Chapter 6

Hamiltonian dynamics

Truth is rarely pure, and never simple.
—Oscar Wilde

You might think that the strangeness of contracting flows, flows such as the Rössler flow of figure 2.5 is of concern only to chemists; real physicists do Hamiltonian dynamics, right? Now, that's full of chaos, too! While it is easier to visualize aperiodic dynamics when a flow is contracting onto a lower-dimensional attracting set, there are plenty examples of chaotic flows that do preserve the full symplectic invariance of Hamiltonian dynamics. The whole story started in fact with Poincaré's restricted 3-body problem, a realization that chaos rules also in general (non-Hamiltonian) flows came much later.

Here we briefly review parts of classical dynamics that we will need later on; symplectic invariance, canonical transformations, and stability of Hamiltonian flows. We discuss billiard dynamics in some detail in chapter 8.

6.1 Hamiltonian flows

(P. Cvitanović and L.V. Vela-Arevalo)

An important class of flows are Hamiltonian flows, given by a Hamiltonian $H(q,p)$ together with the Hamilton's equations of motion

☞ appendix B

$$\dot{q}_i = \frac{\partial H}{\partial p_i}\,, \qquad \dot{p}_i = -\frac{\partial H}{\partial q_i}\,, \tag{6.1}$$

☞ example 7.1

with the $2D$ phase space coordinates x split into the configuration space coordinates and the conjugate momenta of a Hamiltonian system with D degrees of freedom (dof):

☞ sect. 31.1.1

$$x = (\mathbf{q},\mathbf{p})\,, \qquad \mathbf{q} = (q_1, q_2, \ldots, q_D)\,, \qquad \mathbf{p} = (p_1, p_2, \ldots, p_D)\,. \tag{6.2}$$

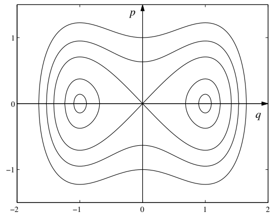

Figure 6.1: Phase plane of the unforced, undamped Duffing oscillator. The trajectories lie on level sets of the Hamiltonian (6.4).

The energy, or the value of the Hamiltonian function at the state space point $x = (\mathbf{q},\mathbf{p})$ is constant along the trajectory $x(t)$,

$$\begin{aligned}\frac{d}{dt}H(\mathbf{q}(t),\mathbf{p}(t)) &= \frac{\partial H}{\partial q_i}\dot{q}_i(t) + \frac{\partial H}{\partial p_i}\dot{p}_i(t) \\ &= \frac{\partial H}{\partial q_i}\frac{\partial H}{\partial p_i} - \frac{\partial H}{\partial p_i}\frac{\partial H}{\partial q_i} = 0\,,\end{aligned} \tag{6.3}$$

so the trajectories lie on surfaces of constant energy, or *level sets* of the Hamiltonian $\{(q,p) : H(q,p) = E\}$. For 1-dof Hamiltonian systems this is basically the whole story.

Example 6.1 Unforced undamped Duffing oscillator: *When the damping term is removed from the Duffing oscillator (2.7), the system can be written in Hamiltonian form with the Hamiltonian*

$$H(q,p) = \frac{p^2}{2} - \frac{q^2}{2} + \frac{q^4}{4}. \tag{6.4}$$

This is a 1-dof Hamiltonian system, with a 2-dimensional state space, the plane (q,p). The Hamilton's equations (6.1) are

$$\dot{q} = p\,, \qquad \dot{p} = q - q^3\,. \tag{6.5}$$

For 1-dof systems, the 'surfaces' of constant energy (6.3) are simply curves in the phase plane (q,p), and the dynamics is very simple: the curves of constant energy are *the trajectories, as shown in figure 6.1.*

Thus all 1-dof systems are *integrable*, in the sense that the entire phase plane is foliated by curves of constant energy, either periodic – as is the case for the harmonic oscillator (a 'bound state')–or open (a 'scattering trajectory'). Add one more degree of freedom, and chaos breaks loose.

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Example 6.2 Collinear helium: *In chapter 35, we shall apply the periodic orbit theory to the quantization of helium. In particular, we will study* collinear helium, *a doubly charged nucleus with two electrons arranged on a line, an electron on each side of the nucleus. The Hamiltonian for this system is*

$$H = \frac{1}{2}p_1^2 + \frac{1}{2}p_2^2 - \frac{2}{r_1} - \frac{2}{r_2} + \frac{1}{r_1 + r_2}\,. \tag{6.6}$$

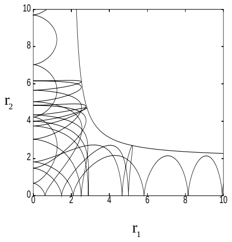

Figure 6.2: A typical collinear helium trajectory in the $[r_1, r_2]$ plane; the trajectory enters along the r_1-axis and then, like almost every other trajectory, after a few bounces escapes to infinity, in this case along the r_2-axis.

Collinear helium has 2 dof, and thus a 4-dimensional phase space $\mathcal{M}$, which energy conservation reduces to 3 dimensions. The dynamics can be projected onto the 2-dimensional configuration plane, the (r_1, r_2), $r_i \geq 0$ quadrant, figure 6.2. It looks messy, and, indeed, it will turn out to be no less chaotic than a pinball bouncing between three disks. As always, a Poincaré section will be more informative than this rather arbitrary projection of the flow.

Note an important property of Hamiltonian flows: if the Hamilton equations (6.1) are rewritten in the $2D$ phase space form $\dot{x}_i = v_i(x)$, the divergence of the velocity field v vanishes, namely the flow is incompressible. The symplectic invariance requirements are actually more stringent than just the phase space volume conservation, as we shall see in the next section.

6.2 Stability of Hamiltonian flows

Hamiltonian flows offer an illustration of the ways in which an invariance of equations of motion can affect the dynamics. In the case at hand, the *symplectic invariance* will reduce the number of independent stability eigenvalues by a factor of 2 or 4.

6.2.1 Canonical transformations

The equations of motion for a time-independent, D-dof Hamiltonian (6.1) can be written

$$\dot{x}_i = \omega_{ij} H_j(x) \,, \qquad \omega = \begin{pmatrix} 0 & \mathbf{I} \\ -\mathbf{I} & 0 \end{pmatrix} \,, \quad H_j(x) = \frac{\partial}{\partial x_j} H(x) \,, \tag{6.7}$$

where $x = (\mathbf{q}, \mathbf{p}) \in \mathcal{M}$ is a phase space point, $H_k = \partial_k H$ is the column vector of partial derivatives of H, $\mathbf{I}$ is the $[D \times D]$ unit matrix, and ω the $[2D \times 2D]$ *symplectic* form

$$\omega^T = -\omega \,, \qquad \omega^2 = -\mathbf{1} \,. \tag{6.8}$$

The evolution of J^t (4.6) is again determined by the stability matrix A, (4.9):

$$\frac{d}{dt} J^t(x) = A(x) J^t(x) \,, \qquad A_{ij}(x) = \omega_{ik} \, H_{kj}(x) \,, \tag{6.9}$$

where the matrix of second derivatives $H_{kn} = \partial_k \partial_n H$ is called the *Hessian matrix*. From the symmetry of H_{kn} it follows that

$$A^T \omega + \omega A = 0 \,. \tag{6.10}$$

This is the defining property for infinitesimal generators of *symplectic* (or canonical) transformations, transformations which leave the symplectic form ω invariant.

Symplectic matrices are by definition linear transformations that leave the (antisymmetric) quadratic form $x_i \omega_{ij} y_j$ invariant. This immediately implies that any symplectic matrix satisfies

$$Q^T \omega Q \;=\; \omega \,, \tag{6.11}$$

and – when Q is close to the identity $Q = \mathbf{1} + \delta t A$ – it follows that that A must satisfy (6.10).

Consider now a smooth nonlinear change of variables of form $y_i = h_i(x)$, and define a new function $K(x) = H(h(x))$. Under which conditions does K generate a Hamiltonian flow? In what follows we will use the notation $\tilde{\partial}_j = \partial/\partial y_j$: by employing the chain rule we have that

$$\omega_{ij} \partial_j K \;=\; \omega_{ij} \tilde{\partial}_l H \frac{\partial h_l}{\partial x_j} \tag{6.12}$$

(Here, as elsewhere in this book, a repeated index implies summation.) By virtue of (6.1) $\tilde{\partial}_l H = -\omega_{lm} \dot{y}_m$, so that, again by employing the chain rule, we obtain

$$\omega_{ij} \partial_j K \;=\; -\omega_{ij} \frac{\partial h_l}{\partial x_j} \omega_{lm} \frac{\partial h_m}{\partial x_n} \dot{x}_n \tag{6.13}$$

The right hand side simplifies to $\dot{x}_i$ (yielding Hamiltonian structure) only if

$$-\,\omega_{ij} \frac{\partial h_l}{\partial x_j} \omega_{lm} \frac{\partial h_m}{\partial x_n} \;=\; \delta_{in} \tag{6.14}$$

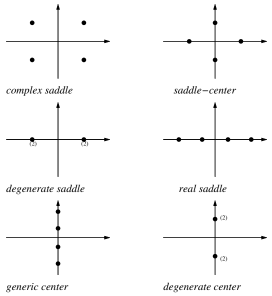

Figure 6.3: Stability exponents of a Hamiltonian equilibrium point, 2-dof.

or, in compact notation, by defining $(\partial h)_{ij} = \frac{\partial h_i}{\partial x_j}$

$$-\,\omega(\partial h)^T\omega(\partial h) \;=\; \mathbf{1} \qquad (6.15)$$

which is equivalent to the requirement that ∂h is symplectic. h is then called a *canonical transformation*. We care about canonical transformations for two reasons. First (and this is a dark art), if the canonical transformation h is very cleverly chosen, the flow in new coordinates might be considerably simpler than the original flow. Second, Hamiltonian flows themselves are a prime example of canonical transformations.

example 7.1

Example 6.3 Hamiltonian flows are canonical: *For Hamiltonian flows it follows from (6.10) that* $\frac{d}{dt}\left(J^T\omega J\right) = 0$, *and since at the initial time* $J^0(x_0) = \mathbf{1}$, *fundamental matrixis a symplectic transformation (6.11). This equality is valid for all times, so a Hamiltonian flow* $f^t(x)$ *is a canonical transformation, with the linearization* $\partial_x f^t(x)$ *a symplectic transformation (6.11): For notational brevity here we have suppressed the dependence on time and the initial point,* $J = J^t(x_0)$. *By elementary properties of determinants it follows from (6.11) that Hamiltonian flows are phase space volume preserving:*

$$|\det J| = 1\,. \qquad (6.16)$$

Actually it turns out that for symplectic matrices (on any field) one always has $\det J = +1$.

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6.2.2 Stability of equilibria of Hamiltonian flows

sect. 4.3.1

For an equilibrium point x_q the stability matrix A is constant. Its eigenvalues describe the linear stability of the equilibrium point. A is the matrix (6.10) with real matrix elements, so its eigenvalues (the stability exponents of (4.30)) are either real or come in complex pairs. In the case of Hamiltonian flows, it follows from (6.10) that the characteristic polynomial of A for an equilibrium x_q satisfies

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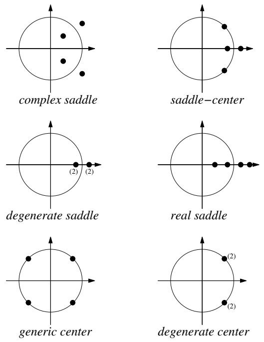

Figure 6.4: Stability of a symplectic map in $\mathbb{R}^4$.

$$\begin{aligned}\det(A-\lambda\mathbf{1}) &= \det\left(\omega^{-1}(A-\lambda\mathbf{1})\omega\right) \;=\; \det(-\omega A\omega-\lambda\mathbf{1})\\ &= \det(A^T+\lambda\mathbf{1}) \;=\; \det(A+\lambda\mathbf{1})\,.\end{aligned} \qquad (6.17)$$

That is, the symplectic invariance implies in addition that if λ is an eigenvalue, then $-\lambda$, λ^* and $-\lambda^*$ are also eigenvalues. Distinct symmetry classes of the stability exponents of an equilibrium point in a 2-dof system are displayed in figure 6.3. It is worth noting that while the linear stability of equilibria in a Hamiltonian system always respects this symmetry, the nonlinear stability can be completely different.

6.3 Symplectic maps

A stability eigenvalue $\Lambda = \Lambda(x_0, t)$ associated to a trajectory is an eigenvalue of the fundamental matrix J. As J is symplectic, (6.11) implies that

$$J^{-1} = -\omega J^T\omega\,, \qquad (6.18)$$

so the characteristic polynomial is reflexive, namely it satisfies

$$\begin{aligned}\det(J-\Lambda\mathbf{1}) &= \det(J^T-\Lambda\mathbf{1}) \;=\; \det(-\omega J^T\omega-\Lambda\mathbf{1})\\ &= \det(J^{-1}-\Lambda\mathbf{1}) \;=\; \det(J^{-1})\det(\mathbf{1}-\Lambda J)\\ &= \Lambda^{2D}\det(J-\Lambda^{-1}\mathbf{1})\,.\end{aligned} \qquad (6.19)$$

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Hence if Λ is an eigenvalue of J, so are $1/\Lambda$, Λ^* and $1/\Lambda^*$. Real eigenvalues always come paired as Λ, $1/\Lambda$. The Liouville conservation of phase space volumes (6.16) is an immediate consequence of this pairing up of eigenvalues. The complex eigenvalues come in pairs Λ, Λ^*, $|\Lambda| = 1$, or in loxodromic quartets Λ, $1/\Lambda$, Λ^* and $1/\Lambda^*$. These possibilities are illustrated in figure 6.4.

Example 6.4 Hamiltonian Hénon map, reversibility: *By (4.53) the Hénon map (3.15) for $b = -1$ value is the simplest 2-d orientation preserving area-preserving map, often studied to better understand topology and symmetries of Poincaré sections of 2 dof Hamiltonian flows. We find it convenient to multiply (3.16) by a and absorb the a factor into x in order to bring the Hénon map for the $b = -1$ parameter value into the form*

$$x_{i+1} + x_{i-1} = a - x_i^2 \,, \quad i = 1, ..., n_p \,, \tag{6.20}$$

The 2-dimensional Hénon map *for $b = -1$ parameter value*

$$\begin{aligned} x_{n+1} &= a - x_n^2 - y_n \\ y_{n+1} &= x_n \,. \end{aligned} \tag{6.21}$$

is Hamiltonian (symplectic) in the sense that it preserves area in the $[x, y]$ plane.

For definitiveness, in numerical calculations in examples to follow we shall fix (arbitrarily) the stretching parameter value to $a = 6$, a value large enough to guarantee that all roots of $0 = f^n(x) - x$ (periodic points) are real.

Example 6.5 2-dimensional symplectic maps: *In the 2-dimensional case the eigenvalues (5.5) depend only on $\mathrm{tr}\, M^t$*

$$\Lambda_{1,2} = \frac{1}{2}\left(\mathrm{tr}\, M^t \pm \sqrt{(\mathrm{tr}\, M^t - 2)(\mathrm{tr}\, M^t + 2)}\right) \,. \tag{6.22}$$

The trajectory is elliptic if the stability residue $|\mathrm{tr}\, M^t| - 2 \le 0$, *with complex eigenvalues* $\Lambda_1 = e^{i\theta t}$, $\Lambda_2 = \Lambda_1^* = e^{-i\theta t}$. *If $|\mathrm{tr}\, M^t| - 2 > 0$, λ is real, and the trajectory is either*

$$\text{hyperbolic} \qquad \Lambda_1 = e^{\lambda t} \,, \quad \Lambda_2 = e^{-\lambda t} \,, \text{ or} \tag{6.23}$$

$$\text{inverse hyperbolic} \qquad \Lambda_1 = -e^{\lambda t} \,, \quad \Lambda_2 = -e^{-\lambda t} \,. \tag{6.24}$$

Example 6.6 Standard map. *Given a smooth function $g(x)$, the map*

$$\begin{aligned} x_{n+1} &= x_n + y_{n+1} \\ y_{n+1} &= y_n + g(x_n) \end{aligned} \tag{6.25}$$

is an area-preserving map. The corresponding nth iterate fundamental matrix (4.48) is

$$M^n(x_0, y_0) = \prod_{k=n}^{1} \begin{pmatrix} 1 + g'(x_k) & 1 \\ g'(x_k) & 1 \end{pmatrix} \,. \tag{6.26}$$

The map preserves areas, $\det M = 1$, and one can easily check that M is symplectic. In particular, one can consider x on the unit circle, and y as the conjugate angular momentum, with a function g periodic with period 1. The phase space of the map is thus the cylinder $S_1 \times \mathbf{R}$ (S_1 stands for the 1-torus, which is fancy way to say "circle"): by taking (6.25) $\mathrm{mod}\ 1$ the map can be reduced on the 2-torus S_2.

The standard map *corresponds to the choice $g(x) = k/2\pi \sin(2\pi x)$. When $k = 0$, $y_{n+1} = y_n = y_0$, so that angular momentum is conserved, and the angle x rotates with uniform velocity*

$$x_{n+1} = x_n + y_0 = x_0 + (n+1)y_0 \qquad \text{mod } 1 \,. \tag{6.27}$$

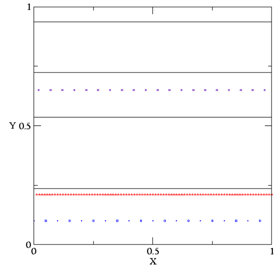

Figure 6.5: Standard map orbits for $k = 0$. Symbols denote periodic orbits, full lines represent quasiperiodic orbits.

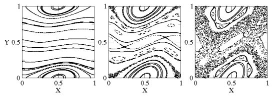

Figure 6.6: Phase portrait for the standard map for $k = 0.3$, $k = 0.85$ and $k = 1.4$: each plot consists of 20 random initial conditions, each iterated 400 times.

The choice of y_0 determines the nature of the motion (in the sense of sect. 2.1.1): for $y_0 = 0$ we have that every point on the $y_0 = 0$ line is stationary, for $y_0 = p/q$ the motion is periodic, and for irrational y_0 any choice of x_0 leads to a quasiperiodic motion (see figure 6.5).

Despite the simple structure of the standard map, a complete description of its dynamics for arbitrary values of the nonlinear parameter k is fairly complex: this can be appreciated by looking at phase portraits of the map for different k values: when k is very small the phase space looks very much like a slightly distorted version of figure 6.5, while, when k is sufficiently large, single trajectories wander erratically on a large fraction of the phase space, as in figure 6.6.

This gives a glimpse of the typical scenario of transition to chaos for Hamiltonian systems.

Note that the map (6.25) provides a stroboscopic view of the flow generated by a (time-dependent) Hamiltonian

$$H(x, y; t) = \frac{1}{2}y^2 + G(x)\delta_1(t) \tag{6.28}$$

where δ_1 denotes the periodic delta function

$$\delta_1(t) = \sum_{m=-\infty}^{\infty} \delta(t - m) \tag{6.29}$$

and

$$G'(x) = -g(x) \,. \tag{6.30}$$

Important features of this map, including transition to global chaos *(destruction of the last invariant torus), may be tackled by detailed investigation of the stability of periodic orbits. A family of periodic orbits of period Q already present in the $k = 0$ rotation maps can be labeled by its* winding number P/Q The Greene residue *describes the stability of a P/Q-cycle:*

$$R_{P/Q} = \frac{1}{4}\left(2 - \mathrm{tr}\, M_{P/Q}\right) \,. \tag{6.31}$$

If $R_{P/Q} \in (0,1)$ the orbit is elliptic, for $R_{P/Q} > 1$ the orbit is hyperbolic orbits, and for $R_{P/Q} < 0$ inverse hyperbolic.

k ??

For $k = 0$ all points on the $y_0 = P/Q$ line are periodic with period Q, winding number P/Q and marginal stability $R_{P/Q} = 0$). As soon as $k > 0$, only a $2Q$ of such orbits survive, according to Poincaré-Birkhoff theorem: half of them elliptic, and half hyperbolic. If we further vary k in such a way that the residue of the elliptic Q-cycle goes through 1, a bifurcation takes place, and two or more periodic orbits of higher period are generated.

6.4 Poincaré invariants

Let C be a region in phase space and $V(0)$ its volume. Denoting the flow of the Hamiltonian system by $f^t(x)$, the volume of C after a time t is $V(t) = f^t(C)$, and using (6.16) we derive the *Liouville theorem*:

$$\begin{aligned} V(t) &= \int_{f^t(C)} dx = \int_C \left| \det \frac{\partial f^t(x')}{\partial x} \right| dx' \\ & \int_C \det(J) dx' = \int_C dx' = V(0) , \end{aligned} \tag{6.32}$$

Hamiltonian flows preserve phase space volumes.

The symplectic structure of Hamilton's equations buys us much more than the 'incompressibility,' or the phase space volume conservation. Consider the symplectic product of two infinitesimal vectors

$$\begin{aligned} (\delta x, \delta \hat{x}) &= \delta x^T \omega \delta \hat{x} = \delta p_i \delta \hat{q}_i - \delta q_i \delta \hat{p}_i \\ &= \sum_{i=1}^{D} \{\text{oriented area in the } (q_i, p_i) \text{ plane}\} . \end{aligned} \tag{6.33}$$

Time t later we have

$$(\delta x', \delta \hat{x}') = \delta x^T J^T \omega J \delta \hat{x} = \delta x^T \omega \delta \hat{x} .$$

This has the following geometrical meaning. We imagine there is a reference phase space point. We then define two other points infinitesimally close so that the vectors δx and $\delta \hat{x}$ describe their displacements relative to the reference point. Under the dynamics, the three points are mapped to three new points which are still infinitesimally close to one another. The meaning of the above expression is that the area of the parallelopiped spanned by the three final points is the same as that spanned by the inital points. The integral (Stokes theorem) version of this infinitesimal area invariance states

that for Hamiltonian flows the D oriented areas $\mathcal{V}_i$ bounded by D loops $\Omega\mathcal{V}_i$, one per each (q_i, p_i) plane, are separately conserved:

$$\int_{\mathcal{V}} dp \wedge dq = \oint_{\Omega\mathcal{V}} p \cdot dq = \text{invariant} . \tag{6.34}$$

Morally a Hamiltonian flow is really D-dimensional, even though its phase space is $2D$-dimensional. Hence for Hamiltonian flows one emphasizes D, the number of the degrees of freedom.


in depth:
appendix B.3, p. 720

In theory there is no difference between theory and practice. In practice there is.
—Yogi Berra

Commentary

Remark 6.1 Hamiltonian dynamics literature. If you are reading this book, in theory you already know everything that is in this chapter. In practice you do not. Try this: Put your right hand on your heart and say: "I understand why nature prefers symplectic geometry". Honest? We make an attempt in sect. 31.1. Out there there are about 2 centuries of accumulated literature on Hamilton, Lagrange, Jacobi etc. formulation of mechanics, some of it excellent. In context of what we will need here, we make a very subjective recommendation–we enjoyed reading Percival and Richards [7.10] and Ozorio de Almeida [7.11].

Remark 6.2 Symplectic. The term symplectic–Greek for twining or plaiting together–was introduced into mathematics by Hermann Weyl. 'Canonical' lineage is church-doctrinal: Greek 'kanon,' referring to a reed used for measurement, came to mean in Latin a rule or a standard.

Remark 6.3 The sign convention of ω. The overall sign of ω, the symplectic invariant in (6.7), is set by the convention that the Hamilton's principal function (for energy conserving flows) is given by $R(q, q', t) = \int_q^{q'} p_i dq_i - Et$. With this sign convention the action along a classical path is minimal, and the kinetic energy of a free particle is positive.

Remark 6.4 Symmetries of the symbol square. For a more detailed discussion of symmetry lines see refs. [12.4, 3.8, 11.49, 6.13]. It is an open question (see remark **??**) as to how time reversal symmetry can be exploited for reductions of cycle expansions. For example, the fundamental domain symbolic dynamics for reflection symmetric systems is discussed in some detail in sect. **??**, but how does one recode from time-reversal symmetric symbol sequences to desymmetrized 1/2 state space symbols?

Remark 6.5 Standard map. Standard maps model free rotators under the influence of short periodic pulses, as can be physically implemented, for instance, by pulsed optical lattices in cold atoms physics. On the theoretical side, standard maps exhibit a number of important features: small k values provide an example of KAM perturbative regime (see ref. [6.8]), while for larger k chaotic deterministic transport is observed [6.9, 6.10]; the transition to global chaos also presents remarkable universality features [6.11, 6.12, 6.13]. Also the quantum counterpart of this model has been widely investigated, being the first example where phenomena like quantum dynamical localization have been observed [6.14]. For some hands-on experience of the standard map, download Meiss simulation code [6.4].

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