MAT_DIM + 1) ;
        apmAssign( earliest->matrix[mat_pos], priz->matrix[mat_pos] ) ;
    }

    for( j=0 ; j < DEG_FREE ; j++ ) {
        apmAssign( earliest->center->z.v[j], priz->center->z.u[j] ) ;

        /*
            Account for imprecision in the starting point.
        */
        mat_pos = STAID_LEW + TWO_DF*MAT_DIM +
                 N_PARMS + DEG_FREE + j * (MAT_DIM + 1) ;
        apmAssign( earliest->matrix[mat_pos], Rstart_size ) ;
    }

    Rglobal_bounds( earliest ) ;
}

```



```

Rbound_btrace( &Rfirst_btrace, earliest );

apmDivide( lip_scratch, precision, (APM)NULL, Rdf_sq, Rmax_slope );
apmCalc( Rfirst_slope, Rfirst_btrace.ub, lip_scratch, APM_SUB,
        max_error, APM_ADD, NULL );

first_slope = apmtodbl( Rfirst_slope ) + DBL_ERR ;

}

# include <stdio.h>
# include <math.h>
# include "apm.h"
# include "apmSpecial.h"
# include "converse.h"
# include "bounding.h"
# include "rows.h"

APM      Rsqrt_disc ;
APM      Ra_term, Rb_term, Rc_term ;
APM      Rtrace_ll, RminBlam_ll, RmaxBlam_ll, Rdenom ;
Bdd_apm  Rbtrace, RminLam, RmaxLam ;
RPrism   *earliest ;

Bdd_dbl  discrim ;
Bdd_dbl  a_sq, b_sq, c_sq ;
Bdd_dbl  *lamFacts[2] ;
Bdd_term ab_term ;

APM      four, lam_scratch ;
Bdd_apm  Rdiscrim ;
Bdd_apm  Ra_sq, Rb_sq, Rc_sq ;
Bdd_apm  *RlamFacts[2] ;
Bapm_term Rab_term ;

APM      RfirstLeastLam, RminLeastLam, RmaxLeastLam, RsumTinyLams ;
double   firstLeastLam, minLeastLam, maxLeastLam, sumTinyLams ;
/* ++++++ */

initLambda()
{
/*
    Do up the APMs
*/
    Ra_term = apmNew( BASE ) ;
    Rb_term = apmNew( BASE ) ;
    Rc_term = apmNew( BASE ) ;

    Rdenom = apmNew( BASE ) ;
    Rtrace_ll = apmNew( BASE ) ;
    Rsqrt_disc = apmNew( BASE ) ;
    RminBlam_ll = apmNew( BASE ) ;
    RmaxBlam_ll = apmNew( BASE ) ;

    RminLeastLam = apmNew( BASE ) ;
    RmaxLeastLam = apmNew( BASE ) ;
    RsumTinyLams = apmNew( BASE ) ;
    RfirstLeastLam = apmNew( BASE ) ;

    newBapm( Ra_sq, BASE ) ;
    newBapm( Rb_sq, BASE ) ;

```

```

newBapm( Rc_sq, BASE );
newBapm( RmaxLam, BASE );
newBapm( RminLam, BASE );
newBapm( RBtrace, BASE );
newBapm( Rdiscrim, BASE );

four = apmInit( 4L, 0, BASE );
lam_scratch = apmNew( BASE );

earliest = conjureRPrism();
/*
    Set up the terms.
*/

ab_term.nfactors = Rab_term.nfactors = 2 ;
ab_term.factors = lamFacts ;
Rab_term.factors = RlamFacts ;
ab_term.coef = -2.0 ;
Rab_term.coef = apmInit( -2L, 0, BASE );
newBapm( Rab_term.bound, BASE );
    ab_term.factors[0] = &a_sin.bound ;
    ab_term.factors[1] = &b_sin.bound ;
    Rab_term.factors[0] = &Ra_sin.bound ;
    Rab_term.factors[1] = &Rb_sin.bound ;
}
/* ++++++ */

Rbd_Blams( leastBlam, bigBlam, trace )

Bdd_apm *leastBlam, *trace, *bigBlam ;
/*
    An APM partner to bd_Blams ;
*/
{
/* Bound the terms for the discriminant. */
    RsetSq( &Ra_sq, &Ra_sin.bound );
    RsetSq( &Rb_sq, &Rb_sin.bound );
    RsetSq( &Rc_sq, &Rc_sin.bound );
    Rbound_term( &Rab_term );

/* Bound the discriminant itself. */

    /* lower bound */
    apmCalc( Rdiscrim.lb, Ra_sq.lb, Rb_sq.lb, APM_ADD,
            four, Rc_sq.lb, APM_MUL, APM_ADD,
            Rab_term.bound.lb, APM_ADD, NULL );

    if( apmCompare( Rdiscrim.lb, zero ) < 1 )
        apmAssign( Rdiscrim.lb, zero );

    /* upper bound */
    apmCalc( Rdiscrim.ub, Ra_sq.ub, Rb_sq.ub, APM_ADD,
            four, Rc_sq.ub, APM_MUL, APM_ADD,
            Rab_term.bound.ub, APM_ADD, NULL );

    if( apmCompare( Rdiscrim.ub, zero ) < 1 )
        apmAssign( Rdiscrim.ub, zero );

/* Do up the final bounds on the eigenvalues.
    First do those requiring
    sqrt( discrim.lb ).
*/

```

```

apmSqrt( Rsqrt_disc, precision, Rdiscrim.lb );
apmCalc( lam_scratch, trace->ub, Rsqrt_disc, APM_SUB,
        max_error, APM_ADD, NULL );
apmDivide( leastBlam->ub, precision, (APM)NULL, lam_scratch, two );

apmCalc( lam_scratch, trace->lb, Rsqrt_disc, APM_ADD,
        max_error, APM_SUB, NULL );
apmDivide( bigBlam->lb, precision, (APM)NULL, lam_scratch, two );

/*
        Next those requiring
        sqrt( discrim.lb )
*/
apmSqrt( Rsqrt_disc, precision, Rdiscrim.ub );
apmCalc( lam_scratch, trace->lb, Rsqrt_disc, APM_SUB,
        max_error, APM_SUB, NULL );
apmDivide( leastBlam->lb, precision, (APM)NULL, lam_scratch, two );

apmCalc( lam_scratch, trace->ub, Rsqrt_disc, APM_ADD,
        max_error, APM_ADD, NULL );
apmDivide( bigBlam->ub, precision, (APM)NULL, lam_scratch, two );
}
/* ++++++ */

setLLbounds( priz )
/*
    Get bounds on the least eigenvalue of the variation of the action
    functional. This is equivalent to the summer's estimate of the
    value of size of the perturbation for which no minimizing state
    can include the maximum of the perturbation.
*/
RPrism *priz ;
{
    int    j, mat_pos ;
    APM    *pmat_pos ;

    for( j=0 ; j < N_PARMS ; j++ )
        apmAssign( earliest->center->p[j], priz->center->p[j] ) ;

    mat_pos = j * (MAT_DIM + 1) ;
    apmAssign( earliest->matrix[mat_pos], priz->matrix[mat_pos] ) ;

    for( j=0 ; j < DEG_FREE ; j++ )
        apmAssign( earliest->center->z.v[j], priz->center->z.u[j] ) ;

/*

    Rglobal_bounds( earliest ) ;
    Rbound_btrace( &RBtrace, earliest ) ;
    Rbd_Blams( &RminLam, &RmaxLam, &RBtrace ) ;

*/

    Account for the imprecision of the starting point
    and the variation of the parameters.
*/
    apmAssignLong( lam_scratch, OL, 0, BASE ) ;
    pmat_pos = priz->matrix ;

    for( j=0 ; j < N_PARMS ; j++ ) {

```

```

    apmCalc( lam_scratch, lam_scratch,
            priz->center->p[j] , Rstart_size,
            APM_MUL, APM_ADD,
            *pmat_pos,
            APM_ABS, APM_ADD, NULL ) ;
    pmat_pos += 1 + MAT_DIM ;
}

apmCalc( RminLam.lb, RminLam.lb, lam_scratch, APM_SUB, NULL ) ;
apmCalc( RminLam.ub, RminLam.ub, lam_scratch, APM_ADD, NULL ) ;

/*
    Exploit the symmetry of the example. The
    largest value for an eigenvalue is
    4.0 - (leastLam.lb).

    The calculation above assumes that the
    u part of the prism's center contains a
    starting point suitable for a least-eigenvalue
    kind of test, i.e. the point where the least ev
    attains its minimum. The bdd_apm RmaxLam will
    contain information about the largest ev of beta
    at the spot where leastLam is small. To get the
    thing we really want for the calculations
    below we must exploit the symmetry described
    above.
*/
apmSubtract( RmaxLam.ub, four, RminLam.lb ) ;
apmCalc( Rdiscrim.ub, RmaxLam.ub, APM_DUP, APM_MUL,
        four, APM_SUB, NULL ) ;
apmSqrt( Rsqrt_disc, precision, Rdiscrim.ub ) ;

/*
    A global lower bound - if the least eigenvalue of
    one of the diagonal blocks (see notes, Jan 10 )
    slips below this value then the next block is
    sure to have a negative eigenvalue.
*/
apmSubtract( lam_scratch, RmaxLam.ub, Rsqrt_disc ) ;
apmDivide( RminLeastLam, precision, (APM) NULL, lam_scratch, two ) ;
apmCalc( RminLeastLam, RminLeastLam, max_error, APM_SUB, NULL ) ;
minLeastLam = apmtodbl( RminLeastLam ) ;

/*
    A lower bound on the sum of the non-maximal eigenvalues
    of a diagonal block.
*/
sumTinyLams = minLeastLam ;
apmAssign( RsumTinyLams, RminLeastLam ) ;

/*
    A global upper bound.
*/
apmAdd( lam_scratch, RmaxLam.ub, Rsqrt_disc ) ;
apmDivide( RmaxLeastLam, precision, (APM) NULL, lam_scratch, two ) ;
apmCalc( RmaxLeastLam, RmaxLeastLam, max_error, APM_ADD, NULL ) ;
maxLeastLam = apmtodbl( RmaxLeastLam ) ;
}
/* ++++++ */
RsetSq( xsq, x )

```

```

Bdd_apm  *x, *xsq ;
{
  if( apmCompare( x->ub, zero ) > 0 ) {
    if( apmCompare( x->lb, zero ) > 0 ) {
      apmMultiply( xsq->ub, x->ub, x->ub ) ;
      apmMultiply( xsq->lb, x->lb, x->lb ) ;
    }
    else {
      apmAbsoluteValue( lam_scratch, x->lb ) ;
      if( apmCompare( x->ub, lam_scratch ) > 0 ) {
        apmMultiply( xsq->ub, x->ub, x->ub ) ;
        apmAssign( xsq->lb, zero ) ;
      }
      else {
        apmMultiply( xsq->ub, x->lb, x->lb ) ;
        apmAssign( xsq->lb, zero ) ;
      }
    }
  }
  else {
    apmMultiply( xsq->ub, x->lb, x->lb ) ;
    apmMultiply( xsq->lb, x->ub, x->ub ) ;
  }
}
/* ++++++ */

setLeastLam( priz )

RPrism *priz ;
/*
   Calculate an upper bound on the largest eigenvalue of beta
   at the initial point, then use it and the global bound,
   maxLeastLam to set firstLeastLam.
*/
{
  int    j, mat_pos ;

  for( j=0 ; j < N_PARMS ; j++ ) {
    earliest->center->p[j] = priz->center->p[j] ;

    mat_pos = j * (MAT_DIM + 1) ;
    earliest->matrix[mat_pos] = priz->matrix[mat_pos] ;
  }

  for( j=0 ; j < DEG_FREE ; j++ )
    earliest->center->z.v[j] = priz->center->z.u[j] ;

  Rglobal_bounds( earliest ) ;
  Rbound_btrace( &RBtrace, earliest ) ;
  Rbd_Blams( &RminLam, &RmaxLam, &RBtrace ) ;

/*
   Obtain an upper bound on the least
   eigenvalue of the block of the Hessian of
   the action functional corresponding to the
   starting point. As in the functions in follow.c,
   compute a whole suite of estimates and choose
   the best one.
*/

```

```

/*
    Rdenom is a global upper bound
    on the size of the largest eigenvalue
    of a diagonal block.
        Rdenom = maximum trace - (n-1) * minimum ev.

    It's used together with the least eigenvalue
    of beta (evaluated at the starting point) :

        LeastLam <= RminBlam.ub - 1.0 / Rdenom
*/
apmCalc( Rdenom, Rdf, one, APM_SUB,
        RminLeastLam, APM_MUL, APM_NEG,
        Rmax_slope, APM_ADD, NULL );
apmDivide( lam_scratch, precision, (APM) NULL, one, Rdenom );
apmSubtract( RminBlam_ll, RminLam.ub, lam_scratch );

/*
    Here we try to attain a small estimate by
    saying :
        LeastLam <= RmaxBlam.ub - 1.0 / maxLeastLam.
*/
apmDivide( lam_scratch, precision, (APM) NULL, one, RmaxLeastLam );
apmSubtract( RmaxBlam_ll, RmaxLam.ub, lam_scratch );

/*
    Finally we make the estimate
        LeastLam <= first_slope / DEG_FREE
*/
apmDivide( Rtrace_ll, precision, (APM) NULL, Rfirst_slope, Rdf );

/*
    Choose the best (smallest) lower bound.
*/
apmAssign( RfirstLeastLam, RmaxBlam_ll );
if( apmCompare( RfirstLeastLam, RminBlam_ll ) == 1 )
    apmAssign( RfirstLeastLam, RminBlam_ll );
if( apmCompare( RfirstLeastLam, Rtrace_ll ) == 1 )
    apmAssign( RfirstLeastLam, Rtrace_ll );

firstLeastLam = apmtodbl( RfirstLeastLam );
}

# include <stdio.h>
# include <math.h>
# include "apm.h"
# include "converse.h"
# include "map.h"
# include "bounding.h"
# include "rows.h"

# define    NUM_FACTS    3
# define    NUM_TERMS    3

Bdd_dbl    *fact_buf[NUM_FACTS] ;
Bdd_expr    b_trc ;
Bdd_term    trace_terms[NUM_TERMS] ;

Bdd_apm    *Rfact_buf[NUM_FACTS] ;
Bapm_expr    Rb_trc ;
Bapm_term    Rtrace_terms[NUM_TERMS] ;

```

```

/* ++++++ */

initTrace()
{
    int      j ;
    Bdd_dbl  **fpt ;
    Bdd_apm  **Rfpt ;

/*      Set up the expressions.
*/
    b_trc.nterms = NUM_TERMS ;
    Rb_trc.nterms = NUM_TERMS ;

    b_trc.const = 4.0 ;
    Rb_trc.const = apmInit( 4L, 0, BASE ) ;

    newBapm( Rb_trc.bound, BASE ) ;

    b_trc.terms = trace_terms ;
    Rb_trc.terms = Rtrace_terms ;

/*      Set up their terms.
*/
    fpt = fact_buf ;
    Rfpt = Rfact_buf ;
    for( j=0 ; j < NUM_TERMS ; j++ ) {
        trace_terms[j].nfactors = 1 ;
        trace_terms[j].coef = -1.0 ;
        trace_terms[j].factors = fpt ;

        Rtrace_terms[j].nfactors = 1 ;
        Rtrace_terms[j].coef = apmInit( -1L, 0, BASE ) ;
        Rtrace_terms[j].factors = Rfpt ;

        newBapm( Rtrace_terms[j].bound, BASE ) ;

        fpt++ ;
        Rfpt++ ;
    }
/*      Fix up the constant in the third term . . . it should be
-2.0.
*/
    trace_terms[2].coef = -2.0 ;
    apmAssignLong( Rtrace_terms[2].coef, -2L, 0, BASE ) ;
/*      Associate the factors - which are only pointers
to bounded objects - to genuine, properly initialized objects.
*/
/* first term */
    b_trc.terms[0].factors[0] = &a_sin.bound ;
    Rb_trc.terms[0].factors[0] = &Ra_sin.bound ;

/* second term */
    b_trc.terms[1].factors[0] = &b_sin.bound ;
    Rb_trc.terms[1].factors[0] = &Rb_sin.bound ;

/* third term */
    b_trc.terms[2].factors[0] = &c_sin.bound ;
    Rb_trc.terms[2].factors[0] = &Rc_sin.bound ;
}

```

```

/* ++++++ */

Rbound_btrace( result, priz )

RPrism *priz ;
Bdd_apm *result ;
/*
   An APM partner to bound_btrace.  Some of the variables
   used here are defined above.
*/
{
   /* Bound the expression */
   Rbound_expr( &Rb_trc ) ;
   apmCalc( Rb_trc.bound.ub, Rb_trc.bound.ub, max_error, APM_ADD, NULL ) ;
   apmCalc( Rb_trc.bound.lb, Rb_trc.bound.lb, max_error, APM_SUB, NULL ) ;

   apmAssign( result->ub, Rb_trc.bound.ub ) ;
   apmAssign( result->lb, Rb_trc.bound.lb ) ;
}

```

C.2.4 control of the computation

the header file converse.h

```

# ifndef YES
# define YES 1 /* Ever popular */
# define NO 0
# endif

# ifndef WORKED
# define WORKED 1
# define FAILED 0
# endif

# define NO_TORI 0 /* A prism of initial conditions */
# define UNTRIED 1 /* has one of these as its in_torus */
# define MAYBE 2 /* attribute according to whether */
# define ACTIVE 3 /* it definitely does not contain */
# define SYMMTRC 4 /* any invariant tori, has not yet
                    been considered, is too hard to
                    decide, is under active
                    consideration, or is equivalent
                    to some symmetrically related,
                    other prism. */

# define N_PARMS 3 /* Details of the particular map */
# define DEG_FREE 2
# define DF_SQ (DEG_FREE * DEG_FREE)
# define TWO_DF (2 * DEG_FREE)

# define MAT_DIM (TWO_DF + N_PARMS) /* Used in finding ones */
# define STAID_LEN (N_PARMS * MAT_DIM) /* place in the matrix */
# define MERC_LEN (TWO_DF * MAT_DIM) /* part of a prism. */
# define MAT_SZ (STAID_LEN + MERC_LEN)

# define DBL_ERR 1.0e-13

# define DFLT_DEPTH 10 /* Default values for various global */
# define DFLT_FRTHST 200 /* variables */

```



```

# define DFLT_PRECIS 30
# define DFLT_GRAPH YES
# define DFLT_ERR YES
# define DFLT_TERSE YES
# define STUBBORN NO
# define SAFETY_PRECIS 5

# define START_SZ 6 /* Numbers bearing on the accuracy */
# define NEWT_TOL 10e-8 /* of the starting point */

# define BASE 10000 /* The base used in APM calculations. */

/*
    Data types for non-rigorous, rough calculations
*/

typedef double *Tor_pt, *Parm_pt ;

typedef struct { Tor_pt u, v ; } Embed_pt ;

typedef struct { Embed_pt z ;
                Parm_pt p ; } Xtnd_pt ;

typedef struct prsm { int in_torus, n_cuts ;
                    char *cuts[N_PARMS+TWO_DF] ;
                    double *matrix ;
                    Xtnd_pt *center ;
                    struct prsm *next ; } Prism ;

/*
    Data types for rigorous, arbitrary precision, calculations
*/

typedef APM *RTor_pt, *RParm_pt ;

typedef struct { RTor_pt u, v ; } REmbed_pt ;

typedef struct { REmbed_pt z ;
                RParm_pt p ; } RXtnd_pt ;

typedef struct Rprsm { int in_torus, n_cuts ;
                    APM *matrix ;
                    char *cuts[MAT_DIM] ;
                    RXtnd_pt *center ;
                    struct Rprsm *next ; } RPrism ;

/* ++++++ */

extern Prism *conjurePrism() ;
extern RPrism *conjureRPrism() ;

/*
    Some variables used throughout the converse KAM calculations
*/

extern int do_graph, do_backup, restoration ;
extern int precision, depth, furthest, terse, stubborn ;
extern int quick_tries, tries, Rtries, max_steps, max_NTsteps ;
extern int HermSuccess, LLSuccess, ll_used[3], most_cuts ;
extern int (*fatten)(), (*row_sums)() ;
extern int fxed_form(), Rfxed_form(), col_rotor(), Rcol_rotor() ;
extern int ff_rows(), Rff_rows(), cr_rows(), Rcr_rows() ;
extern APM Rfirst_slope, Rmin_slope, Rmax_slope, Rdf, Rdf_sq ;
extern APM RminLeastLam, RmaxLeastLam, RfirstLeastLam, RsumTinyLams ;

```

```
extern APM      half, max_error, Rstart_size, RSmBlock_err, RBgBlock_err ;
extern char    *graf_file, *back_name, *rest_name, *parm_names[] ;
extern double  firstLeastLam, minLeastLam, maxLeastLam, sumTinyLams ;
extern double  first_slope, min_slope, max_slope ;
extern double  apmtodbl(), parm_roof[], parm_floor[] ;
extern double  SmBlock_err, BgBlock_err ;
```

main()

```
# include <stdio.h>
# include <math.h>
# include "apm.h"
# include "converse.h"
# include "tree.h"

int      do_graph, do_backup, restoration ;
int      precision, depth, err_hndlr, furthest ;
int      stubborn, terse ;
APM      max_error, RSmBlock_err, RBgBlock_err ;
double   SmBlock_err = DF_SQ * DBL_ERR ;
double   BgBlock_err = DEG_FREE * N_PARMS * DBL_ERR ;
/* ++++++ */

main (argc, argv)

int      argc ;
char    *argv[] ;
{
    int      verdict, Rverdict, tree_verdict, nsteps ;
    Prism   *image_prism ;
    RPrism  *active_prism, *old_prism ;

    handle_opts( argc, argv ) ;
    active_prism = conjureRPrism() ;
    image_prism = conjurePrism() ;
    commence( active_prism ) ;

    /* Study the current prism, cutting it up if need be */
    while( active_prism != NULL ) {
        /*
         Try a preliminary, non-rigorous calculation to see if
         prospects are good.  If they are, do a rigorous check.
         If they aren't, try to refine the prism.  If it has already
         been refined enough, just give up.
         */
        if( do_graph == YES )
            graphPrism( active_prism, ACTIVE ) ;
        /*
         Check the tree to see if an equivalent prism
         is already finished.  If so, record the result
         and press on.  If not, do a detailed analysis.
         */
        tree_verdict = consultTree( active_prism ) ;

        graphPrism( active_prism, SYMMTRC ) ;
        if( do_backup == YES )
            make_backup( active_prism ) ;

        old_prism = active_prism ;
        active_prism = old_prism->next ;
    }
}
```

```

    releaseRPrism( old_prism ) ;
}

else {
    prepare_trial( active_prism ) ;
    verdict = try_prism( active_prism, image_prism, &nsteps ) ;

    Rverdict = UNTRIED ;
    if( verdict == NO_TORI ) {
        Rverdict = Rtry_prism( active_prism, image_prism, &nsteps ) ;
        if( Rverdict == NO_TORI ) {
            active_prism->in_torus = NO_TORI ;

            if( terse == NO )
                printRPrism( active_prism, nsteps ) ;
            if( do_graph == YES )
                graphPrism( active_prism, NO_TORI ) ;
            if( do_backup == YES )
                make_backup( active_prism ) ;

            old_prism = active_prism ;
            active_prism = old_prism->next ;
            releaseRPrism( old_prism ) ;
        }
    }

    if( (Rverdict == MAYBE) || (verdict == MAYBE) ) {

        /* Either refine the prism . . . */
        if( may_refine( active_prism ) == YES ) {
            refinePrism( active_prism, image_prism ) ;
            if( do_graph == YES ) {
                graphPrism( active_prism->next, UNTRIED ) ;
                graphPrism( active_prism, ACTIVE ) ;
            }
        }

        /* . . . or give up and move on. */
        else {
            if( do_graph == YES )
                graphPrism( active_prism, MAYBE ) ;
            if( do_backup == YES )
                make_backup( active_prism ) ;

            active_prism->in_torus = MAYBE ;
            moveEdge_o_Chaos( active_prism, nsteps ) ;
            if( terse == NO )
                printRPrism( active_prism, nsteps ) ;

            old_prism = active_prism ;
            active_prism = old_prism->next ;
            releaseRPrism( old_prism ) ;
        }
    }
}

}

cease() ;
}

```

Rtry_prism()

```

# include <stdio.h>
# include <math.h>
# include "apm.h"
# include "apmSpecial.h"
# include "converse.h"
# include "bounding.h"
# include "rows.h"
# include "pi.h"

# define USE_CR      YES /* Use the column rotor?          */
# define USE_LL      YES /* Use the least eigenvalue test? */
# define USE_QT      YES /* Use the quick, preliminary test */
# define USE_RIGOR   YES /* Use the rigorous tests? */
# define USE_SHIFT   NO

# define FF_CYCLS    1
# define QS_TO_RS    5 /* The ratio of quick steps to rigorous steps
                       to be used in determining how long
                       quick_try should go.
                       */
# define MAX_SUM     PI

# define setLclFurthest( n ) ( (((n)/QS_TO_RS)+3) > furthest ) \
                             ? furthest : ((n)/QS_TO_RS)+3 )

/*
   Declarations for some external variables
   mentioned in converse.h. The APMs are initialized by
   initFollowing().
*/
/*
   The functions in this file manipulate copies of the data
   passed to them. The copies are kept in Prisms and RPrisms
   gotten with the conjuring functions by initFollowing().
*/
Prism      *workPriz[2] ;

double     b_buf[DF_SQ], *b_ptrs[DF_SQ] ;
double     parmbuf[2*N_PARMS], coordbuf[2*TWO_DF] ;

Itnd_pt    xpt_a, xpt_b ;
/*
   Some APM variables needed for orbit
   following and slope watching.
*/
RPrism     *Rwork[2] ;

APM        f_scratch, Rdenom ;
APM        Rsum, Rmax_sum ;
APM        Rtrace_ll, RmaxBlam_ll, RminBlam_ll ;
double     trace_ll, maxBlam_ll, minBlam_ll ;

/*
   The variables declared below don't really need to
   be bounded objects (they did in an earlier version of the code),
   but the .ub in their uses makes the code easier to understand.
*/
Bdd_dbl    b_trace, minBlam, maxBlam, leastLam, slope ;
Bdd_apm    Rb_trace, RminBlam, RmaxBlam, RleastLam, Rslope ;

```

```

int    is_first_trial = YES ;
int    local_furth, ll_used[3] ;
int    HermSuccess, LLSuccess ;
int    max_steps, max_NTsteps, tries, Rtries, quick_tries, most_cuts ;
/* ++++++ */

prepare_trial( priz )

RPrism *priz ;
{
    int    j ;

    if( areNewParms( priz ) == YES ) {

/*
        Unless this is the very first prism,
        record the center point - it will be moved by
        setHermStart() and setLLStart() and will need to be
        restored to its correct value.
*/
        if( is_first_trial == NO ) {
            for ( j=0 ; j < DEG_FREE ; j++ ) {
                apmAssign( xpt_a.z.u[j], priz->center->z.u[j] ) ;
                apmAssign( xpt_a.z.v[j], priz->center->z.v[j] ) ;
            }

            setHermStart( priz ) ;
            setCone( priz ) ;
# if USE_LL
            setLLStart( priz ) ;
            setLLbounds( priz ) ;
# endif
# if USE_SHIFT
            shiftStart( priz ) ;
# endif
/*
            Unless this is the very first trial, restore the
            correct value of the centerpoint before evaluating
            the initial estimates for the slope and least eigenvalue.
*/
            if( is_first_trial == YES )
                is_first_trial = NO ;
            else {
                for ( j=0 ; j < DEG_FREE ; j++ ) {
                    apmAssign( priz->center->z.u[j], xpt_a.z.u[j] ) ;
                    apmAssign( priz->center->z.v[j], xpt_a.z.v[j] ) ;
                }

                setSlopes( priz ) ;

# if USE_LL
                setLeastLam( priz ) ;
# else
                firstLeastLam = 1.0 ;
                minLeastLam = 0.5 ;
                dbltoapm( RfirstLeastLam, BASE, firstLeastLam ) ;
                dbltoapm( RminLeastLam, BASE, minLeastLam ) ;
# endif
            }
        }
    }
}

```

```

}
/* ++++++ */

initFollowing()
{
/*
    Set up the correct connections between the various
    static variables in this file.
*/
    int      j, all_well ;

    all_well = YES ;

/*
    Set up the working prisms.
*/
    workPriz[0] = conjurePrism() ;
    workPriz[1] = conjurePrism() ;
    if( (workPriz[0] == NULL) || (workPriz[1] == NULL) )
        all_well = NO ;

/*
    Set up the APM stuff
*/
    f_scratch = apmNew( BASE ) ;
    Rdenom = apmNew( BASE ) ;

    Rtrace_ll = apmNew( BASE ) ;
    RminBlam_ll = apmNew( BASE ) ;
    RmaxBlam_ll = apmNew( BASE ) ;

    newBapm( Rslope, BASE ) ;
    newBapm( Rb_trace, BASE ) ;
    newBapm( RminBlam, BASE ) ;
    newBapm( RmaxBlam, BASE ) ;
    newBapm( RleastLam, BASE ) ;

# if (USE_LL == NO)
    apmAssignLong( RleastLam.ub, 1L, 0, BASE ) ;
    apmAssignLong( RleastLam.lb, 1L, 0, BASE ) ;
# endif

    Rsum = apmNew( BASE ) ;
    Rmax_sum = apmNew( BASE ) ;
    dbltoapm( Rmax_sum, BASE, MAX_SUM ) ;

    Rwork[0] = conjureRPrism() ;
    Rwork[1] = conjureRPrism() ;
    if( (Rwork[0] == NULL) || (Rwork[1] == NULL) )
        all_well = NO ;

/*
    Set up the extended points - they're used by
    quick_test(), and are pointed to by the
    "center" attributes of the working prisms.
*/
    xpt_a.z.u = coordbuf ;
    xpt_a.z.v = coordbuf + DEG_FREE ;
    xpt_a.p = parmbuf ;

    xpt_b.z.u = coordbuf + TWO_DF ;
    xpt_b.z.v = coordbuf + TWO_DF + DEG_FREE ;
    xpt_b.p = parmbuf + N_PARMS ;

```

```

/*
    Set up pointers to the matrix which receives the
    changeable parts of the jacobian; the one called
    "beta" in most of my notes.
*/
for( j=0 ; j < (sizeof( b_buf ) / sizeof( double )) ; j++ )
    b_ptrs[j] = &b_buf[j] ;

/*
    Initialize various performance data.
*/
most_cuts = 0 ;
max_steps = max_NTsteps = 1 ;
HermSuccess = LLSuccess = 0 ;
tries = Rtries = quick_tries = 0 ;
ll_used[0] = ll_used[1] = ll_used[2] = 0 ;

if( all_well == YES )
    return ;
else {
    fprintf( stderr,
             "initFollowing : Could not prepare for pursuit. Died. \n" ) ;
    cease() ;
}
}
/* ++++++ */

Rtry_prism( initial_priz, final_priz, nsteps )

int      *nsteps ;
Prism    *final_priz ;
RPrism   *initial_priz ;
/*
    Rigorously decides whether a prism of initial data may
    contain any invariant Lagrangian tori, an APM version of
    the routine tryPrism() above.
*/
{
    int      count ;
    RPrism   *priz, *priz_prime, *temp_priz ;

    Rtries++ ;
    priz = Rwork[0] ;
    priz_prime = Rwork[1] ;

/*
    Note that Rtry_prism() does not call setSlopes, setStart or
    setCone. All that should have been done with a call to
    prepare_trial().
*/

    isNewPrism = YES ;
    RcopyRPrism( priz, initial_priz ) ;

    fatten = Rfxed_form ;
    row_sums = Rff_rows ;

    *nsteps = count = 1 ;
    apmAssign( Rslope.ub, Rfirst_slope ) ;
    apmAssign( RleastLam.ub, RfirstLeastLam ) ;
    if( apmCompare(Rslope.ub, Rmin_slope) == -1 ) {
        HermSuccess++ ;
    }
}

```

```

    copyRPrism( final_priz, priz ) ;
    return( NO_TORI ) ;
}
if( apmCompare(RleastLam.ub, RminLeastLam) == -1 ) {
    LLSuccess++ ;
    copyRPrism( final_priz, priz ) ;
    return( NO_TORI ) ;
}

* if (USE_RIGOR == NO)
    copyRPrism( final_priz, priz ) ;
    return( NO_TORI ) ;
* endif

while( big_RPrism( priz ) == NO ) {
/*
    Check the slope.
*/
    count++ ;
/*
    Calculate some bounds useful for both criteria.
*/
    Rglobal_bounds( priz ) ;
    Rbound_btrace( &Rb_trace, priz ) ;

* if USE_LL
    /* mrm's condition */
    Rbd_Blams( &RminBlam, &RmaxBlam, &Rb_trace ) ;

    apmDivide( f_scratch, precision, (APM)NULL, one,
              RleastLam.ub ) ;
    apmSubtract( RmaxBlam_ll, RmaxBlam.ub, f_scratch ) ;

    apmSubtract( Rdenom, Rslope.ub, RsumTinyLams ) ;
    if( apmCompare( Rdenom, zero ) > 0 ) {
        apmDivide( f_scratch, precision, (APM) NULL, one, Rdenom ) ;
        apmSubtract( RminBlam_ll, RminBlam.ub, f_scratch ) ;
    }
    else
        apmAssign( RminBlam_ll, zero ) ;
* endif

    /* Herman's condition */
    apmDivide( f_scratch, precision, (APM) NULL, Rdf_sq, Rslope.ub ) ;
    apmSubtract( Rslope.ub, Rb_trace.ub, f_scratch ) ;

* if USE_LL
    apmDivide( Rtrace_ll, precision, (APM)NULL, Rslope.ub, Rdf ) ;

    Rbest_ll( RleastLam.ub, RmaxBlam_ll,
              RminBlam_ll, Rtrace_ll ) ;

* endif

/*
    Do some truncations to speed things up
*/
* if USE_LL
    apmTruncate( RleastLam.ub, precision ) ;
* endif

```



```

apmTruncate( Rslope.ub, precision ) ;

if( apmCompare(Rslope.ub, Rmin_slope) == -1 ) {
    *nsteps = count ;
    if( count > max_NTsteps )
        max_NTsteps = count ;

    HermSuccess++ ;
    copyRPrism( final_priz, priz ) ;
    return( NO_TORI ) ;
}

else if( apmCompare(RleastLam.ub, RminLeastLam) == -1 ) {
    *nsteps = count ;
    if( count > max_NTsteps )
        max_NTsteps = count ;

    LLSuccess++ ;
    copyRPrism( final_priz, priz ) ;
    return( NO_TORI ) ;
}

else {
    if( count == furthest )
        break ;

    Rprismatic_image( priz_prime, priz ) ;
    m_swap( priz, priz_prime, temp_priz ) ;
}

# if USE_CR
    if( count > FF_CYCLS ) {
        fatten = Rcol_rotor ;
        row_sums = Rcr_rows ;
    }
# endif
}

*nsteps = count ;
copyRPrism( final_priz, priz ) ;
return( MAYBE ) ;
}

/* ++++++ */

big_RPrism( Priz )

RPrism *Priz ;
{
    APM *Rrpt, *Rend_mat, *Rend_row ;

    Rend_mat = Priz->matrix + MAT_SZ ;
    for( Rrpt = Priz->matrix ; Rrpt < Rend_mat ; ) {
        apmAssignLong( Rsum, OL, 0, BASE ) ;
        for( Rend_row = Rrpt + MAT_DIM ; Rend_row < Rend_row ; Rrpt++ )
            apmCalc( Rsum, Rsum, *Rrpt, APM_ABS, APM_ADD, NULL ) ;

        if( apmCompare( Rsum, Rmax_sum) == 1 )
            return( YES ) ;
    }

    return( NO ) ;
}

/* ++++++ */

```

```

Rbest_ll( best, minBlam_ll, maxBlam_ll, trace_ll )

APM  best, minBlam_ll, maxBlam_ll, trace_ll ;
{
  apmAssign( best, maxBlam_ll ) ;
  if( apmCompare( best, minBlam_ll ) == 1 )
    apmAssign( best, minBlam_ll ) ;

  if( apmCompare( best, trace_ll ) == 1 )
    apmAssign( best, trace_ll ) ;
}

```

C.2.5 the map

the header file map.h

```

extern APM      RDeriv[], *Rbeta_ptrs[], *Rgamma_ptrs[] ;
extern double   Deriv[], *beta_ptrs[], *gamma_ptrs[] ;

```

mapping functions

```

/*
  Functions to perform the extended Froeschle map and to
  calculate its jacobian. Each function has a rigorous
  and a non-rigorous form; the former always has a name
  beginning with a "R".

  The functions in this file are quite specific -
  they pertain to maps of the form

  (p,u,v) -> (p',u',v')

  p' = p
  u' = v
  v' = 2v - u -dV(v)

  where u, v, u' and v' are all in 2d Euclidean space,
  p is an element of a space of parameters and
  V(v) = -a * sin( v[0] ) + -b * sin( v[1] ) +
        -c * sin( v[0] + v[1] )

  The parameters a, b, and c are always passed through
  an array called "parms" with

  a = parms[0], b = parms[1], c = parms[2].
*/
#include <stdio.h>
#include <math.h>
#include "apm.h"
#include "apmSpecial.h"
#include "converse.h"
#include "map.h"

APM  Rmixing_term, Rv_sum, map_scratch ;
APM  *Rbeta_ptrs[DF_SQ] ;
APM  *Rgamma_ptrs[DF_SQ], RDeriv[MAT_SZ] ;
double *beta_ptrs[DF_SQ] ;
double *gamma_ptrs[DF_SQ], Deriv[MAT_SZ] ;
/* ++++++

```

```

Rimage()
+++++ */

Rimage( x_prime, x )

Rxtnd_pt  *x, *x_prime ;
/*
    Finds the image, x_prime, of a delay-embedded point, x.
    The parameters of the map are in the parameter-space point
    called "parms".
*/
{
    APM      *x_pt, *xp_pt, *last_x ;
    RParm_pt  parms ;

    parms = x->p ;
    x_pt = x->p ;
    xp_pt = x_prime->p ;
    for( last_x = x_pt + N_PARMS ; x_pt < last_x ; x_pt++ )
        apmAssign( *xp_pt++, *x_pt ) ;

    /* Because of the way delay embedding works,
       the first member of x_prime is the same as
       the second member of x .
    */

    x_pt = x->z.v ;
    xp_pt = x_prime->z.u ;
    for( last_x = x_pt + DEG_FREE ; x_pt < last_x ; x_pt++ )
        apmAssign( *xp_pt++, *x_pt ) ;

    /* Do up the actual map. One could
       write a version of image() which worked for
       any standard-type symplectic map; it would
       rely on another function, perturb(), to
       completely define the map. Instead we
       incorporate the perturbation to the
       generating function right into our map -
       we hope to save a little time.
    */
    apmAdd( Rv_sum, x->z.v[0], x->z.v[1] ) ;
    apmCos( map_scratch, Rv_sum ) ;
    apmMultiply( Rmixing_term, map_scratch, parms[2] ) ;

    apmCos( map_scratch, x->z.v[0] ) ;
    apmCalc( x_prime->z.v[0], two, x->z.v[0], APM_MUL,
             x->z.u[0], APM_SUB,
             parms[0], map_scratch, APM_MUL,
             Rmixing_term, APM_ADD,
             APM_ADD, NULL ) ;

    apmCos( map_scratch, x->z.v[1] ) ;
    apmCalc( x_prime->z.v[1], two, x->z.v[1], APM_MUL,
             x->z.u[1], APM_SUB,
             parms[1], map_scratch, APM_MUL,
             Rmixing_term, APM_ADD,
             APM_ADD, NULL ) ;
}
/* +++++
    find_Rbeta()

```

In the interest of speed, we provide functions which only

```

        calculate those parts of the Jacobian that actually
        depend on parms and (u,v). The other parts are
        assumed to have been correctly set by a call to
        initJacobian() or initRjacobian(), both of which
        may be found below.
    ++++++ */

find_Rbeta( b_block, x )

APM      *b_block[] ;
RItnd_pt *x ;
{
    apmAdd( Rv_sum, x->z.v[0], x->z.v[1] ) ;
    apmSin( map_scratch, Rv_sum ) ;
    apmMultiply( Rmixing_term, x->p[2], map_scratch ) ;

    apmSin( map_scratch, x->z.v[0] ) ;
    apmCalc( *b_block[0], x->p[0], map_scratch, APM_MUL,
              two, APM_SWAP, APM_SUB,
              Rmixing_term, APM_SUB, NULL ) ;

    apmNegate( *b_block[1], Rmixing_term ) ;
    apmNegate( *b_block[2], Rmixing_term ) ;

    apmSin( map_scratch, x->z.v[1] ) ;
    apmCalc( *b_block[3], x->p[1], map_scratch, APM_MUL,
              two, APM_SWAP, APM_SUB,
              Rmixing_term, APM_SUB, NULL ) ;
}
/* ++++++

    Rgamma() : calculate the dependence of
    v' on the parameters. Even as the functions
    above, gamma() and Rgamma() change only those components
    pointed to by elements of a block of pointers.
    ++++++ */

find_Rgamma( g_block, x )

APM      *g_block[] ;
RItnd_pt *x ;
{
    apmAdd( Rv_sum, x->z.v[0], x->z.v[1] ) ;
    apmCos( Rmixing_term, Rv_sum ) ;

    apmCos( *g_block[0], x->z.v[0] ) ;
    apmAssign( *g_block[1], Rmixing_term ) ;
    apmCos( *g_block[2], x->z.v[1] ) ;
    apmAssign( *g_block[3], Rmixing_term ) ;
}
/* ++++++ */

initRjacobian( jac )
/*
    Set the constant parts of a jacobian matrix
*/

APM *jac ;
{
    int      j ;
    APM      *end_jac, *jpt ;

```

```

/*
    If the array of APM's called jac has not yet been
    initialized, do that first.
*/
if( apmValidate(jac[0]) != APM_OK ) {
    end_jac = jac + MAT_SZ ;
    for( jpt=jac ; jpt < end_jac ; jpt++ )
        *jpt = apmNew( BASE ) ;
}

end_jac = jac + MAT_SZ ;          /* Set all the entries */
for( jpt=jac ; jpt < end_jac ; jpt++ ) /* to zero. */
    apmAssignLong( *jpt, 0L, 0, BASE ) ;

/*
    Put the identity in the (p,p) position. */
jpt = jac ;
for( j=0 ; j < N_PARMS ; j++ ) {
    apmAssignLong( *jpt, 1L, 0, BASE ) ;
    jpt += MAT_DIM + 1 ;
}

/*
    Put the identity in the (u,v) position. */
jpt = jac + STAID_LEN + N_PARMS + DEG_FREE ;
for( j=0 ; j < DEG_FREE ; j++ ) {
    apmAssignLong( *jpt, 1L, 0, BASE ) ;
    jpt += MAT_DIM + 1 ;
}

/*
    Put -1 times the identity in the (v,u) position. */
jpt = jac + STAID_LEN + (DEG_FREE * MAT_DIM) + N_PARMS ;
for( j=0 ; j < DEG_FREE ; j++ ) {
    apmAssignLong( *jpt, -1L, 0, BASE ) ;
    jpt += MAT_DIM + 1 ;
}
}
/* ++++++ */

initMap()
{
/*
    This function depends in detail on the choice of map.
*/
    beta_ptrs[0] = Deriv + STAID_LEN + (DEG_FREE * MAT_DIM) +
        N_PARMS + DEG_FREE ;
    beta_ptrs[1] = beta_ptrs[0] + 1 ;
    beta_ptrs[2] = beta_ptrs[0] + MAT_DIM ;
    beta_ptrs[3] = beta_ptrs[2] + 1 ;

    gamma_ptrs[0] = Deriv + STAID_LEN + (DEG_FREE * MAT_DIM) ;
    gamma_ptrs[1] = gamma_ptrs[0] + 2 ;
    gamma_ptrs[2] = gamma_ptrs[0] + MAT_DIM + 1 ;
    gamma_ptrs[3] = gamma_ptrs[1] + MAT_DIM ;

/*
    APM stuff
*/
    Rbeta_ptrs[0] = RDeriv + STAID_LEN + (DEG_FREE * MAT_DIM) +
        N_PARMS + DEG_FREE ;
    Rbeta_ptrs[1] = Rbeta_ptrs[0] + 1 ;
    Rbeta_ptrs[2] = Rbeta_ptrs[0] + MAT_DIM ;
    Rbeta_ptrs[3] = Rbeta_ptrs[2] + 1 ;
}

```

```

Rgamma_ptrs[0] = RDeriv + STAID_LEN + (DEG_FREE * MAT_DIM) ;
Rgamma_ptrs[1] = Rgamma_ptrs[0] + 2 ;
Rgamma_ptrs[2] = Rgamma_ptrs[0] + MAT_DIM + 1 ;
Rgamma_ptrs[3] = Rgamma_ptrs[1] + MAT_DIM ;

initJacobian( Deriv ) ;
initRjacobian( RDeriv ) ;

/*
    Further APM stuff - constants and scratch variables.
*/
Rv_sum = apmNew( BASE ) ;
map_scratch = apmNew( BASE ) ;
Rmixing_term = apmNew( BASE ) ;
}
/* ++++++ */

Rjacobian( xpt )

RXtnd_pt *xpt ;
{
    find_Rbeta( Rbeta_ptrs, xpt ) ;
    find_Rgamma( Rgamma_ptrs, xpt ) ;
}

# include <stdio.h>
# include <math.h>
# include "apm.h"
# include "apmSpecial.h"
# include "converse.h"
# include "bounding.h"
# include "map.h"

int          (* fatten)(), (* row_sums)() ;
APM          Rw[MAT_DIM] ;
/* ++++++ */

Rprismatic_image( pz_prime, pz )

RPrism *pz_prime, *pz ;
{
    int      j ;
    APM      *mpt, *end_mat, *wpt, *end_w ;

/*
    Find the image of the center of the prism.
*/
    Rimage( pz_prime->center, pz->center ) ;

    Rjacobian( pz->center ) ; /* Calculate the derivative
                               of the map. */

/*
    Fatten the matrix Deriv * pz->matrix so that it isn't too
    singular.
*/
    (* fatten) ( pz_prime->matrix, RDeriv, pz->matrix ) ;

/*
    Get upper bounds on the rows of the fattened matrix,
    and use them to get the matrix of a prism gauranteed

```

```

        to enclose the image of pz.
*/
(* row_sums)( Rw, pz_prime->matrix, RDeriv, pz );

end_w = Rw + MAT_DIM ;
end_mat = pz_prime->matrix + MAT_SZ ;
for( mpt = pz_prime->matrix ; mpt < end_mat ; ) {
    for( wpt = Rw ; wpt < end_w ; wpt++, mpt++ )
        apmCalc( *mpt, *mpt, *wpt, max_error,
                 APM_ADD, APM_MUL, NULL ) ;
}

truncateRPrism( pz_prime, precision ) ;

}
/* ++++++ */

initPrismatic()
{
    int j ;

    for( j=0 ; j < N_PARMS ; j++ ) {
        Rw[j] = apmNew( BASE ) ;
        apmAssign( Rw[j], one ) ;
        w[j] = 1.0 ;
    }

    for( j=N_PARMS ; j < (N_PARMS + DEG_FREE) ; j++ )
        Rw[j] = apmNew( BASE ) ;

    for( j=(N_PARMS + DEG_FREE) ; j < MAT_DIM ; j++ ) {
        w[j] = 1.0 + DBL_ERR ;
        Rw[j] = apmNew( BASE ) ;
        apmAdd( Rw[j], one, max_error ) ;
    }
}

```

C.2.6 images of prisms

the header file rows.h

```

extern int      isNewPrism ;

extern int      global_bounds(), Rglobal_bounds() ;
extern int      Rbeta_dif_star(), Rgamdif_star() ;
extern double   beta_dif_star(), gamdif_star() ;

extern Bdd_dbl  cos_zero, cos_one, cos_sum ;
extern Bdd_expr a_sin, b_sin, c_sin ;

extern Bdd_apm  Rcos_zero, Rcos_one, Rcos_sum ;
extern Bapm_expr Ra_sin, Rb_sin, Rc_sin ;

extern APM      neg_one, neg_two, Rrow_abs[] ;
/* ++++++ */

```

Rglobal_bounds()

```

* include <stdio.h>

```

```

# include <math.h>
# include "apm.h"
# include "apmSpecial.h"
# include "converse.h"
# include "bounding.h"
# include "rows.h"

# define NUM_FACTS 14
# define NUM_TERMS 11
# define DET_TOL 1e-13

APM      neg_one, neg_two ;
APM      Rrows[DEG_FREE], Rrow_abs[DEG_FREE] ;

Bdd_dbl  a, b, c, cos_zero, cos_one, cos_sum ;
Bdd_dbl  sin_zero, sin_one, sin_sum, theta ;
Bdd_dbl  *row_factors[NUM_FACTS] ;
Bdd_term row_terms[NUM_TERMS] ;
Bdd_expr beta_dif[3], gamma_dif[3] ;
Bdd_expr a_sin, b_sin, c_sin ;

Bdd_apm  Ra, Rb, Rc, Rcos_zero, Rcos_one, Rcos_sum ;
Bdd_apm  Rsin_zero, Rsin_one, Rsin_sum, Rtheta ;
Bdd_apm  *Rrow_factors[NUM_FACTS] ;
Bapm_term Rrow_terms[NUM_TERMS] ;
Bapm_expr Rbeta_dif[3], Rgamma_dif[3] ;
Bapm_expr Ra_sin, Rb_sin, Rc_sin ;
/* ++++++ */

initRowSums()
/*
    Set up the expressions and terms as described in my notes
    from 11/14.
*/
{
    int      j, k ;
    Bdd_dbl  **dpt ;
    Bdd_apm  **apt ;
    Bdd_term *tpt ;
    Bapm_term *Rtpt ;

/*
    Set up some APM's to be used to hold intermediate
    results.
*/
    newBapm( Ra, BASE ) ;
    newBapm( Rb, BASE ) ;
    newBapm( Rc, BASE ) ;
    newBapm( Rtheta, BASE ) ;

    newBapm( Rcos_zero, BASE ) ;
    newBapm( Rcos_one, BASE ) ;
    newBapm( Rcos_sum, BASE ) ;
    newBapm( Rsin_zero, BASE ) ;
    newBapm( Rsin_one, BASE ) ;
    newBapm( Rsin_sum, BASE ) ;

    neg_one = apmInit( -1L, 0, BASE ) ;
    neg_two = apmInit( -2L, 0, BASE ) ;

    for( j=0 ; j < DEG_FREE ; j++ ) {

```



```

    Rrows[j] = apmNew( BASE ) ;
    Rrow_abs[j] = apmNew( BASE ) ;
}

/*
    Set the number of terms in the bounded expressions
*/
a_sin.nterms = Ra_sin.nterms = 1 ;
b_sin.nterms = Rb_sin.nterms = 1 ;
c_sin.nterms = Rc_sin.nterms = 1 ;

beta_dif[0].nterms = Rbeta_dif[0].nterms = 2 ;
beta_dif[1].nterms = Rbeta_dif[1].nterms = 1 ;
beta_dif[2].nterms = Rbeta_dif[2].nterms = 2 ;

gamma_dif[0].nterms = Rgamma_dif[0].nterms = 1 ;
gamma_dif[1].nterms = Rgamma_dif[1].nterms = 1 ;
gamma_dif[2].nterms = Rgamma_dif[2].nterms = 1 ;

/*
    Assign terms
*/

tpt = row_terms ;
Rtpt = Rrow_terms ;
for( j=0 ; j < 3 ; j++ ) {
    beta_dif[j].terms = tpt ;
    Rbeta_dif[j].terms = Rtpt ;
    tpt += beta_dif[j].nterms ;
    Rtpt += Rbeta_dif[j].nterms ;

    gamma_dif[j].terms = tpt ;
    Rgamma_dif[j].terms = Rtpt ;
    tpt += gamma_dif[j].nterms ;
    Rtpt += Rgamma_dif[j].nterms ;
}

a_sin.terms = tpt++ ;
Ra_sin.terms = Rtpt++ ;

b_sin.terms = tpt++ ;
Rb_sin.terms = Rtpt++ ;

c_sin.terms = tpt++ ;
Rc_sin.terms = Rtpt++ ;

/*
    Set nfactors.
*/

Rbeta_dif[0].terms[0].nfactors = beta_dif[0].terms[0].nfactors = 1 ;
Rbeta_dif[0].terms[1].nfactors = beta_dif[0].terms[1].nfactors = 1 ;
Rbeta_dif[1].terms[0].nfactors = beta_dif[1].terms[0].nfactors = 1 ;
Rbeta_dif[2].terms[0].nfactors = beta_dif[2].terms[0].nfactors = 1 ;
Rbeta_dif[2].terms[1].nfactors = beta_dif[2].terms[1].nfactors = 1 ;

Rgamma_dif[0].terms->nfactors = gamma_dif[0].terms->nfactors = 1 ;
Rgamma_dif[1].terms->nfactors = gamma_dif[1].terms->nfactors = 1 ;
Rgamma_dif[2].terms->nfactors = gamma_dif[2].terms->nfactors = 1 ;

a_sin.terms->nfactors = Ra_sin.terms->nfactors = 2 ;
b_sin.terms->nfactors = Rb_sin.terms->nfactors = 2 ;

```

```

c_sin.terms->nfactors = Rc_sin.terms->nfactors = 2 ;
/*
  Assign factors.
*/

dpt = row_factors ;
apt = Rrow_factors ;
for( j=0 ; j < 3 ; j++ ) {
  /*
    beta_dif
  */
  for( k=0 ; k < beta_dif[j].nterms ; k++ ) {
    beta_dif[j].terms[k].factors = dpt ;
    Rbeta_dif[j].terms[k].factors = apt ;

    dpt += beta_dif[j].terms[k].nfactors ;
    apt += Rbeta_dif[j].terms[k].nfactors ;
  }

  /*
    gamma_dif
  */
  for( k=0 ; k < gamma_dif[j].nterms ; k++ ) {
    gamma_dif[j].terms[k].factors = dpt ;
    Rgamma_dif[j].terms[k].factors = apt ;

    dpt += gamma_dif[j].terms[k].nfactors ;
    apt += Rgamma_dif[j].terms[k].nfactors ;
  }
}

a_sin.terms->factors = dpt ;
Ra_sin.terms->factors = apt ;
dpt += 2 ;
apt += 2 ;

b_sin.terms->factors = dpt ;
Rb_sin.terms->factors = apt ;
dpt += 2 ;
apt += 2 ;

c_sin.terms->factors = dpt ;
Rc_sin.terms->factors = apt ;

/*
  Set up those of the "bound" attributes which are
  bounded APM's.
*/

for( j=0 ; j < NUM_TERMS ; j++ ) {
  newBapm( Rrow_terms[j].bound, BASE ) ;
}

for( j=0 ; j < 3 ; j++ ) {
  newBapm( Rbeta_dif[j].bound, BASE ) ;
  newBapm( Rgamma_dif[j].bound, BASE ) ;
}

newBapm( Ra_sin.bound, BASE ) ;
newBapm( Rb_sin.bound, BASE ) ;
newBapm( Rc_sin.bound, BASE ) ;

```

```

/*
    Set up the terms and expressions.
*/

/* a_sin */

a_sin.const = 0.0 ;
Ra_sin.const = apmNew( BASE ) ;
a_sin.terms->coef = 1.0 ;
Ra_sin.terms->coef = apmInit( 1L, 0, BASE ) ;

a_sin.terms->factors[0] = &a ;
a_sin.terms->factors[1] = &sin_zero ;
Ra_sin.terms->factors[0] = &Ra ;
Ra_sin.terms->factors[1] = &Rsin_zero ;

/* b_sin */

b_sin.const = 0.0 ;
Rb_sin.const = apmNew( BASE ) ;
b_sin.terms->coef = 1.0 ;
Rb_sin.terms->coef = apmInit( 1L, 0, BASE ) ;

b_sin.terms->factors[0] = &b ;
b_sin.terms->factors[1] = &sin_one ;
Rb_sin.terms->factors[0] = &Rb ;
Rb_sin.terms->factors[1] = &Rsin_one ;

/* c_sin */

c_sin.const = 0.0 ;
Rc_sin.const = apmNew( BASE ) ;
c_sin.terms->coef = 1.0 ;
Rc_sin.terms->coef = apmInit( 1L, 0, BASE ) ;

c_sin.terms->factors[0] = &c ;
c_sin.terms->factors[1] = &sin_sum ;
Rc_sin.terms->factors[0] = &Rc ;
Rc_sin.terms->factors[1] = &Rsin_sum ;

/* beta_dif */

/* beta_dif[0] = ( 2.0 - a * sin(v[0]) - c * sin(v[0] + v[1]) )
   -{ 2.0 - ac * sin(vc[0]) - cc * sin(vc[0] + vc[1])
   Where ac, cc, vc[0], and vc[1] are the values of these
   numbers at the center of the prism. The whole second
   term ( enclosed in braces ) is an entry in the jacobian
   of the map
*/

Rbeta_dif[0].const = apmNew( BASE ) ;
beta_dif[0].terms[0].coef = -1.0 ;
Rbeta_dif[0].terms[0].coef = neg_one ;

beta_dif[0].terms[0].factors[0] = &a_sin.bound ;
Rbeta_dif[0].terms[0].factors[0] = &Ra_sin.bound ;

beta_dif[0].terms[1].coef = -1.0 ;
Rbeta_dif[0].terms[1].coef = neg_one ;

beta_dif[0].terms[1].factors[0] = &c_sin.bound ;
Rbeta_dif[0].terms[1].factors[0] = &Rc_sin.bound ;

```

```

/* beta_dif[1] =      -2.0 * c * sin.bound( v[0] + v[1] )
   - { -2.0 * cc * sin.bound( vc[0] + vc[1] ) }
*/
Rbeta_dif[1].const = apmNew( BASE );
beta_dif[1].terms[0].coef = -2.0 ;
Rbeta_dif[1].terms[0].coef = neg_two ;

    beta_dif[1].terms[0].factors[0] = &c_sin.bound ;
    Rbeta_dif[1].terms[0].factors[0] = &Rc_sin.bound ;

/* beta_dif[2] = 2.0 - b * sin.bound(v[1]) - c * sin(v[1] + v[0])
   -{ 2.0 - bc * sin.bound(vc[1]) - cc * sin(vc[1] + vc[0]) }
*/
Rbeta_dif[2].const = apmNew( BASE );
beta_dif[2].terms[0].coef = -1.0 ;
Rbeta_dif[2].terms[0].coef = neg_one ;

    beta_dif[2].terms[0].factors[0] = &b_sin.bound ;
    Rbeta_dif[2].terms[0].factors[0] = &Rb_sin.bound ;

beta_dif[2].terms[1].coef = -1.0 ;
Rbeta_dif[2].terms[1].coef = neg_one ;

    beta_dif[2].terms[1].factors[0] = &c_sin.bound ;
    Rbeta_dif[2].terms[1].factors[0] = &Rc_sin.bound ;

/* gamma_dif */

/* gamma_dif[0] = da * ( cos(v[0]) - cos(vc[0]) )
   Where da is half the prism's width as measured
   along the a-axis and vc is as above.          */
Rgamma_dif[0].const = apmNew( BASE );

    Rgamma_dif[0].terms[0].coef = apmNew( BASE );

    gamma_dif[0].terms[0].factors[0] = &cos_zero ;
    Rgamma_dif[0].terms[0].factors[0] = &Rcos_zero ;

/* gamma_dif[1] = db * ( cos(v[1]) - cos(vc[1]) ) */
Rgamma_dif[1].const = apmNew( BASE );

    Rgamma_dif[1].terms[0].coef = apmNew( BASE );

    gamma_dif[1].terms[0].factors[0] = &cos_one ;
    Rgamma_dif[1].terms[0].factors[0] = &Rcos_one ;

/* gamma_dif[2] = dc * ( cos(v[0] + v[1]) -
   cos(vc[0] + vc[1]) ) */
Rgamma_dif[2].const = apmNew( BASE );

    Rgamma_dif[2].terms[0].coef = apmNew( BASE );

    gamma_dif[2].terms[0].factors[0] = &cos_sum ;
    Rgamma_dif[2].terms[0].factors[0] = &Rcos_sum ;
}
/* ++++++ */

Rglobal_bounds( pz )

```

```

RPrism *pz ;
{
    int      j ;
    APM      *apt, *end_row ;

    apmAdd( Ra.ub, pz->center->p[0], pz->matrix[0] ) ;
    apmSubtract( Ra.lb, pz->center->p[0], pz->matrix[0] ) ;

    apmAdd( Rb.ub, pz->center->p[1], pz->matrix[MAT_DIM+1] ) ;
    apmSubtract( Rb.lb, pz->center->p[1], pz->matrix[MAT_DIM+1] ) ;

    apmAdd( Rc.ub, pz->center->p[2], pz->matrix[2*MAT_DIM+2] ) ;
    apmSubtract( Rc.lb, pz->center->p[2], pz->matrix[2*MAT_DIM+2] ) ;

    apt = pz->matrix + STAID_LEN + (DEG_FREE * MAT_DIM) ;
    for( j=0 ; j < DEG_FREE ; j++ ) {
        apmAssign( Rows[j], zero ) ;
        for( end_row=apt + MAT_DIM ; apt < end_row ; apt++ ) {
            apmCalc( Rows[j], Rows[j], *apt,
                    APM_ABS, APM_ADD, NULL ) ;
        }
    }

    apmAdd( Rtheta.ub, pz->center->z.v[0], Rows[0] ) ;
    apmSubtract( Rtheta.lb, pz->center->z.v[0], Rows[0] ) ;
    Rbd_sin( &Rsin_zero, &Rtheta ) ;
    Rbd_cos( &Rcos_zero, &Rtheta ) ;

    apmAdd( Rtheta.ub, pz->center->z.v[1], Rows[1] ) ;
    apmSubtract( Rtheta.lb, pz->center->z.v[1], Rows[1] ) ;
    Rbd_sin( &Rsin_one, &Rtheta ) ;
    Rbd_cos( &Rcos_one, &Rtheta ) ;

    apmCalc( Rtheta.ub, Rtheta.ub, pz->center->z.v[0], Rows[0],
            APM_ADD, APM_ADD, NULL ) ;
    apmCalc( Rtheta.lb, Rtheta.lb, pz->center->z.v[0], Rows[0],
            APM_SUB, APM_ADD, NULL ) ;

    Rbd_sin( &Rsin_sum, &Rtheta ) ;
    Rbd_cos( &Rcos_sum, &Rtheta ) ;

    Rbound_expr( &Ra_sin ) ;
    Rbound_expr( &Rb_sin ) ;
    Rbound_expr( &Rc_sin ) ;
}
/* ++++++ */
Rbeta_dif_star( answer, deriv )
APM  answer, *deriv ;
{
    APM  *dpt ;

    dpt = deriv + STAID_LEN + (MAT_DIM*DEG_FREE) + N_PARMS + DEG_FREE ;
    apmSubtract( Rbeta_dif[0].const, two, *dpt++ ) ;
    apmMultiply( Rbeta_dif[1].const, neg_two, *dpt ) ;
    dpt += MAT_DIM ;
    apmSubtract( Rbeta_dif[2].const, two, *dpt ) ;

    Rbound_expr( &Rbeta_dif[0] ) ;
    Rbound_expr( &Rbeta_dif[1] ) ;
    Rbound_expr( &Rbeta_dif[2] ) ;
}

```

```

RmaxAbs( answer, Rbeta_dif[0].bound.ub, Rbeta_dif[0].bound.lb ) ;
RmaxAbs( Rrow_abs[0], Rbeta_dif[1].bound.ub, Rbeta_dif[1].bound.lb ) ;
RmaxAbs( Rrow_abs[1], Rbeta_dif[2].bound.ub, Rbeta_dif[2].bound.lb ) ;

/*
    Add max_error to the answer to account for the uncertainties
    in beta**(center).
*/
apmCalc( answer, answer, Rrow_abs[0], Rrow_abs[1], max_error,
          APM_ADD, APM_ADD, APM_ADD, NULL ) ;
}
/* ++++++ */
Rgamdif_star( answer, deriv, pmat )

APM  answer, *deriv, *pmat ;
{
    APM  *apt, *Rda, *Rdb, *Rdc ;

    Rda = pmat ;
    Rdb = pmat + MAT_DIM + 1 ;
    Rdc = pmat + ( 2 * MAT_DIM ) + 2 ;

    apmAssign( Rgamma_dif[0].terms[0].coef, *Rda ) ;
    apmAssign( Rgamma_dif[1].terms[0].coef, *Rdb ) ;
    apmMultiply( Rgamma_dif[2].terms[0].coef, two, *Rdc ) ;

    apt = deriv + STAID_LEN + (DEG_FREE * MAT_DIM) ;
    apmCalc( Rgamma_dif[0].const, *Rda, APM_NEG, *apt, APM_MUL, NULL ) ;
    apt += MAT_DIM + 1 ;
    apmCalc( Rgamma_dif[1].const, *Rdb, APM_NEG, *apt, APM_MUL, NULL ) ;
    apt++ ;
    apmCalc( Rgamma_dif[2].const, two, APM_NEG, *Rdc, *apt,
            APM_MUL, APM_MUL, NULL ) ;

    Rbound_expr( &Rgamma_dif[0] ) ;
    Rbound_expr( &Rgamma_dif[1] ) ;
    Rbound_expr( &Rgamma_dif[2] ) ;

    RmaxAbs( answer, Rgamma_dif[0].bound.ub, Rgamma_dif[0].bound.lb ) ;
    RmaxAbs( Rrow_abs[0], Rgamma_dif[1].bound.ub, Rgamma_dif[1].bound.lb ) ;
    RmaxAbs( Rrow_abs[1], Rgamma_dif[2].bound.ub, Rgamma_dif[2].bound.lb ) ;
/*
    Add max_error to the answer to account for the uncertainties
    in beta**(center).
*/
apmCalc( answer, answer, Rrow_abs[0], Rrow_abs[1], max_error,
          APM_ADD, APM_ADD, APM_ADD, NULL ) ;
}

```

column-rotor

```

# include <stdio.h>
# include <math.h>
# include "apm.h"
# include "apmSpecial.h"
# include "converse.h"
# include "bounding.h"
# include "rows.h"

```

```

# include "pi.h"

# define  m_sign( x )          ( ( x > 0.0 ) ? 1.0 : -1.0 )
# define  Rm_sign( x, a )     apmAssignLong((x),(long)apmSign((a)),0,BASE)

# define  USE_ROT             YES

# define  THETA_ROT           0.5      /* The angle for rotations - it's
                                        recorded here in units of pi.    */

APM      Rcthet, Rsthet, Rsmall_sinsq ;
APM      Rarea, Rsin_sq, Rnorm_one, Rnorm_two, Rsign ;
APM      Rnorm_prod, Rsign, Rx, Ry ;
double   cthet, sthet, small_sinsq ;
/* ++++++ */

initRotor()
{
    Rcthet = apmNew( BASE ) ;
    Rsthet = apmNew( BASE ) ;

    Rx = apmNew( BASE ) ;
    Ry = apmNew( BASE ) ;
    Rarea = apmNew( BASE ) ;
    Rsign = apmNew( BASE ) ;
    Rsin_sq = apmNew( BASE ) ;
    Rnorm_one = apmNew( BASE ) ;
    Rnorm_two = apmNew( BASE ) ;
    Rnorm_prod = apmNew( BASE ) ;
    Rsmall_sinsq = apmNew( BASE ) ;

    cthet = cos( PI * THETA_ROT ) ;
    sthet = sin( PI * THETA_ROT ) ;
    small_sinsq = sthet * sthet ;

    dbltoapm( Rx, BASE, THETA_ROT ) ;
    apmMultiply( Ry, pi, Rx ) ;
    apmCos( Rcthet, Ry ) ;
    apmSin( Rsthet, Ry ) ;
    apmMultiply( Rsmall_sinsq, Rsthet, Rsthet ) ;
}
/* ++++++ */

Rcol_rotor( Amat, Deriv, Prizmat )

APM *Amat, *Deriv, *Prizmat ;
/*
    Prepares the matrix called "A" in my notes.  Mostly we want to
    have A = DF*Priz, but we want to ensure that A is not singular.
    In the interest of speed we have coded the calculations below with
    pointers.  Our hope is that the resulting function will scream along
    at ultrasonic speed.  Unfortunately it is quite unreadable.
*/
{
    int          j, k ;
    APM          *Aend, *Dend, *Pend ;
    register APM  *Apt, *Dpt, *Ppt ;

/*
    Copy the few terms which appear in the top rows of Amat.
*/

```

```

Aend = Amat + N_PARMS * (MAT_DIM + 1) ;
for( Apt = Amat, Ppt = Prizmat ; Apt < Aend ; Apt += (MAT_DIM + 1 ),
      Ppt += (MAT_DIM + 1 ) )
    apmAssign( *Apt, *Ppt ) ;

/*
    Clear out those parts of Amat which change from iteration to
    iteration.
*/

Aend = Amat + MAT_SZ ;
for( Apt = Amat + STAID_LEN ; Apt < Aend ; Apt++ )
    apmAssignLong( *Apt, OL, O, BASE ) ;

/*
    Set the (u,p) part of A
    It's equal to the (v,p) part of Prizmat.
*/

Aend = Amat + STAID_LEN + (DEG_FREE * MAT_DIM) ;
Ppt = Prizmat + STAID_LEN + (DEG_FREE * MAT_DIM) ;
for( Apt = Amat + STAID_LEN ; Apt < Aend ; Apt += TWO_DF ) {
    for( Pend = Ppt + N_PARMS ; Ppt < Pend ; Ppt++ )
        apmAssign( *Apt++, *Ppt ) ;

    Ppt += TWO_DF ;
}

/*
    Set the (v,p) part - three terms.
*/

/* First term - equal to Deriv(v,p) * Prizmat(p,p) */

Dpt = Deriv + STAID_LEN + (DEG_FREE * MAT_DIM) ;
Apt = Amat + STAID_LEN + (DEG_FREE * MAT_DIM) ;
for( Aend = Apt + (DEG_FREE * MAT_DIM) ; Apt < Aend ; Apt += TWO_DF ) {
    Ppt = Prizmat ;
    for( Dend = Dpt + N_PARMS ; Dpt < Dend ; Dpt++ ) {
        apmCalc( *Apt, *Apt, *Dpt, *Ppt, APM_MUL, APM_ADD, NULL ) ;
        Apt++ ;
        Ppt += MAT_DIM + 1 ;
    }

    Dpt += TWO_DF ;
}

/* Second term - equal to negative Prizmat(u,p) */

Ppt = Prizmat + STAID_LEN ;
Apt = Amat + STAID_LEN + (DEG_FREE * MAT_DIM) ;
for( Pend = Ppt + (DEG_FREE * MAT_DIM) ; Ppt < Pend ; Ppt += TWO_DF ) {
    for( Aend = Apt + N_PARMS ; Apt < Aend ; Apt++ )
        apmCalc( *Apt, *Apt, *Ppt++, APM_SUB, NULL ) ;

    Apt += TWO_DF ;
}

/* Third term - equal to Deriv(v,v) * Prizmat(v,p) */

Dpt = Deriv + STAID_LEN + (DEG_FREE * (MAT_DIM + 1)) + N_PARMS ;
Dend = Deriv + MAT_SZ ;

```



```

Apt = Amat + STAID_LEN + (DEG_FREE * MAT_DIM) ;
while( Dpt < Dend ) {
  Ppt = Prizmat + STAID_LEN + (DEG_FREE * MAT_DIM) ;
  Pend = Prizmat + MAT_SZ ;
  while( Ppt < Pend ) {
    Aend = Apt + N_PARMS ;
    while( Apt < Aend ) {
      apmCalc( *Apt, *Apt, *Dpt, *Ppt, APM_MUL, APM_ADD, NULL ) ;
      Apt++ ;
      Ppt++ ;
    }

    Dpt++ ;
    Ppt += TWO_DF ;
    Apt -= N_PARMS ;
  }

  Dpt += N_PARMS + DEG_FREE ;
  Apt += MAT_DIM ;
}

/*
  (u,u) part
  equals Priz(v,u)
*/

Apt = Amat + STAID_LEN + N_PARMS ;
Aend = Amat + STAID_LEN + (DEG_FREE * MAT_DIM) ;
Ppt = Prizmat + STAID_LEN + (DEG_FREE * MAT_DIM) + N_PARMS ;
while( Apt < Aend ) {
  Pend = Ppt + DEG_FREE ;
  while( Ppt < Pend ) {
    apmAssign( *Apt++, *Ppt ++ ) ;
  }

  Apt += N_PARMS + DEG_FREE ;
  Ppt += N_PARMS + DEG_FREE ;
}

/*
  (u,v) part
  equals Priz(v,v)
*/

Apt = Amat + STAID_LEN + N_PARMS + DEG_FREE ;
Aend = Amat + STAID_LEN + (DEG_FREE * MAT_DIM) ;
Ppt = Prizmat + STAID_LEN + (DEG_FREE * MAT_DIM) + N_PARMS + DEG_FREE ;
while( Apt < Aend ) {
  Pend = Ppt + DEG_FREE ;
  while( Ppt < Pend )
    apmAssign( *Apt++, *Ppt++ ) ;

  Apt += N_PARMS + DEG_FREE ;
  Ppt += N_PARMS + DEG_FREE ;
}

/*
  The (v,u) part - equal to Deriv(v,v) * Priz(v,u) - Priz(u,u) ,
*/

```

```

/* First term */
Apt = Amat + STAID_LEN + (DEG_FREE * MAT_DIM) + N_PARMS ;
Aend = Apt + (DEG_FREE * MAT_DIM) ;
Dpt = Deriv + STAID_LEN + (DEG_FREE*MAT_DIM) + N_PARMS + DEG_FREE ;
while( Apt < Aend ) {
  Ppt = Prizmat + STAID_LEN + (DEG_FREE * MAT_DIM) + N_PARMS ;
  Pend = Ppt + DEG_FREE ;
  while( Ppt < Pend ) {
    Dend = Dpt + DEG_FREE ;
    while( Dpt < Dend ) {
      apmCalc( *Apt, *Apt, *Dpt++, *Ppt, APM_MUL,
              APM_ADD, NULL ) ;

      Ppt += MAT_DIM ;
    }
    Apt++ ;
    Dpt -= DEG_FREE ;
    Ppt -= (DEG_FREE * MAT_DIM) - 1 ;
  }
  Dpt += MAT_DIM ;
  Apt += N_PARMS + DEG_FREE ;
}

/* Second term */
Apt = Amat + STAID_LEN + (DEG_FREE * MAT_DIM) + N_PARMS + DEG_FREE ;
Ppt = Prizmat + STAID_LEN + N_PARMS ;
Pend = Ppt + (MAT_DIM * DEG_FREE) ;
while( Ppt < Pend ) {
  Aend = Apt + DEG_FREE ;
  while( Apt < Aend ) {
    apmCalc( *Apt, *Apt, *Ppt, APM_SUB, NULL ) ;
    Apt++ ;
    Ppt++ ;
  }

  Ppt += N_PARMS + DEG_FREE ;
  Apt += N_PARMS + DEG_FREE ;
}

/*
(v,v) part - equals Deriv(v,v) * Priz(v,v) - Priz(u,v)
*/

/* First term */
Apt = Amat + STAID_LEN + (DEG_FREE * MAT_DIM) + N_PARMS + DEG_FREE ;
Aend = Apt + (DEG_FREE * MAT_DIM) ;
Dpt = Deriv + STAID_LEN + (DEG_FREE*MAT_DIM) + N_PARMS + DEG_FREE ;
while( Apt < Aend ) {
  Ppt = Prizmat + STAID_LEN + (DEG_FREE*MAT_DIM) +
      N_PARMS + DEG_FREE ;
  Pend = Ppt + DEG_FREE ;
  while( Ppt < Pend ) {
    Dend = Dpt + DEG_FREE ;
    while( Dpt < Dend ) {
      apmCalc( *Apt, *Apt, *Dpt++, *Ppt, APM_MUL,
              APM_ADD, NULL ) ;

      Ppt += MAT_DIM ;
    }
    Apt++ ;
  }
}

```

```

        Dpt -= DEG_FREE ;
        Ppt -= (DEG_FREE * MAT_DIM) - 1 ;
    }
    Dpt += MAT_DIM ;
    Apt += N_PARMS + DEG_FREE ;
}

/* Second term */
Apt = Amat + STAID_LEN + (DEG_FREE * MAT_DIM) + N_PARMS + DEG_FREE ;
Ppt = Prizmat + STAID_LEN + N_PARMS + DEG_FREE ;
Pend = Ppt + (MAT_DIM * DEG_FREE) ;
while( Ppt < Pend ) {
    Aend = Apt + DEG_FREE ;
    while( Apt < Aend ) {
        apmCalc( *Apt, *Apt, *Ppt, APM_SUB, NULL ) ;
        Apt++ ;
        Ppt++ ;
    }

    Ppt += N_PARMS + DEG_FREE ;
    Apt += N_PARMS + DEG_FREE ;
}

# if USE_ROT
/*
    Do up the rotations.
*/
for( j=0 ; j < TWO_DF ; j++ )
    for( k=(j+1) ; k < TWO_DF ; k++ )
        Rsubspace_rot( Amat, j, k ) ;
# endif
}
/* ++++++ */

Rsubspace_rot( Amat, col_one, col_two )

int    col_one, col_two ;
APM    *Amat ;
{
    APM    *Apt, *Apt2 ;

    Apt = Amat + STAID_LEN + N_PARMS +
            (col_two - col_one - 1) * MAT_DIM +
            col_one ;
    Apt2 = Apt + col_two - col_one ;

    apmCalc( Rarea, *Apt, Apt2[MAT_DIM], APM_MUL,
            Apt[MAT_DIM], *Apt2, APM_MUL,
            APM_SUB, NULL ) ;
    apmCalc( Rnorm_one, *Apt, APM_DUP, APM_MUL,
            Apt[MAT_DIM], APM_DUP, APM_MUL,
            APM_ADD, NULL ) ;
    apmCalc( Rnorm_two, *Apt2, APM_DUP, APM_MUL,
            Apt2[MAT_DIM], APM_DUP, APM_MUL,
            APM_ADD, NULL ) ;
    apmMultiply( Rnorm_prod, Rnorm_one, Rnorm_two ) ;
    if( apmCompare( Rnorm_prod, zero ) == 1 ) {
        apmMultiply( Rx, Rarea, Rarea ) ;
        apmDivide( Rsin_sq, precision, (APM) NULL, Rx, Rnorm_prod ) ;
    }
}

```

```

if( apmCompare( Rsin_sq, Rsmall_sinsq ) == -1 ) {
    Rm_sign( Rsign, Rarea ) ;

    if( apmCompare( Rnorm_two, Rnorm_one ) != 1 ) {
        apmCalc( Rx, Rcthet, *Apt2, APM_MUL,
            Rsign, Rsthet, Apt2[MAT_DIM], APM_MUL, APM_MUL,
            APM_SUB, NULL ) ;
        apmCalc( Ry, Rsthet, *Apt2, Rsign, APM_MUL, APM_MUL,
            Rcthet, Apt2[MAT_DIM], APM_MUL,
            APM_ADD, NULL ) ;

        apmAssign( *Apt2, Rx ) ;
        apmAssign( Apt2[MAT_DIM], Ry ) ;
    }
    else {
        apmCalc( Rsign, Rsign, APM_NEG, NULL ) ;
        apmCalc( Rx, Rcthet, *Apt, APM_MUL,
            Rsign, Rsthet, Apt[MAT_DIM], APM_MUL, APM_MUL,
            APM_SUB, NULL ) ;
        apmCalc( Ry, Rsthet, *Apt, Rsign, APM_MUL, APM_MUL,
            Rcthet, Apt[MAT_DIM], APM_MUL,
            APM_ADD, NULL ) ;

        apmAssign( *Apt, Rx ) ;
        apmAssign( Apt[MAT_DIM], Ry ) ;
    }
}
}
}

# include <stdio.h>
# include <math.h>
# include "apm.h"
# include "apmSpecial.h"
# include "converse.h"
# include "bounding.h"
# include "rows.h"

# define NUM_FACTS 3
# define NUM_TERMS 3
# define DET_TOL 1e-13

int isNewPrism ;

APM cr_scratch ;
APM RBmat[MAT_SZ], Rconst_mat[DF_SQ], Rcopy[4 * DF_SQ] ;
APM *Rcopy_rows[TWO_DF] ;
APM RBu_rows[DEG_FREE], RBv_rows[DEG_FREE] ;
APM Rbd_star, Rgd_star, Rstar, RPvp_star ;
APM Rcenter_err[MAT_DIM] ;
APM Rup_rows[DEG_FREE], Ruu_rows[DEG_FREE], Ruv_rows[DEG_FREE] ;
APM Rvp_rows[DEG_FREE], Rvu_rows[DEG_FREE], Rvv_rows[DEG_FREE] ;

double Bmat[MAT_SZ], const_mat[DF_SQ], copy[4 * DF_SQ] ;
double *copy_rows[TWO_DF] ;
double Bu_rows[DEG_FREE], Bv_rows[DEG_FREE] ;
double bd_star, gd_star, star, Pvp_star ;
double center_err[MAT_DIM] ;
double up_rows[DEG_FREE], uu_rows[DEG_FREE], uv_rows[DEG_FREE] ;
double vp_rows[DEG_FREE], vu_rows[DEG_FREE], vv_rows[DEG_FREE] ;

```

```

Bdd_dbl  *cr_factors[NUM_FACTS] ;
Bdd_term cr_terms[NUM_TERMS] ;
Bdd_expr beta_prod ;

Bdd_apm  *Rcr_factors[NUM_FACTS] ;
Bapm_term Rcr_terms[NUM_TERMS] ;
Bapm_expr Rbeta_prod ;
/* ++++++ */

init_crRows()
/*
    Set up the expressions and terms as described in my notes
    from 12/3 and 12/4.
*/
{
    int      j, k ;
    APM      *Rcpt ;
    double   *cpt ;
    Bdd_dbl  **dpt ;
    Bdd_apm  **apt ;

/*
    Initialize a batch of APM's.
*/
    for(j=0 ; j < DEG_FREE ; j++ ) {
        Rvp_rows[j] = apmNew( BASE ) ;
        Rup_rows[j] = apmNew( BASE ) ;
        Ruu_rows[j] = apmNew( BASE ) ;
        Ruv_rows[j] = apmNew( BASE ) ;
        Rvu_rows[j] = apmNew( BASE ) ;
        Rvv_rows[j] = apmNew( BASE ) ;
        RBu_rows[j] = apmNew( BASE ) ;
        RBv_rows[j] = apmNew( BASE ) ;
    }

    Rstar = apmNew( BASE ) ;
    Rgd_star = apmNew( BASE ) ;
    Rbd_star = apmNew( BASE ) ;
    RPvp_star = apmNew( BASE ) ;
    cr_scratch = apmNew( BASE ) ;
    for( j=0 ; j < MAT_SZ ; j++ ) {
        Bmat[j] = 0.0 ;
        RBmat[j] = apmNew( BASE ) ;
    }

    for( j=0 ; j < DF_SQ ; j++ )
        Rconst_mat[j] = apmNew( BASE ) ;

    for( j=0 ; j < (4 * DF_SQ) ; j++ )
        Rcopy[j] = apmNew( BASE ) ;

    for( j=0 ; j < MAT_DIM ; j++ )
        Rcenter_err[j] = apmNew( BASE ) ;

    cpt = copy ;
    Rcpt = Rcopy ;
    for( j=0 ; j < TWO_DF ; j++ ) {
        copy_rows[j] = cpt ;
        Rcopy_rows[j] = Rcpt ;

        cpt += TWO_DF ;
        Rcpt += TWO_DF ;
    }
}

```

```

    }

/*
    Set the number of terms in the bounded expressions
*/
    beta_prod.nterms = Rbeta_prod.nterms = 3 ;

/*
    Assign terms
*/
    beta_prod.terms = cr_terms ;
    Rbeta_prod.terms = Rcr_terms ;

/*
    Set nfactored.
*/
    Rbeta_prod.terms[0].nfactors = beta_prod.terms[0].nfactors = 1 ;
    Rbeta_prod.terms[1].nfactors = beta_prod.terms[1].nfactors = 1 ;
    Rbeta_prod.terms[2].nfactors = beta_prod.terms[2].nfactors = 1 ;

/*
    Assign factors.
*/
    dpt = cr_factors ;
    apt = Rcr_factors ;
    for( k=0 ; k < beta_prod.nterms ; k++ ) {
        beta_prod.terms[k].factors = dpt ;
        Rbeta_prod.terms[k].factors = apt ;

        dpt += beta_prod.terms[k].nfactors ;
        apt += Rbeta_prod.terms[k].nfactors ;
    }

/*
    Set up those of the "bound" attributes which are
    bounded APM's.
*/
    newBapm( Rbeta_prod.bound, BASE ) ;
    for( j=0 ; j < NUM_TERMS ; j++ ) {
        newBapm( Rcr_terms[j].bound, BASE ) ;
    }

/*
    Set up the terms and expressions.
*/

/* beta_prod */
    Rbeta_prod.const = apmNew( BASE ) ;
    Rbeta_prod.terms[0].coef = apmNew( BASE ) ;

    beta_prod.terms[0].factors[0] = #a_sin.bound ;
    Rbeta_prod.terms[0].factors[0] = #Ra_sin.bound ;

    Rbeta_prod.terms[1].coef = apmNew( BASE ) ;

    beta_prod.terms[1].factors[0] = #c_sin.bound ;

```

```

        Rbeta_prod.terms[1].factors[0] = #Rc_sin.bound ;

        Rbeta_prod.terms[2].coef = apmNew( BASE ) ;

        beta_prod.terms[2].factors[0] = #b_sin.bound ;
        Rbeta_prod.terms[2].factors[0] = #Rb_sin.bound ;
    }
    /* ++++++ */

Rcr_rows( Rw, Amat, Deriv, Priz )

APM      *Rw, *Amat, *Deriv ;
RPrism   *Priz ;
/*
    Obtain bounds on the sums of the absolute values of
    the entries in the rows of
    -1
    [A] * Deriv * Pmat,

    put the results in w.
*/
{
    int      j ;
    APM      *end_row, *end_mat, *Pmat, *inv_pt ;
    APM      *pipt, *p2pt, *bipt, *b2pt, *wu_pt, *wv_pt ;

    Pmat = Priz->matrix ;
    Rset_inverse( Amat ) ;

/*
    Do up some row sums for the inverse; these
    are used to calculate center_err[].
*/
    bipt = REmat + STAID_LEN + N_PARMS ;
    b2pt = bipt + MAT_DIM * DEG_FREE ;
    for( j=0 ; j < DEG_FREE ; j++ ) {
        apmAssign( RBU_rows[j], zero ) ;
        apmAssign( RBV_rows[j], zero ) ;

        for( end_row = bipt + TWO_DF ; bipt < end_row ; ) {
            apmCalc( RBU_rows[j], RBU_rows[j], *bipt++,
                    APM_ABS, APM_ADD, NULL ) ;
            apmCalc( RBV_rows[j], RBV_rows[j], *b2pt++,
                    APM_ABS, APM_ADD, NULL ) ;
        }
    }

/*
    Call functions which calculate upper bound on the
    sums of the elements of various matrices.
    Before any bounding of matrices, one must invoke
    global_bounds( Pmat ) to set such global variables,
    as cos_one, and sin_sum. This is done in Rtry_prism.
*/
    Rbeta_dif_star( Rbd_star, Deriv ) ;
    Rgamdif_star( Rgd_star, Deriv, Pmat ) ;

/*
    Calculate bounds on the sums of the absolute values
    of the elements in various blocks.
*/

```

```

/* up & vp blocks */

apmAssignLong( RPvp_star, OL, O, BASE ) ;
pipt = Pmat + STAID_LEN + (MAT_DIM * DEG_FREE) ;
end_mat = pipt + (DEG_FREE * MAT_DIM) ;
for( ; pipt < end_mat ; pipt += TWO_DF ) {
    for( end_row = pipt + N_PARMS ; pipt < end_row ; pipt++ )
        apmCalc( RPvp_star, RPvp_star, *pipt, APM_ABS,
                APM_ADD, NULL ) ;
}

apmCalc( Rstar, Rgd_star, Rbd_star, RPvp_star,
        APM_MUL, APM_ADD, NULL ) ;
bipt = RBmat + STAID_LEN + N_PARMS + DEG_FREE ;
b2pt = RBmat + STAID_LEN + N_PARMS + DEG_FREE + (MAT_DIM * DEG_FREE) ;
for( j=0 ; j < DEG_FREE ; j++ ) {
    apmAssignLong( Rup_rows[j], OL, O, BASE ) ;
    apmAssignLong( Rvp_rows[j], OL, O, BASE ) ;
    for( end_row = bipt + DEG_FREE ; bipt < end_row ;
        bipt++, b2pt++ ) {
        apmCalc( Rup_rows[j], Rup_rows[j], *bipt, APM_ABS,
                APM_ADD, NULL ) ;
        apmCalc( Rvp_rows[j], Rvp_rows[j], *b2pt, APM_ABS,
                APM_ADD, NULL ) ;
    }

    apmCalc( Rup_rows[j], Rup_rows[j], Rstar, APM_MUL, NULL ) ;
    apmCalc( Rvp_rows[j], Rvp_rows[j], Rstar, APM_MUL, NULL ) ;

    bipt += N_PARMS + DEG_FREE ;
    b2pt += N_PARMS + DEG_FREE ;
}

/*
Do the remaining blocks - those that actually arise
from the derivatives of the (u,v) -> (u',v') part of
the map. This section uses the mighty bound_rows(),
which may be found below.
*/

/* (u,u) block :

$$B(u,u) * P(v,u) + B(u,v) * \{ \beta * P(v,u) - P(u,u) \}$$

*/

pipt = Pmat + STAID_LEN + (DEG_FREE * MAT_DIM) + N_PARMS ;
p2pt = Pmat + STAID_LEN + N_PARMS ;

bipt = RBmat + STAID_LEN + N_PARMS ;
b2pt = RBmat + STAID_LEN + N_PARMS + DEG_FREE ;
Rbound_rows( Ruu_rows, bipt, pipt, b2pt, p2pt ) ;

/* (u,v) block :

$$B(u,u) * P(v,v) + B(u,v) * \{ \beta * P(v,v) - P(u,v) \}$$

*/

pipt = Pmat + STAID_LEN + (DEG_FREE * MAT_DIM) + N_PARMS + DEG_FREE ;
p2pt = Pmat + STAID_LEN + N_PARMS + DEG_FREE ;

```



```

/*      The same parts of RBmat as used to find uu_rows. */
Rbound_rows( Ruv_rows, b1pt, p1pt, b2pt, p2pt ) ;

/* (v,u) block :
      B(v,u) * P(v,u) + B(v,v) * { beta * P(v,u) -
                                  P(u,u) }
*/

p1pt = Pmat + STAID_LEN + (DEG_FREE*MAT_DIM) + N_PARMS ;
p2pt = Pmat + STAID_LEN + N_PARMS ;

b1pt = RBmat + STAID_LEN + (DEG_FREE*MAT_DIM) + N_PARMS ;
b2pt = RBmat + STAID_LEN + (DEG_FREE*MAT_DIM) + N_PARMS + DEG_FREE ;
Rbound_rows( Rvu_rows, b1pt, p1pt, b2pt, p2pt ) ;

/* (v,v) block :
      B(v,u) * P(v,v) + B(v,v) * { beta * P(v,v) -
                                  P(u,v) }
*/

p1pt = Pmat + STAID_LEN + (DEG_FREE*MAT_DIM) + N_PARMS + DEG_FREE ;
p2pt = Pmat + STAID_LEN + N_PARMS + DEG_FREE ;

/*      Same parts of RBmat as are used to find vu_rows. */
Rbound_rows( Rvv_rows, b1pt, p1pt, b2pt, p2pt ) ;

/*

Get the contributions to Rw[] that arise from
errors in the computation of the image of the
prism's center.

*/
for( j=0 ; j < DEG_FREE ; j++ ) {
center_err[j+N_PARMS] = Bu_rows[j] * DBL_ERR ;
center_err[j+N_PARMS+DEG_FREE] = Bv_rows[j] * DBL_ERR ;
apmMultiply( Rcenter_err[j+N_PARMS], RBu_rows[j], max_error ) ;
apmMultiply( Rcenter_err[j+N_PARMS+DEG_FREE], RBu_rows[j],
max_error ) ;
}

/*

Compute the components of w[].

*/
wu_pt = &Rw[N_PARMS] ;
wv_pt = &Rw[N_PARMS + DEG_FREE] ;
for( j=0 ; j < DEG_FREE ; j++, wu_pt++, wv_pt++ ) {
apmCalc( *wu_pt, Rup_rows[j], Ruu_rows[j], Ruv_rows[j], max_error,
APM_ADD, APM_ADD, APM_ADD, NULL ) ;
apmCalc( *wv_pt, Rvp_rows[j], Rvu_rows[j], Rvv_rows[j], max_error,
APM_ADD, APM_ADD, APM_ADD, NULL ) ;
}

/*

Include errors due to miscalculation of
prism's center.

*/

for( j= N_PARMS ; j < MAT_DIM ; j++ )
apmCalc( Rw[j], Rw[j], Rcenter_err[j], APM_ADD, NULL ) ;

return ;
}
/* ++++++ */

```

```

Rbound_rows( rows, first_b, first_p, second_b, second_p )
APM *rows, *first_b, *second_b, *first_p, *second_p ;
{
/*
    Obtain upper bounds on the sums of the absolute
    values of rows of matrices given by expressions
    like:
        B1 * S1 + B2 * ( [beta] * S1 - S2 ).

    Expressions like these arise in cr_rows() above.
    The idea is to cast these rows as bounded expressions
    and then use the usual machinery to find their limits.
*/
    int    j, k ;
    APM    *bpt_b, *ppt_a, *ppt_b, *end_row, *cpt ;

/*
    Evaluate the constant part of the matrix expression.
    It's :
        (B1 + 2.0 * B2) * S1 - B2 * S2
*/
    cpt = Rconst_mat ;
    for( j=0 ; j < DEG_FREE ; j++ ) {

        bpt_a = first_b + j * MAT_DIM ;
        bpt_b = second_b + j * MAT_DIM ;
        for( k=0 ; k < DEG_FREE ; k++ ) {
            apmAssignLong( *cpt, OL, 0, BASE ) ;

            ppt_a = first_p + k ;
            ppt_b = second_p + k ;
            for( end_row = bpt_a + DEG_FREE ; bpt_a < end_row ; ) {
                apmCalc( *cpt, *cpt, *bpt_a,
                        *bpt_b, two, APM_MUL,
                        APM_ADD,
                        *ppt_a, APM_MUL,
                        *bpt_b, *ppt_b,
                        APM_MUL, APM_SUB,
                        APM_ADD, NULL ) ;

                bpt_a++, bpt_b++ ;
                ppt_a += MAT_DIM ;
                ppt_b += MAT_DIM ;
            }

            bpt_a -= DEG_FREE ;
            bpt_b -= DEG_FREE ;
            cpt++ ;
        }
    }

    cpt = Rconst_mat ;
    for( j=0 ; j < DEG_FREE ; j++ ) {
        apmAssignLong( rows[j], OL, 0, BASE ) ;

        bpt_a = second_b + j * MAT_DIM ;
        bpt_b = bpt_a + 1 ;
        for( k=0 ; k < DEG_FREE ; k++ ) {
            ppt_a = first_p + k ;
            ppt_b = ppt_a + MAT_DIM ;
        }
    }
}

```

```

/* a * sin( v[0] ) term */
    apmMultiply( cr_scratch, *bpt_a, *ppt_a );
    apmNegate( Rbeta_prod.terms[0].coef, cr_scratch );

/* c * sin( v[0] + v[1] ) term */
    apmCalc( cr_scratch, *bpt_a, *bpt_b, APM_ADD,
             *ppt_a, *ppt_b, APM_ADD,
             APM_MUL, NULL );
    apmNegate( Rbeta_prod.terms[1].coef, cr_scratch );

/* b * sin( v[0] + v[1] ) term */
    apmMultiply( cr_scratch, *bpt_b, *ppt_b );
    apmNegate( Rbeta_prod.terms[2].coef, cr_scratch );

    apmAssign( Rbeta_prod.const, *cpt++ );
    Rbound_expr( &Rbeta_prod );

    RmaxAbs( cr_scratch, Rbeta_prod.bound.ub,
             Rbeta_prod.bound.lb );
    apmCalc( rows[j], rows[j], cr_scratch, APM_ADD, NULL );
}
}
}
/* ++++++ */

Rset_inverse( mat )

APM *mat ;
{
    APM *end_row, *end_block, *end_col ;
    APM *ipt_a, *ipt_b, *ipt_c, *ipt_set, *mpt_a, *mpt_b ;

    if( isNewPrism == YES ) {
        end_block = RBmat + N_PARMS * (MAT_DIM + 1) ;
        for( ipt_a=RBmat, mpt_a=mat ; ipt_a < end_block ; ) {
            apmDivide( *ipt_a, precision, (APM)NULL, one, *mpt_a ) ;

            mpt_a += MAT_DIM + 1 ;
            ipt_a += MAT_DIM + 1 ;
        }

        isNewPrism = NO ;
    }

    Rinvert_corner( mat ) ;

/*
Set the (u,p) part of the inverse.
*/
    ipt_a = RBmat + STAID_LEN + N_PARMS ;
    ipt_b = RBmat + STAID_LEN + N_PARMS + DEG_FREE ;

    ipt_set = RBmat + STAID_LEN ;
    end_block = ipt_set + (MAT_DIM * DEG_FREE) ;
    for( ; ipt_set < end_block ; ipt_set += TWO_DF ) {
        ipt_c = RBmat ;

        mpt_a = mat + STAID_LEN ;
        mpt_b = mat + STAID_LEN + (DEG_FREE * MAT_DIM) ;

        end_row = ipt_set + N_PARMS ;

```

```

for( ; ipt_set < end_row ; ipt_set++ ) {
    apmAssignLong( *ipt_set, OL, O, BASE ) ;

    end_col = mpt_a + (DEG_FREE * MAT_DIM) ;
    for( ; mpt_a < end_col ; mpt_a += MAT_DIM ) {
        apmCalc( *ipt_set, *ipt_a, *mpt_a, APM_MUL,
                *ipt_b, *mpt_b, APM_MUL,
                APM_ADD, APM_NEG,
                *ipt_set, APM_ADD, NULL ) ;

        ipt_a++ ;
        ipt_b++ ;
        mpt_b += MAT_DIM ;
    }
    apmCalc( *ipt_set, *ipt_set, *ipt_c, APM_MUL, NULL ) ;

    ipt_a -= DEG_FREE ;
    ipt_b -= DEG_FREE ;
    ipt_c += MAT_DIM + 1 ;

    mpt_a -= (MAT_DIM * DEG_FREE) - 1 ;
    mpt_b -= (MAT_DIM * DEG_FREE) - 1 ;
}

ipt_a += MAT_DIM ;
ipt_b += MAT_DIM ;
mpt_a -= DEG_FREE ;
mpt_b -= DEG_FREE ;
}

/*
Set the (v,p) part of the inverse.
*/
ipt_a = RBmat + STAID_LEN + N_PARMS + (DEG_FREE * MAT_DIM) ;
ipt_b = RBmat + STAID_LEN + N_PARMS + (DEG_FREE+MAT_DIM) + DEG_FREE ;

ipt_set = RBmat + STAID_LEN + (DEG_FREE * MAT_DIM) ;
end_block = ipt_set + (MAT_DIM * DEG_FREE) ;
for( ; ipt_set < end_block ; ipt_set += TWO_DF ) {
    ipt_c = RBmat ;

    mpt_a = mat + STAID_LEN ;
    mpt_b = mat + STAID_LEN + (DEG_FREE * MAT_DIM) ;

    end_row = ipt_set + N_PARMS ;
    for( ; ipt_set < end_row ; ipt_set++ ) {
        apmAssignLong( *ipt_set, OL, O, BASE ) ;

        end_col = mpt_a + (DEG_FREE * MAT_DIM) ;
        for( ; mpt_a < end_col ; mpt_a += MAT_DIM ) {
            apmCalc( *ipt_set, *ipt_a, *mpt_a, APM_MUL,
                    *ipt_b, *mpt_b, APM_MUL,
                    APM_ADD, APM_NEG,
                    *ipt_set, APM_ADD, NULL ) ;

            ipt_a++ ;
            ipt_b++ ;
            mpt_b += MAT_DIM ;
        }
        apmCalc( *ipt_set, *ipt_set, *ipt_c, APM_MUL, NULL ) ;

        ipt_a -= DEG_FREE ;

```

```

    ipt_b -= DEG_FREE ;
    ipt_c += MAT_DIM + 1 ;

    mpt_a -= (MAT_DIM * DEG_FREE) - 1 ;
    mpt_b -= (MAT_DIM * DEG_FREE) - 1 ;
}

    ipt_a += MAT_DIM ;
    ipt_b += MAT_DIM ;
    mpt_a -= DEG_FREE ;
    mpt_b -= DEG_FREE ;
}
}
/* ++++++ */

Rinvert_corner( mat )

APM *mat ;
{
/*
    Set up matrices to prepare 'em for use by Rgauss().
    Note that we use the matrix called const_mat[].
    At the times this function is called const_mat[]
    doesn't contain anything important.
*/
    int      j ;
    APM      *end_row, *mpt, *bpt, *cpt ;

/*
    Copy the matrix.
*/
    mpt = mat + STAID_LEN + N_PARMS ;
    for( j=0 ; j < TWO_DF ; j++ ) {

        cpt = Rcopy_rows[j] ;
        end_row = mpt + TWO_DF ;
        while( mpt < end_row )
            apmAssign( *cpt++, *mpt++ ) ;

        mpt += N_PARMS ;
    }

/*
    Do the inversion.
*/
    Rgauss( Rcopy_rows ) ;

/*
    Copy the answer.
*/

    bpt = RBmat + STAID_LEN + N_PARMS ;
    for( j=0 ; j < TWO_DF ; j++ ) {

        cpt = Rcopy_rows[j] ;
        end_row = bpt + TWO_DF ;
        while( bpt < end_row )
            apmAssign( *bpt++, *cpt++ ) ;

        bpt += N_PARMS ;
    }
}

```

}

fixed-form

```

* include <stdio.h>
* include <math.h>
* include "apm.h"
* include "apmSpecial.h"
* include "converse.h"

/* ++++++ */

fixed_form( Amat, Deriv, Prizmat )

double *Amat, *Deriv, *Prizmat ;
/*
    Prepares the matrix called "A" in my notes. Eventually we want to
    have A = DF*Priz, but early in a calculation, when Priz is singular,
    we want to fatten A up by requiring it to have a certain fixed form.
    In the interest of speed we have coded the calculations below with
    pointers. Our hope is that the resulting function will scream along
    at ultrasonic speed. Unfortunately it is quite unreadable.
*/
{
    double      *Aend, *Aend2, *Dend, *Pend, *Pend2 ;
    register double *Apt, *Apt2, *Dpt, *Ppt, *Ppt2 ;

/*
    Copy the few terms which appear in the top rows of Amat.
*/
    Aend = Amat + N_PARMS * ( MAT_DIM + 1 ) ;
    for( Apt = Amat, Ppt = Prizmat ; Apt < Aend ; Apt += ( MAT_DIM + 1 ),
        Ppt += ( MAT_DIM + 1 ) )
        *Apt = *Ppt ;

/*
    Clear out those parts of Amat which change from iteration to
    iteration.
*/
    Aend = Amat + MAT_SZ ;
    for( Apt = Amat + STAID_LEN ; Apt < Aend ; Apt++ )
        *Apt = 0.0 ;

/*
    Set the (u,p) part of A
    It's equal to the (v,p) part of Prizmat.
*/
    Aend = Amat + STAID_LEN + ( DEG_FREE * MAT_DIM ) ;
    Ppt = Prizmat + STAID_LEN + ( DEG_FREE * MAT_DIM ) ;
    for( Apt = Amat + STAID_LEN ; Apt < Aend ; Apt += TWO_DF ) {
        for( Pend = Ppt + N_PARMS ; Ppt < Pend ; Ppt++ )
            *Apt++ = *Ppt ;

        Ppt += TWO_DF ;
    }

/*
    Set the (v,p) part - three terms.

```

```

*/
/* First term - equal to Deriv(v,p) * Prizmat(p,p) */
Dpt = Deriv + STAID_LEN + (DEG_FREE * MAT_DIM) ;
Apt = Amat + STAID_LEN + (DEG_FREE * MAT_DIM) ;
for( Aend = Apt + (DEG_FREE * MAT_DIM) ; Apt < Aend ; Apt += TWO_DF ) {
    Ppt = Prizmat ;
    for( Dend = Dpt + N_PARMS ; Dpt < Dend ; Dpt++ ) {
        *Apt++ += *Dpt * (*Ppt) ;
        Ppt += MAT_DIM + 1 ;
    }

    Dpt += TWO_DF ;
}

/* Second term - equal to negative Prizmat(u,p) */
Ppt = Prizmat + STAID_LEN ;
Apt = Amat + STAID_LEN + (DEG_FREE * MAT_DIM) ;
for( Pend = Ppt + (DEG_FREE * MAT_DIM) ; Ppt < Pend ; Ppt += TWO_DF ) {
    for( Aend = Apt + N_PARMS ; Apt < Aend ; Apt++ )
        *Apt -= *Ppt++ ;

    Apt += TWO_DF ;
}

/* Third term - equal to Deriv(v,v) * Prizmat(v,p) */
Dpt = Deriv + STAID_LEN + (DEG_FREE * (MAT_DIM + 1)) + N_PARMS ;
Dend = Deriv + MAT_SZ ;
Apt = Amat + STAID_LEN + (DEG_FREE * MAT_DIM) ;
while( Dpt < Dend ) {
    Ppt = Prizmat + STAID_LEN + (DEG_FREE * MAT_DIM) ;
    Pend = Prizmat + MAT_SZ ;
    while( Ppt < Pend ) {
        Aend = Apt + N_PARMS ;
        while( Apt < Aend )
            *Apt++ += *Dpt * (*Ppt++) ;

        Dpt++ ;
        Ppt += TWO_DF ;
        Apt -= N_PARMS ;
    }

    Dpt += N_PARMS + DEG_FREE ;
    Apt += MAT_DIM ;
}

/*
(u,v) part
equals Priz(v,u) + Priz(v,v)
*/

Apt = Amat + STAID_LEN + N_PARMS + DEG_FREE ;
Aend = Amat + STAID_LEN + (DEG_FREE * MAT_DIM) ;
Ppt = Prizmat + STAID_LEN + (DEG_FREE * MAT_DIM) + N_PARMS ;
Ppt2 = Ppt + DEG_FREE ;
while( Apt < Aend ) {
    Pend = Ppt + DEG_FREE ;
    while( Ppt < Pend )
        *Apt++ += ( *Ppt++ + *Ppt2++ ) ;
}

```

```

    Apt += N_PARMS + DEG_FREE ;
    Ppt += N_PARMS + DEG_FREE ;
    Ppt2 += N_PARMS + DEG_FREE ;
}

/*
    The (v,u) part
    equal to Deriv(v,v) * { Priz(v,u) + Priz(v,v) },
    which also equals Deriv(v, v) * A(u,v)
*/

Apt = Amat + STAID_LEN + (DEG_FREE * MAT_DIM) + N_PARMS ;
Dpt = Deriv + STAID_LEN + (DEG_FREE * MAT_DIM) + N_PARMS + DEG_FREE ;
Dend = Deriv + MAT_SZ ;
while( Dpt < Dend ) {
    Apt2 = Amat + STAID_LEN + N_PARMS + DEG_FREE ;
    Aend2 = Apt2 + (DEG_FREE * MAT_DIM) ;
    while( Apt2 < Aend2 ) {
        Aend = Apt + DEG_FREE ;
        while( Apt < Aend ) {
            *Apt++ += *Dpt * (*Apt2++) ;
        }

        Dpt++ ;
        Apt -= DEG_FREE ;
        Apt2 += DEG_FREE + N_PARMS ;
    }

    Apt += MAT_DIM ;
    Dpt += N_PARMS + DEG_FREE ;
}

/*
    (v,v) part - equals Deriv(v,v) * Priz(v,v) - Priz(u,v)
*/

/* First term */
Apt = Amat + STAID_LEN + (DEG_FREE * MAT_DIM) + N_PARMS + DEG_FREE ;
Dpt = Deriv + STAID_LEN + (DEG_FREE * MAT_DIM) + N_PARMS + DEG_FREE ;
Dend = Deriv + MAT_SZ ;
while( Dpt < Dend ) {
    Ppt = Prizmat + STAID_LEN + (DEG_FREE * MAT_DIM) + N_PARMS + DEG_FREE ;
    Pend = Prizmat + MAT_SZ ;
    while( Ppt < Pend ) {
        Aend = Apt + DEG_FREE ;
        while( Apt < Aend ) {
            *Apt++ += *Dpt * (*Ppt++) ;
        }

        Dpt++ ;
        Apt -= DEG_FREE ;
        Ppt += DEG_FREE + N_PARMS ;
    }

    Apt += MAT_DIM ;
    Dpt += N_PARMS + DEG_FREE ;
}

/* Second term */
Apt = Amat + STAID_LEN + (DEG_FREE * MAT_DIM) + N_PARMS + DEG_FREE ;
Ppt = Prizmat + STAID_LEN + N_PARMS + DEG_FREE ;

```



```

Pend = Ppt + (MAT_DIM * DEG_FREE) ;
while( Ppt < Pend ) {
    Aend = Apt + DEG_FREE ;
    while( Apt < Aend )
        *Apt++ -= *Ppt++ ;

    Ppt += N_PARMS + DEG_FREE ;
    Apt += N_PARMS + DEG_FREE ;
}

}

/* ++++++ */

Rfixed_form( Amat, Deriv, Prizmat )

APM *Amat, *Deriv, *Prizmat ;
/*
    Prepares the matrix called "A" in my notes. Eventually we want to
    have A = DF*Priz, but early in a calculation, when Priz is singular,
    we want to fatten A up by requiring it to have a certain fixed form.
    In the interest of speed we have coded the calculations below in
    terms of pointers. Our hope is that the resulting function will
    scream along at ultrasonic speed. Unfortunately it is quite
    unreadable.
*/
{
    APM      *Aend, *Aend2, *Dend, *Pend, *Pend2 ;
    register APM *Apt, *Apt2, *Dpt, *Ppt, *Ppt2 ;

    /*
        Copy the few terms which appear in the top rows of Amat.
    */
    Aend = Amat + N_PARMS * (MAT_DIM + 1) ;
    for( Apt = Amat, Ppt = Prizmat ; Apt < Aend ; Apt += (MAT_DIM + 1),
        Ppt += (MAT_DIM + 1) )
        apmAssign( *Apt, *Ppt ) ;

    /*
        Clear out those parts of Amat which change from iteration to
        iteration.
    */

    Aend = Amat + MAT_SZ ;
    for( Apt = Amat + STAID_LEN ; Apt < Aend ; Apt++ )
        apmAssignLong( *Apt, OL, O, O ) ;

    /*
        Set the (u,p) part of A
        It's equal to the (v,p) part of Prizmat.
    */

    Aend = Amat + STAID_LEN + (DEG_FREE * MAT_DIM) - TWO_DF ;
    Ppt = Prizmat + STAID_LEN + (DEG_FREE * MAT_DIM) ;
    for( Apt = Amat + STAID_LEN ; Apt < Aend ; Apt += TWO_DF ) {
        for( Pend = Ppt + N_PARMS ; Ppt < Pend ; Ppt++, Apt++ )
            apmCalc( *Apt, *Apt, *Ppt, APM_ADD, NULL ) ;

        Ppt += TWO_DF ;
    }

    /*
        Set the (v,p) part - three terms.
    */

```

```

/* First term - equal to Deriv(v,p) * Prizmat(p,p) */
Dpt = Deriv + STAID_LEN + (DEG_FREE * MAT_DIM) ;
Apt = Amat + STAID_LEN + (DEG_FREE * MAT_DIM) ;
for( Aend = Apt + (DEG_FREE * MAT_DIM) ; Apt < Aend ; Apt += TWO_DF ) {
    Ppt = Prizmat ;
    for( Dend = Dpt + N_PARMS ; Dpt < Dend ; Dpt++ ) {
        apmMultiply( *Apt++, *Dpt, *Ppt ) ;
        Ppt += MAT_DIM + 1 ;
    }
    Dpt += TWO_DF ;
}

/* Second term - equal to negative Prizmat(u,p) */
Ppt = Prizmat + STAID_LEN ;
Apt = Amat + STAID_LEN + (DEG_FREE * MAT_DIM) ;
for( Pend = Ppt + (DEG_FREE * MAT_DIM) ; Ppt < Pend ; Ppt += TWO_DF ) {
    for( Aend = Apt + N_PARMS ; Apt < Aend ; Apt++, Ppt++ )
        apmCalc( *Apt, *Apt, *Ppt, APM_SUB, NULL ) ;
    Apt += TWO_DF ;
}

/* Third term - equal to Deriv(v,v) * Prizmat(v,p) */
Dpt = Deriv + STAID_LEN + (DEG_FREE * (MAT_DIM + 1)) + N_PARMS ;
Dend = Deriv + MAT_SZ ;
Apt = Amat + STAID_LEN + (DEG_FREE * MAT_DIM) ;
while( Dpt < Dend ) {
    Ppt = Prizmat + STAID_LEN + (DEG_FREE * MAT_DIM) ;
    Pend = Prizmat + MAT_SZ - TWO_DF ;
    while( Ppt < Pend ) {
        Aend = Apt + N_PARMS ;
        while( Apt < Aend ) {
            apmCalc( *Apt, *Dpt, *Ppt, APM_MUL, *Apt, APM_ADD, NULL ) ;
            Apt++ ;
            Ppt++ ;
        }
        Dpt++ ;
        Ppt += TWO_DF ;
        Apt -= N_PARMS ;
    }
    Dpt += N_PARMS + DEG_FREE ;
    Apt += MAT_DIM ;
}

/*
(u,v) part
equals Priz(v,u) + Priz(v,v)
*/

Apt = Amat + STAID_LEN + N_PARMS + DEG_FREE ;
Aend = Amat + STAID_LEN + (DEG_FREE * MAT_DIM) ;
Ppt = Prizmat + STAID_LEN + (DEG_FREE * MAT_DIM) + N_PARMS ;
Ppt2 = Ppt + DEG_FREE ;
while( Apt < Aend ) {
    Pend = Ppt + DEG_FREE ;
    while( Ppt < Pend ) {
        apmCalc( *Apt, *Ppt, *Ppt2, APM_ADD, *Apt, APM_ADD, NULL ) ;
    }
}

```

```

        Apt++ ;
        Ppt++ ;
        Ppt2++ ;
    }

    Apt += N_PARMS + DEG_FREE ;
    Ppt += N_PARMS + DEG_FREE ;
    Ppt2 += N_PARMS + DEG_FREE ;
}

/*
The (v,u) part
equal to Deriv(v,v) * [ Priz(v,u) + Priz(v,v) ],
which also equals Deriv(v, v) * A(u,v)
*/

Apt = Amat + STAID_LEN + (DEG_FREE * MAT_DIM) + N_PARMS ;
Dpt = Deriv + STAID_LEN + (DEG_FREE * MAT_DIM) + N_PARMS + DEG_FREE ;
Dend = Deriv + MAT_SZ ;
while( Dpt < Dend ) {
    Apt2 = Amat + STAID_LEN + N_PARMS + DEG_FREE ;
    Aend2 = Apt2 + (DEG_FREE * MAT_DIM) ;
    while( Apt2 < Aend2 ) {
        Aend = Apt + DEG_FREE ;
        while( Apt < Aend ) {
            apmCalc( *Apt, *Apt, *Dpt, *Apt2, APM_MUL, APM_ADD, NULL ) ;
            Apt++ ;
            Apt2++ ;
        }

        Dpt++ ;
        Apt -= DEG_FREE ;
        Apt2 += DEG_FREE + N_PARMS ;
    }

    Apt += MAT_DIM ;
    Dpt += N_PARMS + DEG_FREE ;
}

/*
(v,v) part - equals Deriv(v,v) * Priz(v,v) - Priz(u,v)
*/

/* First term */
Apt = Amat + STAID_LEN + (DEG_FREE * MAT_DIM) + N_PARMS + DEG_FREE ;
Dpt = Deriv + STAID_LEN + (DEG_FREE * MAT_DIM) + N_PARMS + DEG_FREE ;
Dend = Deriv + MAT_SZ ;
while( Dpt < Dend ) {
    Ppt = Prizmat + STAID_LEN + (DEG_FREE * MAT_DIM) + N_PARMS + DEG_FREE ;
    Pend = Prizmat + MAT_SZ ;
    while( Ppt < Pend ) {
        Aend = Apt + DEG_FREE ;
        while( Apt < Aend ) {
            apmCalc( *Apt, *Apt, *Dpt, *Ppt, APM_MUL, APM_ADD, NULL ) ;

            Apt++ ;
            Ppt++ ;
        }

        Dpt++ ;
        Apt -= DEG_FREE ;
        Ppt += DEG_FREE + N_PARMS ;
    }
}

```

```

    }

    Apt += MAT_DIM ;
    Dpt += N_PARMS + DEG_FREE ;
}

/* Second term */
Apt = Amat + STAID_LEN + (DEG_FREE * MAT_DIM) + N_PARMS + DEG_FREE ;
Ppt = Prizmat + STAID_LEN + N_PARMS + DEG_FREE ;
Pend = Ppt + (MAT_DIM * DEG_FREE) ;
while( Ppt < Pend ) {
    Aend = Apt + DEG_FREE ;
    while( Apt < Aend ) {
        apmCalc( *Apt, *Apt, *Ppt, APM_SUB, NULL ) ;

        Apt++ ;
        Ppt++ ;
    }

    Ppt += N_PARMS + DEG_FREE ;
    Apt += N_PARMS + DEG_FREE ;
}
}

```

```

# include <stdio.h>
# include <math.h>
# include "apm.h"
# include "apmSpecial.h"
# include "converse.h"
# include "bounding.h"
# include "rows.h"

# define NUM_FACTS 5
# define NUM_TERMS 5
# define DET_TOL 1e-13

APM Rerr_star ;
APM ff_scratch ;
APM Rcenter_err[MAT_DIM] ;
APM Rdet_vu, Rdet_uv, Rstar ;
APM RAvv_star, RAuvInv_star ;
APM Rb_star, Rbd_star, Rgd_star ;
APM RPvv_star, RPvp_star, RPvu_star ;

double beta_star() ;
double center_err[MAT_DIM] ;
Bdd_dbl *ff_factors[NUM_FACTS] ;
Bdd_term ff_terms[NUM_TERMS] ;
Bdd_expr beta[3] ;

Bdd_apm *Rff_factors[NUM_FACTS] ;
Bapm_term Rff_terms[NUM_TERMS] ;
Bapm_expr Rbeta[3] ;
/* ++++++ */

init_ffRows()
/*
    Set up the expressions and terms as described in my notes
    from 11/14.
*/
{
    int j, k ;

```

```

Bdd_dbl  **dpt ;
Bdd_apm  **apt ;
Bdd_term *tpt ;
Bapm_term *Rtpt ;

/*
  Set up some APM's to be used to hold intermediate
  results.
*/
Rstar = apmNew( BASE ) ;
Rdet_uv = apmNew( BASE ) ;
Rdet_vu = apmNew( BASE ) ;
Rb_star = apmNew( BASE ) ;
Rbd_star = apmNew( BASE ) ;
Rgd_star = apmNew( BASE ) ;
Rerr_star = apmNew( BASE ) ;
RAvv_star = apmNew( BASE ) ;
RPvv_star = apmNew( BASE ) ;
RPvp_star = apmNew( BASE ) ;
RPvu_star = apmNew( BASE ) ;
ff_scratch = apmNew( BASE ) ;
RAuvInv_star = apmNew( BASE ) ;

for( j = 0 ; j < MAT_DIM ; j++ )
  Rcenter_err[j] = apmNew( BASE ) ;

/*
  Set the number of terms in the bounded expressions
*/
beta[0].nterms = Rbeta[0].nterms = 2 ;
beta[1].nterms = Rbeta[1].nterms = 1 ;
beta[2].nterms = Rbeta[2].nterms = 2 ;

/*
  Assign terms
*/
tpt = ff_terms ;
Rtpt = Rff_terms ;
for( j=0 ; j < 3 ; j++ ) {
  beta[j].terms = tpt ;
  Rbeta[j].terms = Rtpt ;
  tpt += beta[j].nterms ;
  Rtpt += Rbeta[j].nterms ;
}

/*
  Set nfactors.
*/
Rbeta[0].terms[0].nfactors = beta[0].terms[0].nfactors = 1 ;
Rbeta[0].terms[1].nfactors = beta[0].terms[1].nfactors = 1 ;
Rbeta[1].terms[0].nfactors = beta[1].terms[0].nfactors = 1 ;
Rbeta[2].terms[0].nfactors = beta[2].terms[0].nfactors = 1 ;
Rbeta[2].terms[1].nfactors = beta[2].terms[1].nfactors = 1 ;

/*
  Assign factors.
*/
dpt = ff_factors ;

```

```

apt = Rff_factors ;
for( j=0 ; j < 3 ; j++ ) {
/*
  beta
*/
  for( k=0 ; k < beta[j].nterms ; k++ ) {
    beta[j].terms[k].factors = dpt ;
    Rbeta[j].terms[k].factors = apt ;

    dpt += beta[j].terms[k].nfactors ;
    apt += Rbeta[j].terms[k].nfactors ;
  }
}

/*
  Set up those of the "bound" attributes which are
  bounded APM's.
*/

for( j=0 ; j < NUM_TERMS ; j++ ) {
  newBapm( Rff_terms[j].bound, BASE ) ;
}

for( j=0 ; j < 3 ; j++ ) {
  newBapm( Rbeta[j].bound, BASE ) ;
}

/*
  Set up the terms and expressions.
*/

/* beta */

/* beta[0] = 2.0 - a * sin(v[0]) - c * sin(v[0] + v[1]) */
beta[0].const = 2.0, Rbeta[0].const = two ;
beta[0].terms[0].coef = -1.0 ;
Rbeta[0].terms[0].coef = neg_one ;

  beta[0].terms[0].factors[0] = &a_sin.bound ;
  Rbeta[0].terms[0].factors[0] = &Ra_sin.bound ;

beta[0].terms[1].coef = -1.0 ;
Rbeta[0].terms[1].coef = neg_one ;

  beta[0].terms[1].factors[0] = &c_sin.bound ;
  Rbeta[0].terms[1].factors[0] = &Rc_sin.bound ;

/* beta[1] = - 2.0 * c * sin( v[0] + v[1] ) */
beta[1].const = 0.0, Rbeta[1].const = zero ;
beta[1].terms[0].coef = -2.0 ;
Rbeta[1].terms[0].coef = neg_two ;

  beta[1].terms[0].factors[0] = &c_sin.bound ;
  Rbeta[1].terms[0].factors[0] = &Rc_sin.bound ;

/* beta[2] = 2.0 - b * sin(v[1]) - c * sin(v[1] + v[0]) */
beta[2].const = 2.0, Rbeta[2].const = two ;
beta[2].terms[0].coef = -1.0 ;
Rbeta[2].terms[0].coef = neg_one ;

  beta[2].terms[0].factors[0] = &b_sin.bound ;
  Rbeta[2].terms[0].factors[0] = &Rb_sin.bound ;

```

```

    beta[2].terms[1].coef = -1.0 ;
    Rbeta[2].terms[1].coef = neg_one ;

    beta[2].terms[1].factors[0] = &c_sin.bound ;
    Rbeta[2].terms[1].factors[0] = &Rc_sin.bound ;
}
/* ++++++ */

ff_rows( w, Amat, Deriv, Priz )

Prism *Priz ;
double *w, *Amat, *Deriv ;
/*
    Obtain bounds on the sums of the absolute values of
    the entries in the rows of
        -1
    [A] * Deriv * Pmat,

    put the results in w.
*/
{
    double *apt, *mpt, *end_row, *end_mat, *Pmat ;
    double det_uv, det_uv_star ;
    double Avv_star, AuvInv_star ;
    double b_star, bd_star, gd_star ;
    double Pvv_star, Pvp_star, Pvu_star ;

/*
    Check that A(u,v) is invertible. If not, die.
*/
    Pmat = Priz->matrix ;

    apt = Amat + STAID_LEN + N_PARMS + DEG_FREE ;
    det_uv = *apt * ( *(apt + MAT_DIM + 1) ) ;
    apt++ ;
    det_uv -= *apt * ( *(apt + MAT_DIM -1) ) ;

    if( fabs( det_uv ) < DET_TOL ) {
        fprintf( stderr,
            "The determinant of A(u,v) = %.14e. Died. \n",
                det_uv ) ;
        cease() ;
    }
/*
    Call functions which calculate upper bound on the
    sums of the elements of various matrices.
    Before any bounding of matrices, one must invoke
    global_bounds( Pmat ) to set such global variables,
    as cos_one, and sin_sum. It is called in try_prism().
*/
    b_star = beta_star() ;
    bd_star = beta_dif_star( Deriv ) ;
    gd_star = gamdif_star( Deriv, Pmat ) ;

/*
    Find sums of the absolute values of the entries
    of A(v,v), AInv(u,v), Pmat(v,v), Pmat(v,u), and Pmat(v,p)
*/
    end_mat = Pmat + MAT_SZ ;

```

```

Pvv_star = 0.0 ;
mpt = Pmat + STAID_LEN + (DEG_FREE * MAT_DIM) + N_PARMS + DEG_FREE ;
for( ; mpt < end_mat ; mpt += (N_PARMS + DEG_FREE) ) {
    for( end_row = mpt + DEG_FREE ; mpt < end_row ; mpt++ ) {
        Pvv_star += fabs( *mpt ) ;
    }
}

Pvu_star = 0.0 ;
mpt = Pmat + STAID_LEN + (DEG_FREE * MAT_DIM) + N_PARMS ;
for( ; mpt < end_mat ; mpt += (N_PARMS + DEG_FREE) ) {
    for( end_row = mpt + DEG_FREE ; mpt < end_row ; mpt++ ) {
        Pvu_star += fabs( *mpt ) ;
    }
}

Pvp_star = 0.0 ;
mpt = Pmat + STAID_LEN + (DEG_FREE * MAT_DIM) ;
for( ; mpt < end_mat ; mpt += TWO_DF ) {
    for( end_row = mpt + N_PARMS ; mpt < end_row ; mpt++ ) {
        Pvp_star += fabs( *mpt ) ;
    }
}

Avv_star = Smblock_err ;
mpt = Amat + STAID_LEN + DEG_FREE * MAT_DIM + DEG_FREE + N_PARMS ;
for( ; mpt < end_mat ; mpt += TWO_DF ) {
    for( end_row = mpt + N_PARMS ; mpt < end_row ; mpt++ ) {
        Avv_star += fabs( *mpt ) ;
    }
}

AuvInv_star = Smblock_err ;
mpt = Amat + STAID_LEN + N_PARMS + DEG_FREE ;
for( ; mpt < end_mat ; mpt += TWO_DF ) {
    for( end_row = mpt + N_PARMS ; mpt < end_row ; mpt++ ) {
        AuvInv_star += fabs( *mpt ) ;
    }
}

AuvInv_star /= det_uv ;

/*
    Check that A(v,u) is invertible.  If not, die.
    If it is, set the harder-to-compute elements of w.
*/

apt = Amat + STAID_LEN + N_PARMS + (DEG_FREE * MAT_DIM) ;
det_vu = *apt * ( *(apt + MAT_DIM + 1) ) ;
apt++ ;
det_vu -= *apt * ( *(apt + MAT_DIM - 1) ) ;

if( fabs( det_vu ) < DET_TOL ) {
    fprintf( stderr,
        "The determinant of A(v,u) = %.14e. Died. \n",
            det_vu ) ;
    cease() ;
}
else {
    w[3] = fabs( Amat[MAT_SZ - DEG_FREE - 1] ) +
        fabs( Amat[STAID_LEN + (DEG_FREE * MAT_DIM) + N_PARMS + 1] ) +

```



```

        DBL_ERR ;
w[4] = fabs( Amat[MAT_SZ - TWO_DF] ) +
      fabs( Amat[STAIID_LEN + (DEG_FREE*MAT_DIM) + N_PARMS] ) +
      DBL_ERR ;

center_err[3] = w[3] * (1 + Avv_star * AuvInv_star) * DBL_ERR ;
center_err[4] = w[4] * (1 + Avv_star * AuvInv_star) * DBL_ERR ;
center_err[5] = AuvInv_star * DBL_ERR ;
center_err[6] = center_err[5] ;

star = (gd_star + bd_star * (Pvp_star + Pvv_star) +
        b_star * Pvu_star) / det_vu ;
w[3] *= star + center_err[3] / det_vu ;
w[4] *= star + center_err[4] / det_vu ;
w[5] = 1.0 + center_err[5] ;
w[6] = 1.0 + center_err[6] ;
}

return ;
}
/* ++++++ */

double beta_star()
{
    double answer ;

    bound_expr( &beta[0] ) ;
    bound_expr( &beta[1] ) ;
    bound_expr( &beta[2] ) ;

    answer = maxAbs( beta[0].bound.ub, beta[0].bound.lb ) +
            maxAbs( beta[1].bound.ub, beta[1].bound.lb ) +
            maxAbs( beta[2].bound.ub, beta[2].bound.lb ) ;

    return( answer ) ;
}
/* ++++++ */

Rff_rows( w, Amat, Deriv, Priz )

APM      *w, *Amat, *Deriv ;
RPrism   *Priz ;
/*
    Obtain bounds on the sums of the absolute values of
    the entries in the rows of
    -1
    [A] * Deriv * Pmat,

    put the results in w.
*/
{
    APM      *apt, *mpt, *end_row, *end_mat, *Pmat ;

/*
    Check that A(u,v) is invertible.  If not, die.
*/
    Pmat = Priz->matrix ;

    apt = Amat + STAIID_LEN + N_PARMS + DEG_FREE ;
    apmMultiply( Rdet_uv, *apt, *(apt + MAT_DIM + 1) ) ;
    apt++ ;

```

```

apmCalc( Rdet_uv, Rdet_uv, *apt, *(apt + MAT_DIM -1),
        APM_MUL, APM_SUB, NULL );
apmAbsoluteValue( ff_scratch, Rdet_uv );

if( apmCompare( ff_scratch, max_error ) != 1 ) {
    fprintf( stderr,
            "The determinant of A(u,v) is too small. Died. \n" );
    fprintf( stderr, "\t %.12e \n", apmtodbl( ff_scratch ) );
    cease();
}

/*
    Call functions which calculate upper bound on the
    sums of the elements of various matrices.
    Before any bounding of matrices, one must invoke
    global_bounds( Pmat ) to set such global variables,
    as cos_one, and sin_sum. It is called in Rtry_prism().
*/
Rbeta_star( Rb_star );
Rbeta_dif_star( Rbd_star, Deriv );
Rgamdif_star( Rgd_star, Deriv, Pmat );

/*
    Find sums of the absolute values of the entries
    of Pmat(v,v), Pmat(v,u), and Pmat(v,p)
*/
end_mat = Pmat + MAT_SZ ;

apmAssign( RPvv_star, zero );
mpt = Pmat + STAID_LEN + (DEG_FREE * MAT_DIM) + N_PARMS + DEG_FREE ;
for( ; mpt < end_mat ; mpt += (N_PARMS + DEG_FREE) ) {
    for( end_row = mpt + DEG_FREE ; mpt < end_row ; mpt++ ) {
        apmCalc( RPvv_star, RPvv_star, *mpt, APM_ABS,
                APM_ADD, NULL );
    }
}

apmAssign( RPvu_star, zero );
mpt = Pmat + STAID_LEN + (DEG_FREE * MAT_DIM) + N_PARMS ;
for( ; mpt < end_mat ; mpt += (N_PARMS + DEG_FREE) ) {
    for( end_row = mpt + DEG_FREE ; mpt < end_row ; mpt++ ) {
        apmCalc( RPvu_star, RPvu_star, *mpt, APM_ABS,
                APM_ADD, NULL );
    }
}

apmAssign( RPvp_star, zero );
mpt = Pmat + STAID_LEN + (DEG_FREE * MAT_DIM) ;
for( ; mpt < end_mat ; mpt += TWO_DF ) {
    for( end_row = mpt + N_PARMS ; mpt < end_row ; mpt++ ) {
        apmCalc( RPvp_star, RPvp_star, *mpt, APM_ABS,
                APM_ADD, NULL );
    }
}

apmAssign( RAvv_star, RSmBlock_err );
mpt = Amat + STAID_LEN + DEG_FREE * MAT_DIM + DEG_FREE + N_PARMS ;
for( ; mpt < end_mat ; mpt += TWO_DF ) {
    for( end_row = mpt + N_PARMS ; mpt < end_row ; mpt++ ) {
        apmCalc( RAvv_star, RAvv_star, *mpt,
                APM_ABS, APM_ADD, NULL );
    }
}

```

```

}

apmAssign( RAuvInv_star, RSmBlock_err );
mpt = Amat + STAID_LEN + N_PARMS + DEG_FREE ;
for( ; mpt < end_mat ; mpt += TWO_DF ) {
    for( end_row = mpt + N_PARMS ; mpt < end_row ; mpt++ ) {
        apmCalc( RAuvInv_star, RAuvInv_star, *mpt,
                APM_ABS, APM_ADD, NULL ) ;
    }
}

apmDivide( ff_scratch, precision, (APM) NULL,
          RAuvInv_star, Rdet_uv ) ;
apmAssign( RAuvInv_star, ff_scratch ) ;

/*
    Check that A(v,u) is invertible.  If not, die.
    If it is, set the harder-to-compute elements of w.
*/

apm = Amat + STAID_LEN + N_PARMS + (DEG_FREE * MAT_DIM) ;
apmMultiply( Rdet_vu, *apm, *(apm + MAT_DIM + 1) ) ;
apm++ ;
apmCalc( Rdet_vu, Rdet_vu, *apm, *(apm + MAT_DIM - 1),
        APM_MUL, APM_SUB, NULL ) ;
apmAbsoluteValue( ff_scratch, Rdet_vu ) ;

if( apmCompare( ff_scratch, max_error ) != 1 ) {
    fprintf( stderr,
            "The determinant of A(v,u) is too small. Died. \n" ) ;
    fprintf( stderr, "\t %.12e \n", apmtodbl( ff_scratch ) ) ;
    cease() ;
}

/*
    Note that the sums below seem to contain some misplaced
    elements of Amat.  These are to be thought of as elements
    of A(v,u) inverse.
*/

else {
    apmCalc( w[3], Amat[MAT_SZ-DEG_FREE-1], APM_ABS,
            Amat[STAID_LEN+(DEG_FREE*MAT_DIM)+N_PARMS+1],
            APM_ABS, max_error, APM_ADD, APM_ADD, NULL ) ;

    apmCalc( w[4], Amat[MAT_SZ-TWO_DF], APM_ABS,
            Amat[STAID_LEN+(DEG_FREE*MAT_DIM)+N_PARMS],
            APM_ABS, max_error, APM_ADD, APM_ADD, NULL ) ;

    apmCalc( Rerr_star, RAuv_star, RAuvInv_star, APM_MUL,
            one, APM_ADD, NULL ) ;
    apmCalc( Rcenter_err[3], w[3], Rerr_star, max_error,
            APM_MUL, APM_MUL, NULL ) ;
    apmCalc( Rcenter_err[4], w[4], Rerr_star, max_error,
            APM_MUL, APM_MUL, NULL ) ;
    apmMultiply( Rcenter_err[5], RAuvInv_star, max_error ) ;
    apmAssign( Rcenter_err[6], Rcenter_err[5] ) ;

    apmCalc( Rstar, RPvp_star, RPvv_star, APM_ADD,
            Rbd_star, APM_MUL,
            Rb_star, RPvu_star, APM_MUL,
            Rgd_star, APM_ADD, APM_ADD, NULL ) ;

    apmCalc( ff_scratch, Rcenter_err[3], Rstar, w[3],

```

```

                                APM_MUL, APM_ADD, NULL ) ;
apmDivide( w[3], precision, (APM) NULL, ff_scratch, Rdet_vu ) ;
apmCalc( ff_scratch, Rcenter_err[4], Rstar, w[4],
                                APM_MUL, APM_ADD, NULL ) ;
apmDivide( w[4], precision, (APM) NULL, ff_scratch, Rdet_vu ) ;
apmAdd( w[5], one, Rcenter_err[5] ) ;
apmAdd( w[6], one, Rcenter_err[6] ) ;
}

return ;
}
/* ++++++ */

Rbeta_star( answer )

APM    answer ;
{
    Rbound_expr( &Rbeta[0] ) ;
    Rbound_expr( &Rbeta[1] ) ;
    Rbound_expr( &Rbeta[2] ) ;

    RmaxAbs( answer, Rbeta[0].bound.ub, Rbeta[0].bound.lb ) ;
    RmaxAbs( Rrow_abs[0], Rbeta[1].bound.ub, Rbeta[1].bound.lb ) ;
    RmaxAbs( Rrow_abs[1], Rbeta[2].bound.ub, Rbeta[2].bound.lb ) ;

    apmCalc( answer, answer, Rrow_abs[0], Rrow_abs[1],
                                APM_ADD, APM_ADD, NULL ) ;
}
/* ++++++ */

```

matrix inverter

```

# include <stdio.h>
# include <math.h>
# include "apm.h"
# include "apmSpecial.h"
# include "converse.h"

# define BUF_SZ          66

# define OOM_DF          1
# define MAX_RECUR      2
# define DFLT_XDP        5

# define Rm_swap(x,y,t)  (apmAssign(t, x), apmAssign(x, y), \
                          apmAssign(y, t) )

/*
The Numerical Recipes Gauss-Jordan matrix inverter as adapted
for a converse KAM code.
I have removed the dimension arguments n and m and replaced
them with TWO_DF and 1. I have also changed all the floats
into doubles and replaced some automatically allocated
arrays with arrays of fixed dimension. Finally, I have
replaced the error handling code with some of my own.

Rgauss, the rigorous version, also does a host of checks to
guarantee that the inverse it produces, when multiplied by
the original matrix, a, gives something equal to the
identity to the accuracy specified by the global variable,
"precision".
*/

```

```

int    extra_dp, last_inv_dp ;
int    inv_depth ;    /* Used to make sure that we don't keep trying
                       to invert singular matrices by using
                       ever increasing precision. */

APM    a_abs, Rbig, Rdum, Rpinv, Rtemp ;
APM    Rrow_max, Rcol_max, Rmat_min, Rmat_max ;
APM    *Rmat[TWO_DF], Rmat_block[4*DF_SQ] ;
APM    Rdiv_err, Rrow_err, Rinv_err, Rtotal_err, Rpiv_err ;
/* ++++++ */

initGauss()
{
    int    j, k ;
    APM    *mpt ;

    inv_depth = 0 ;
    extra_dp = 0 ;

    Rbig = apmNew( BASE ) ;
    Rdum = apmNew( BASE ) ;
    a_abs = apmNew( BASE ) ;
    Rtemp = apmNew( BASE ) ;
    Rpinv = apmNew( BASE ) ;
    Rinv_err = apmNew( BASE ) ;
    Rrow_err = apmNew( BASE ) ;
    Rpiv_err = apmNew( BASE ) ;
    Rdiv_err = apmNew( BASE ) ;
    Rrow_max = apmNew( BASE ) ;
    Rcol_max = apmNew( BASE ) ;
    Rmat_min = apmNew( BASE ) ;
    Rmat_max = apmNew( BASE ) ;
    Rtotal_err = apmNew( BASE ) ;

    mpt = Rmat_block ;
    for( j=0 ; j < TWO_DF ; j++ ) {
        Rmat[j] = mpt ;
        for( k=0 ; k < TWO_DF ; k++ )
            *mpt++ = apmNew( BASE ) ;
    }
}
/* ++++++ */

Rgauss( a )
APM    **a ;
{
    int    indxc[TWO_DF], indxr[TWO_DF], ipiv[TWO_DF] ;
    int    i, icol, irow, j, k, l, ll ;
    int    inv_dp, err_dp ;

    if( ++inv_depth > MAX_RECUR ) {
        fprintf( stderr, "Singular matrix in Rgauss. Died. \n" ) ;
        cease() ;
    }

    for( j=0 ; j < TWO_DF ; j++ ) {
        ipiv[j] = 0 ;
        indxr[j] = 0 ;
        indxc[j] = 0 ;
    }
}

```

```

}
/*
    If this is the attempt to invert a,
    copy the matrix in case of a loss of precision.
    Also, choose
    the precision to which to do the inversion calculations.
*/
if( inv_depth == 1 ) {
    copyRmat( Rmat, a );
    inv_dp = choosePrecis( a );
}
else {
    if( extra_dp == 0 )
        inv_dp = last_inv_dp + DFLT_XDP ;
    else
        inv_dp = last_inv_dp + extra_dp ;
}
last_inv_dp = inv_dp ;

/*
    Initialize the error propagation stuff.
*/
apmAssignLong( Rdiv_err, 1L, -inv_dp, BASE ) ;
apmAssignLong( Rinv_err, 0L, 0, BASE ) ;
apmAssign( Rpiv_err, Rinv_err ) ;

for (i=0;i<TWO_DF;i++) {
    apmAssignLong( Rbig, 0L, 0, BASE ) ;
    for (j=0;j<TWO_DF;j++) {
        if (ipiv[j] != 1) {
            for (k=0;k<TWO_DF;k++) {
                if (ipiv[k] == 0) {
                    apmAbsoluteValue( a_abs, a[j][k] ) ;
                    if( apmCompare(a_abs, Rbig) != -1 ) {
                        apmAssign( Rbig, a_abs ) ;
                        irow=j;
                        icol=k;
                    }
                }
                else if (ipiv[k] > 1) {
                    fprintf( stderr,
                        "Singular matrix in gauss. Died.\n" ) ;
                    cease() ;
                }
            }
        }
    }
    ++(ipiv[icol]);
    if(irow != icol) {
        for (l=0;l<TWO_DF;l++)
            Rm_swap(a[irow][l],a[icol][l],Rtemp) ;
    }

    indxr[i]=irow;
    indxc[i]=icol;

/*
    Check that the pivot interval does not
    contain zero. If it does, restart the
    calculation and carry more decimal places.
*/
    apmCalc( Rtemp, a[icol][icol], APM_ABS,

```

```

        Rinv_err, APM_SUB, NULL ) ;
if( apmCompare( Rtemp, zero ) != 1 ) {
    copyRmat( a, Rmat ) ;
    Rgauss( a ) ;
    return ;
}
/*
    Get the new pivot error. It is here that we face
    the possibility of catastrophic loss of precision.
*/
apmDivide( Rpiv_err, inv_dp, (APM)NULL, Rinv_err, Rtemp ) ;
apmCalc( Rpiv_err, Rpiv_err, Rdiv_err, Rdiv_err,
        APM_ADD, APM_ADD, NULL ) ;
apmDivide( Rpivinv, inv_dp, (APM)NULL, one, a[icol][icol] ) ;
apmAssignLong( a[icol][icol], 1L, 0, BASE ) ;

apmAssignLong( Rrow_max, OL, 0, BASE ) ;
for (l=0;l<TWO_DF;l++) {
    if( l != icol ) {
        apmAbsoluteValue( Rtemp, a[icol][l] ) ;
        if( apmCompare( Rtemp, Rrow_max ) < 0 )
            apmAssign( Rrow_max, Rtemp ) ;
    }

    apmCalc( a[icol][l], a[icol][l], Rpivinv, APM_MUL, NULL ) ;
}

/*
    Get a bound on the size of the errors in the elements
    of the pivot row.
*/
apmCalc( Rrow_err, Rinv_err, Rpivinv, APM_MUL,
        Rrow_max, Rinv_err, APM_ADD,
        Rpiv_err, APM_MUL, APM_ADD, NULL ) ;

apmAssignLong( Rcol_max, OL, 0, BASE ) ;
for (ll=0;ll<TWO_DF;ll++) {
    if (ll != icol) {
        apmAssign( Rdum, a[ll][icol] ) ;
        apmAbsoluteValue( Rtemp, Rdum ) ;
        if( apmCompare( Rtemp, Rcol_max ) == 1 )
            apmAssign( Rcol_max, Rtemp ) ;

        apmAssignLong( a[ll][icol], OL, 0, BASE ) ;
        for (l=0;l<TWO_DF;l++)
            apmCalc( a[ll][l], a[ll][l], a[icol][l], Rdum,
                    APM_MUL, APM_SUB, NULL ) ;
    }
}

/*
    Calculate the new upper bound on errors in the matrix.
*/
apmCalc( Rinv_err, Rrow_max, Rrow_err, APM_ADD,
        Rinv_err, APM_MUL,
        Rcol_max, Rrow_err, APM_MUL,
        Rinv_err, APM_ADD,
        APM_ADD, APM_ADD, NULL ) ;

/*
    Add an extra Rdiv_err to Rinv_err and truncate everything.
    This will probably speed the calculation considerably.
*/

```

```

    apmCalc( Rinv_err, Rinv_err, Rdiv_err, APM_ADD, NULL ) ;

    apmTruncate( Rinv_err, inv_dp ) ;
    for( l = 0 ; l < TWO_DF ; l++ )
        for( ll=0 ; ll < TWO_DF ; ll++ )
            apmTruncate( a[l][ll], inv_dp ) ;
}

for (l=(TWO_DF-1);l>=0;l--) {
    if (indxr[l] != indxc[l])
        for (k=0;k<TWO_DF;k++)
            Rm_swap(a[k][indxr[l]],a[k][indxc[l]],Rtemp);
}

/*
    Check the overall size of the error.
    If it is too big, set extra_dp and try again.
*/
err_dp = -(apmLogBd( Rinv_err ) + OOM_DF) ;
if( err_dp < precision ) {
    extra_dp = precision - err_dp + 2 ;
    copyRmat( a, Rmat ) ;
    Rgauss( a ) ;
    return ;
}

/*
    Tidy up.
    If we reach this line, all is well, the inversion is
    good to the desired precision, so all we want to do is
    restore the recursive variables to their initial state.
*/
inv_depth = 0 ;
extra_dp = 0 ;
return ;
}
/* ++++++ */

copyRmat( copy, mat )

APM **copy, **mat ;
{
    int j, k ;

    for( j=0 ; j < TWO_DF ; j++ )
        for( k=0 ; k < TWO_DF ; k++ )
            apmAssign( copy[j][k], mat[j][k] ) ;
}
/* ++++++ */

choosePrecis( mat )

APM **mat ;
{
    APM *mpt, *end_mat ;
    int oom_min, oom_max, oom_err, oom_twos ;

/*
    Find the minimum and maximum entries of the matrix.
    If none of the entries has absolute value bigger than
    one, use one as the maximum; this ensures that the
    resulting inverse will have entries good to at least

```



```

    "precision" decimal places.
*/
mpt = mat[0] ;
apmAssignLong( Rmat_min, 0L, 0, BASE ) ;
apmAssignLong( Rmat_max, 1L, 0, BASE ) ;

for( end_mat = mpt + (TWO_DF*TWO_DF) ; mpt < end_mat ; mpt++ ) {
    apmAbsoluteValue( Rtemp, *mpt ) ;
    if( apmCompare( Rmat_min, Rtemp ) > 0 )
        apmAssign( Rmat_min, Rtemp ) ;
    else if( apmCompare( Rmat_max, Rtemp ) < 0 )
        apmAssign( Rmat_max, Rtemp ) ;
}

/*
    Do a basic estimate of the number of digits one must carry
    to get an answer whose precision is as good as the code
    requires.
    First find the orders of magnitude ("oom"'s) of various things.
*/
oom_max = apmLogBd( Rmat_max ) ;
oom_twos = (TWO_DF / 3) ;

oom_err = oom_twos + OOM_DF + (2 * TWO_DF + 1) * abs( oom_max ) ;

if( oom_err < 0 )
    return( precision ) ;
else
    return( precision + oom_err ) ;
}

```

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