# **Chapter 8**

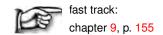
# Hamiltonian dynamics

Conservative mechanical systems have equations of motion that are symplectic and can be expressed in Hamiltonian form. The generic properties within the class of symplectic vector fields are quite different from those within the class of all smooth vector fields: the system always has a first integral ("energy") and a preserved volume, and equilibrium points can never be asymptotically stable in their energy level.

- John Guckenheimer

OU MIGHT THINK that the strangeness of contracting flows, flows such as the Rössler flow of figure 2.6 is of concern only to chemists or biomedical engineers or the weathermen; 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 of examples of chaotic flows that do preserve the full symplectic invariance of Hamiltonian dynamics. The whole story started 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. If your eventual destination are applications such as chaos in quantum and/or semiconductor systems, read this chapter. If you work in neuroscience or fluid dynamics, skip this chapter, continue reading with the billiard dynamics of chapter 9 which requires no incantations of symplectic pairs or loxodromic quartets.



### 8.1 Hamiltonian flows

"... to do this business right is a thing of far greater difficulty than I was aware of."

— Sir Isaac Newton, in a letter to Edmund Halley

(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 A4 remark 2.1

$$\dot{q}_i = \frac{\partial H}{\partial p_i}, \qquad \dot{p}_i = -\frac{\partial H}{\partial q_i},$$
 (8.1)

with the d = 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):

$$x = (\mathbf{q}, \mathbf{p}), \qquad \mathbf{q} = (q_1, q_2, \dots, q_D), \qquad \mathbf{p} = (p_1, p_2, \dots, p_D).$$
 (8.2)

The equations of motion (8.1) for a time-independent, D-dof Hamiltonian can be written compactly as

$$\dot{x}_i = \omega_{ij} H_{,j}(x), \qquad H_{,j}(x) = \frac{\partial}{\partial x_j} H(x),$$
(8.3)

where  $x = (\mathbf{q}, \mathbf{p}) \in \mathcal{M}$  is a phase-space point, and the a derivative of  $(\cdot)$  with respect to  $x_j$  is denoted by comma-index notation  $(\cdot)_{,j}$ ,

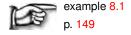
$$\omega = \begin{bmatrix} 0 & \mathbf{I} \\ -\mathbf{I} & 0 \end{bmatrix}, \tag{8.4}$$

is an antisymmetric  $[d \times d]$  matrix, and **I** is the  $[D \times D]$  unit matrix.

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

$$\frac{d}{dt}H(\mathbf{q}(t),\mathbf{p}(t)) = \frac{\partial H}{\partial q_i}\dot{q}_i(t) + \frac{\partial H}{\partial p_i}\dot{p}_i(t) 
= \frac{\partial H}{\partial q_i}\frac{\partial H}{\partial p_i} - \frac{\partial H}{\partial p_i}\frac{\partial H}{\partial q_i} = 0,$$
(8.5)

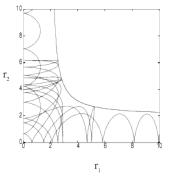
so the trajectories lie on surfaces of constant energy, or *level sets* of the Hamiltonian  $\{(q, p) : H(q, p) = E\}$ . For 1-dof Hamiltonian systems this is basically the whole story.



Thus all 1-dof systems are *integrable*, in the sense that the entire phase plane is stratified by curves of constant energy, either periodic, as is the case for the

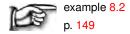
**Figure 8.1:** Phase plane of the unforced, undamped Duffing oscillator. The trajectories lie on level sets of the Hamiltonian (8.25).

**Figure 8.2:** 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. In this example the energy is set to H = E = -1, and the trajectory is bounded by the kinetic energy = 0 line.



harmonic oscillator (a 'bound state'), or open (a 'scattering trajectory'). Add one more degree of freedom, and chaos breaks loose.

example A2.1



Note an important property of Hamiltonian flows: if the Hamilton equations (8.1) 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,  $\nabla \cdot v = \partial_i v_i = \omega_i H_{,ij} = 0$ . The symplectic invariance requirements are actually more stringent than just the phase-space volume conservation, as we shall see in sect. 8.3.

Throughout ChaosBook we reserve the term 'phase space' to Hamiltonian flows. A 'state space' is the stage on which any flow takes place. 'Phase space' is a special but important case, a state space with symplectic structure, preserved by the flow. For us the distinction is necessary, as ChaosBook covers dissipative, mechanical, stochastic and quantum systems, all as one happy family.

## 8.2 Symplectic group

Either you're used to this stuff... or you have to get used to it.

-Maciej Zworski

A matrix transformation g is called *symplectic*,

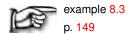
$$g^{\mathsf{T}}\omega g = \omega\,,\tag{8.6}$$

if it preserves the *symplectic bilinear form*  $\langle \hat{x}|x\rangle = \hat{x}^{\top}\omega x$ , where  $g^{\top}$  denotes the transpose of g, and  $\omega$  is a non-singular  $[2D\times 2D]$  antisymmetric matrix which satisfies

remark 8.3

$$\omega^{\mathsf{T}} = -\omega \,, \qquad \omega^2 = -1 \,. \tag{8.7}$$

While these are defining requirements for any symplectic bilinear form,  $\omega$  is often conventionally taken to be of form (8.4).



If g is symplectic, so is its inverse  $g^{-1}$ , and if  $g_1$  and  $g_2$  are symplectic, so is their product  $g_2g_1$ . Symplectic matrices form a Lie group called the *symplectic group* Sp(d). Use of the symplectic group necessitates a few remarks about Lie groups in general, a topic that we study in more depth in chapter 12. A *Lie group* is a group whose elements  $g(\phi)$  depend smoothly on a finite number N of parameters  $\phi_a$ . In calculations one has to write these matrices in a specific basis, and for infinitesimal transformations they take form (repeated indices are summed throughout this chapter, and the dot product refers to a sum over Lie algebra generators):

$$g(\delta\phi) \simeq 1 + \delta\phi \cdot \mathbf{T}, \quad \delta\phi \in \mathbb{R}^N, \quad |\delta\phi| \ll 1,$$
 (8.8)

where  $\{\mathbf{T}_1, \mathbf{T}_2 \cdots, \mathbf{T}_N\}$ , the *generators* of infinitesimal transformations, are a set of N linearly independent  $[d \times d]$  matrices which act linearly on the d-dimensional phase space  $\mathcal{M}$ . The infinitesimal statement of symplectic invariance follows by substituting (8.8) into (8.6) and keeping the terms linear in  $\delta \phi$ ,

$$\mathbf{T}_{a}^{\mathsf{T}}\omega + \omega \mathbf{T}_{a} = 0. \tag{8.9}$$

This is the defining property for infinitesimal generators of *symplectic* transformations. Matrices that satisfy (8.9) are sometimes called *Hamiltonian matrices*. A linear combination of Hamiltonian matrices is a Hamiltonian matrix, so Hamiltonian matrices form a linear vector space, the *symplectic Lie algebra* sp(d). By the antisymmetry of  $\omega$ ,

$$(\omega \mathbf{T}_a)^{\mathsf{T}} = \omega \mathbf{T}_a \,. \tag{8.10}$$

is a symmetric matrix. Its number of independent elements gives the dimension (the number of independent continuous parameters) of the symplectic group Sp(d),

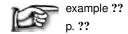
$$N = d(d+1)/2 = D(2D+1). (8.11)$$

The lowest-dimensional symplectic group Sp(2), of dimension N = 3, is isomorphic to SU(2) and SO(3). The first interesting case is Sp(3) whose dimension is N = 10.

It is easily checked that the exponential of a Hamiltonian matrix

$$g = e^{\phi \cdot \mathbf{T}} \tag{8.12}$$

is a symplectic matrix; Lie *group* elements are related to the Lie *algebra* elements by exponentiation.



### 8.3 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 Floquet multipliers by a factor of 2 or 4.

#### 8.3.1 Canonical transformations

The evolution of  $J^t$  (4.5) is determined by the stability matrix A, (4.10):

$$\frac{d}{dt}J^{t}(x) = A(x)J^{t}(x), \qquad A_{ij}(x) = \omega_{ik} H_{,kj}(x), \qquad (8.13)$$

where the symmetric matrix of second derivatives of the Hamiltonian,  $H_{,kn} = \partial_k \partial_n H$ , is called the *Hessian matrix*. From (8.13) and the symmetry of  $H_{,kn}$  it follows that for Hamiltonian flows (8.3)

$$A^{\mathsf{T}}\omega + \omega A = 0. \tag{8.14}$$

This is the defining property (8.9) for infinitesimal generators of *symplectic* (or canonical) transformations.

Consider now a smooth nonlinear coordinate change form  $y_i = h_i(x)$  (see sect. 2.3 for a discussion), and define a 'Kamiltonian' function K(x) = H(h(x)). Under which conditions does K generate a Hamiltonian flow? In what follows we will use the notation  $\partial_{\tilde{j}} = \partial/\partial y_j$ ,  $s_{i,j} = \partial h_i/\partial x_j$ . By employing the chain rule we have that

$$K_{,j} = H_{\tilde{j}} s_{\tilde{l},j} \tag{8.15}$$

(Here, as elsewhere in this book, a repeated index implies summation.) By virtue of (8.1),  $\tilde{\partial}_l H = -\omega_{lm} \dot{y}_m$ , so that, again by employing the chain rule, we obtain

$$\omega_{ij}\partial_j K = -\omega_{ij} s_{i,l} \omega_{lm} s_{m,n} \dot{x}_n \tag{8.16}$$

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

$$-\omega_{ij}s_{l,j}\omega_{lm}s_{m,n} = \delta_{in} \tag{8.17}$$

or, in compact notation,

$$-\omega(\partial h)^{\mathsf{T}}\omega(\partial h) = \mathbf{1} \tag{8.18}$$

which is equivalent to the requirement (8.6) that  $\partial h$  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 A2.1

Dream student Henriette Roux: "I hate these  $s_{m,n}$ . Can't you use a more sensible notation?" A: "Be my guest."



### 8.3.2 Stability of equilibria of Hamiltonian flows

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 (8.14) with real matrix elements, so its eigenvalues (the Floquet exponents of (5.1)) are either real or come in complex pairs. In the case of Hamiltonian flows, it follows from (8.14) that the characteristic polynomial of A for an equilibrium  $x_q$  satisfies

section 5.1 exercise 8.4 exercise 8.5

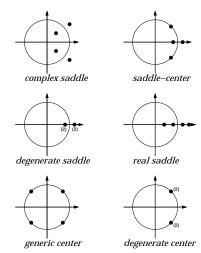
$$\det(A - \lambda \mathbf{1}) = \det(\omega^{-1}(A - \lambda \mathbf{1})\omega) = \det(-\omega A\omega - \lambda \mathbf{1})$$
$$= \det(A^{\top} + \lambda \mathbf{1}) = \det(A + \lambda \mathbf{1}). \tag{8.19}$$

That is, the symplectic invariance implies in addition that if  $\lambda$  is an eigenvalue, then  $-\lambda$ ,  $\lambda^*$  and  $-\lambda^*$  are also eigenvalues. Distinct symmetry classes of the Floquet exponents of an equilibrium point in a 2-dof system are displayed in figure 8.4. 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.

## 8.4 Symplectic maps

So far we have considered only the continuous time Hamiltonian flows. As discussed in sect. 4.4 for finite time evolution mappings, and in sect. 4.5 the iterated discrete time mappings, the stability of maps is characterized by eigenvalues of their Jacobian matrices, or 'multipliers.' A multiplier  $\Lambda = \Lambda(x_0, t)$  associated to a trajectory is an eigenvalue of the Jacobian matrix J. As J is symplectic, (8.6) implies that

$$J^{-1} = -\omega J^{\mathsf{T}} \omega \,, \tag{8.20}$$



**Figure 8.3:** Stability of a symplectic map in  $\mathbb{R}^4$ .

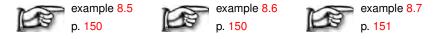
so the characteristic polynomial is reflexive, namely it satisfies

$$\det(J - \Lambda \mathbf{1}) = \det(J^{\top} - \Lambda \mathbf{1}) = \det(-\omega J^{\top} \omega - \Lambda \mathbf{1})$$

$$= \det(J^{-1} - \Lambda \mathbf{1}) = \det(J^{-1}) \det(\mathbf{1} - \Lambda J)$$

$$= \Lambda^{2D} \det(J - \Lambda^{-1} \mathbf{1}). \tag{8.21}$$

Hence if  $\Lambda$  is an eigenvalue of J, so are  $1/\Lambda$ ,  $\Lambda^*$  and  $1/\Lambda^*$ . Real eigenvalues always come paired as  $\Lambda$ ,  $1/\Lambda$ . The Liouville conservation of phase-space volumes (8.30) is an immediate consequence of this pairing up of eigenvalues. The complex eigenvalues come in pairs  $\Lambda$ ,  $\Lambda^*$ ,  $|\Lambda| = 1$ , or in loxodromic quartets  $\Lambda$ ,  $1/\Lambda$ ,  $\Lambda^*$  and  $1/\Lambda^*$ . These possibilities are illustrated in figure 8.3.



### 8.5 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 (8.30) we derive the *Liouville theorem*:

$$V(t) = \int_{f'(C)} dx = \int_{C} \left| \det \frac{\partial f'(x')}{\partial x} \right| dx'$$
$$\int_{C} \det (J) dx' = \int_{C} dx' = V(0), \qquad (8.22)$$

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

$$\langle \delta x | \delta \hat{x} \rangle = \delta x^{\top} \omega \delta \hat{x} = \delta p_{i} \delta \hat{q}_{i} - \delta q_{i} \delta \hat{p}_{i}$$

$$= \sum_{i=1}^{D} \{ \text{oriented area in the } (q_{i}, p_{i}) \text{ plane} \}.$$
(8.23)

Time t later we have

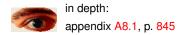
$$\langle \delta x' | \delta \hat{x}' \rangle = \delta x^{\mathsf{T}} J^{\mathsf{T}} \omega J \delta \hat{x} = \delta x^{\mathsf{T}} \omega \delta \hat{x}.$$

This has the following geometrical meaning. Imagine that there is a reference phase-space point. Take two other points infinitesimally close, with the vectors  $\delta x$  and  $\delta \hat{x}$  describing 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 parallelepiped spanned by the three final points is the same as that spanned by the initial points. The integral (Stokes theorem) version of this infinitesimal area invariance states that for Hamiltonian flows the sum of D oriented areas  $V_i$  bounded by D loops  $\Omega V_i$ , one per each  $(q_i, p_i)$  plane, is conserved:

$$\int_{\mathcal{V}} dp \wedge dq = \oint_{\mathcal{O}\mathcal{V}} p \cdot dq = \text{invariant}. \tag{8.24}$$

One can show that also the 4, 6,  $\cdots$ , 2D phase-space volumes are preserved. The phase space is 2D-dimensional, but as there are D coordinate combinations conserved by the flow, morally a Hamiltonian flow is D-dimensional. Hence for Hamiltonian flows the key notion of dimensionality is D, the number of the degrees of freedom (dof), rather than the phase-space dimensionality d = 2D.

Dream student Henriette Roux: "Would it kill you to draw some pictures here?" A: "Be my guest."



### Résumé

Physicists do Lagrangians and Hamiltonians. Many know of no world other than the perfect world of quantum mechanics and quantum field theory in which the energy and much else is conserved. From the dynamical point of view, a Hamiltonian flow is just a flow, but a flow with a symmetry: the stability matrix  $A_{ij} = \omega_{ik} H_{,kj}(x)$  of a Hamiltonian flow  $\dot{x}_i = \omega_{ij} H_{,j}(x)$  satisfies  $A^T \omega + \omega A = 0$ . Its integral along the trajectory, the linearization of the flow J that we call the 'Jacobian matrix', is symplectic, and a Hamiltonian flow is thus a canonical transformation in the sense that the Hamiltonian time evolution  $x' = f^t(x)$  is a transformation whose linearization (Jacobian matrix)  $J = \partial x'/\partial x$  preserves the symplectic form,

 $J^{\top}\omega J=\omega$ . This implies that A are in the symplectic algebra sp(2D), and that the 2D-dimensional Hamiltonian phase-space flow preserves D oriented infinitesimal volumes, or Poincaré invariants. The Liouville phase-space volume conservation is one consequence of this invariance.

While symplectic invariance enforces  $|\Lambda|=1$  for complex eigenvalue pairs and precludes existence of attracting equilibria and limit cycles typical of dissipative flows, for hyperbolic equilibria and periodic orbits  $|\Lambda|>1$ , and the pairing requirement only enforces a particular value on the  $1/\Lambda$  contracting direction. Hence the description of chaotic dynamics as a sequence of saddle visitations is the same for the Hamiltonian and dissipative systems. You might find symplecticity beautiful. Once you understand that every time you have a symmetry, you should use it, you might curse the day [17] you learned to say 'symplectic'.

chapter 12

### Commentary

In theory there is no difference between theory and practice. In practice there is.

-Anonymous

**Remark 8.1.** Hamiltonian dynamics, sources. 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?

Where does the skew-symmetric  $\omega$  come from? Newton f = ma law for a motion in a potential is  $m\ddot{q} = -\partial V$ . Rewrite this as a pair of first order ODEs,  $\dot{q} = p/m$ ,  $\dot{p} = -\partial V$ , define the total energy  $H(q,p) = p^2/2m + V(q)$ , and voila, the equation of motion take on the symplectic form (8.3). What makes this important is the fact that the evolution in time (and more generally any canonical transformation) preserves this symplectic structure, as shown in sect. 8.3.1. Another way to put it: a gradient flow  $\dot{x} = -\partial V(x)$  contracts a state space volume into a fixed point. When that happens, V(x) is a 'Lyapunov function', and the equilibrium x = 0 is 'Lyapunov asymptotically stable'. In contrast, the '-' sign in the symplectic action on (q, p) coordinates,  $\dot{p} = -\partial V$  induces a rotation, and conservation of phase-space areas: for a symplectic flow there can be no volume contraction.

Out there there are 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 [23] and Ozorio de Almeida [21]. In a fine overview, Gotay and Isenberg [11] go as far as to claim that all of science will be symplectized, and with continuing mathematicians' deep dive into symplectic geometry, they might well be right. Exposition of sect. 8.2 follows Dragt [5]. There are two conventions in literature for what the integer argument of  $Sp(\cdots)$  stands for: either Sp(D) or Sp(d) (used, for example, in refs. [4, 5]), where D = dof, and d = 2D. As explained in Chapter 13 of ref. [4], symplectic groups are the 'negative dimensional',  $d \rightarrow -d$  sisters of the orthogonal groups, so only the second notation makes sense in the grander scheme of things. Mathematicians can even make sense of the d =odd-dimensional case, see Proctor [9, 24], by dropping the requirement that  $\omega$  is non-degenerate, and defining a symplectic group  $Sp(\mathcal{M}, \omega)$  acting on a vector space  $\mathcal{M}$  as a subgroup of  $Gl(\mathcal{M})$  which preserves a skew-symmetric bilinear form  $\omega$  of

maximal possible rank. The odd symplectic groups Sp(2D + 1) are not semisimple. If you care about group theory for its own sake (the dynamical systems symmetry reduction techniques of chapter 12 are still too primitive to be applicable to Quantum Field Theory), chapter 14 of ref. [4] is fun, too.

Referring to the Sp(d) Lie algebra elements as 'Hamiltonian matrices' as one sometimes does [5, 28] conflicts with what is meant by a 'Hamiltonian matrix' in quantum mechanics: the quantum Hamiltonian sandwiched between vectors taken from any complete set of quantum states. We are not sure where this name comes from; Dragt cites refs. [8, 10], and chapter 17 of his own book in progress [6]. Fulton and Harris [8] use it. Certainly Van Loan [22] uses in 1981, and Taussky in 1972. Might go all the way back to Sylvester?

Dream student Henriette Roux wants to know: "Dynamics equals a Hamiltonian plus a bracket. Why don't you just say it?" A: "It is true that in the tunnel vision of atomic mechanicians the world is Hamiltonian. But it is much more wondrous than that. This chapter starts with Newton 1687: force equals acceleration, and we always replace a higher order time derivative with a set of first order equations. If there are constraints, or fully relativistic Quantum Field Theory is your thing, the tool of choice is to recast Newton equations as a Lagrangian 1788 variational principle. If you still live in material but non-relativistic world and have not gotten beyond Heisenberg 1925, you will find Hamilton's 1827 principal function handy. The question is not whether the world is Hamiltonian - it is not - but why is it so often profitably formulated this way. For Maupertuis 1744 variational principle was a proof of God's existence; for Lagrange who made it mathematics, it was just a trick. Our sect. 37.1.1 "Semiclassical evolution" is an attempt to get inside 17 year old Hamilton's head, but it is quite certain that he did not get to it the way we think about it today. He got to the 'Hamiltonian' by studying optics, where the symplectic structure emerges as the leading WKB approximation to wave optics; higher order corrections destroy it again. In dynamical systems theory, the densities of trajectories are transported by Liouville evolution operators, as explained here in sect. 19.6. Evolution in time is a one-parameter Lie group, and Lie groups act on functions infinitesimally by derivatives. If the evolution preserves additional symmetries, these derivatives have to respect them, and so 'brackets' emerge as a statement of symplectic invariance of the flow. Dynamics with a symplectic structure are just a special case of how dynamics moves densities of trajectories around. Newton is deep, Poisson brackets are technology and thus they appear naturally only by the time we get to chapter 19. Any narrative is of necessity linear, and putting Poisson ahead of Newton [27] would be a disservice to you, the student. But if you insist: Dragt and Habib [5, 7] offer a concise discussion of symplectic Lie operators and their relation to Poisson brackets."

**Remark 8.2.** 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 8.3.** The sign convention of  $\omega$ . The overall sign of  $\omega$ , the symplectic invariant in (8.3), 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. Any finite-dimensional symplectic vector space has a *Darboux basis* such that  $\omega$  takes form (8.6). Dragt [5] convention for phase-space variables is as in (8.2). He calls the dynamical trajectory  $x_0 \to x(x_0, t)$  the 'transfer map', something that we will avoid here, as it conflicts with the well established use of 'transfer matrices' in statistical mechanics.

**Remark 8.4.** Loxodromic quartets. For symplectic flows, real eigenvalues always come paired as  $\Lambda$ ,  $1/\Lambda$ , and complex eigenvalues come either in  $\Lambda$ ,  $\Lambda^*$  pairs,  $|\Lambda| = 1$ , or

 $\Lambda$ ,  $1/\Lambda$ ,  $\Lambda^*$ ,  $1/\Lambda^*$  loxodromic quartets. As most maps studied in introductory nonlinear dynamics are 2d, you have perhaps never seen a loxodromic quartet. How likely are we to run into such things in higher dimensions? According to a very extensive study of periodic orbits of a driven billiard with a four dimensional phase space, carried in ref. [16], the three kinds of eigenvalues occur with about the same likelihood.

**Remark 8.5.** Standard map. Standard maps model free rotors 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 illustrate a number of important features: small k values provide an example of KAM perturbative regime (see ref. [14]), while larger k's illustrate deterministic chaotic transport [3, 18], and the transition to global chaos presents remarkable universality features [12, 13, 25]. The quantum counterpart of this model has been widely investigated, as the first example where phenomena like quantum dynamical localization have been observed [1]. Stability residue was introduced by Greene [12]. For some hands-on experience of the standard map, download Meiss simulation code [19].

**Remark 8.6.** Diagnosing chaos. In sect. 1.3.1 we have stated that a deterministic system exhibits 'chaos' if its orbits are locally unstable (positive Lyapunov exponent) and globally mixing (positive entropy). In sect. 6.2 we shall define Lyapunov exponents and discuss their evaluation, but already at this point it would be handy to have a few quick numerical methods to diagnose chaotic dynamics. Laskar's *frequency analysis* method [15] is useful for extracting quasi-periodic and weakly chaotic regions of state space in Hamiltonian dynamics with many degrees of freedom. For pointers to other numerical methods, see ref. [26].

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**Example 8.1.** Unforced undamped Duffing oscillator. When the damping term is removed from the Duffing oscillator (2.22), the system can be written in Hamiltonian form,

$$H(q,p) = \frac{p^2}{2} - \frac{q^2}{2} + \frac{q^4}{4}.$$
 (8.25)

This is a 1-dof Hamiltonian system, with a 2-dimensional state space, the plane (q, p). The Hamilton's equations (8.1) are

$$\dot{q} = p \,, \qquad \dot{p} = q - q^3 \,. \tag{8.26}$$

For 1-dof systems, the 'surfaces' of constant energy (8.5) are curves that stratify the phase plane (q, p), and the dynamics is very simple: the curves of constant energy *are* the trajectories, as shown in figure 8.1.

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**Example 8.2.** Collinear helium. In the quantum chaos part of ChaosBook.org 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

$$H = \frac{1}{2}p_1^2 + \frac{1}{2}p_2^2 - \frac{2}{r_1} - \frac{2}{r_2} + \frac{1}{r_1 + r_2}.$$
 (8.27)

Collinear helium has 2 dof, and thus a 4-dimensional phase space  $\mathcal{M}$ , which energy conservation stratified by 3-dimensional constant energy hypersurfaces. In order to visualize it, we often project the dynamics onto the 2-dimensional configuration plane, the  $(r_1, r_2)$ ,  $r_i \geq 0$  quadrant, figure 8.2. 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. The difference is that in such *projection* we see the flow from an arbitrary perspective, with trajectories crisscrossing. In a *Poincaré section* the flow is decomposed into intrinsic coordinates, a pair along the marginal stability time and energy directions, and the rest transverse, revealing the phase-space structure of the flow.

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**Example 8.3. Symplectic form for** D = 2**.** For two degrees of freedom the phase space is 4-dimensional,  $x = (q_1, q_2, p_1, p_2)$ , and the symplectic 2-form is

$$\omega = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix},\tag{8.28}$$

The symplectic bilinear form  $\langle x^{(1)}|x^{(2)}\rangle$  is the sum over the areas of the parallelepipeds spanned pairwise by components of the two vectors,

$$\langle x^{(1)}|x^{(2)}\rangle = (x^{(1)})^{\top}\omega \, x^{(2)} = (q_1^{(1)}p_1^{(2)} - q_1^{(2)}p_1^{(1)}) + (q_2^{(1)}p_2^{(2)} - q_2^{(2)}p_2^{(1)}) \,. \tag{8.29}$$

It is this sum over oriented areas (not the Euclidean distance between the two vectors,  $|x^{(2)} - x^{(1)}|$ ) that is preserved by the symplectic transformations.

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**Example 8.4. Hamiltonian flows are canonical.** For Hamiltonian flows it follows from (8.14) that  $\frac{d}{dt}(J^{\top}\omega J) = 0$ , and since at the initial time  $J^0(x_0) = 1$ , Jacobian matrix is a symplectic transformation (8.6). 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 (8.6): For notational brevity here we have suppressed the dependence on time

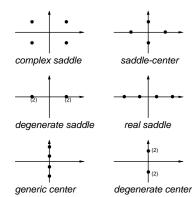


Figure 8.4: Stability exponents of a Hamiltonian equilibrium point, 2-dof.

and the initial point,  $J = J'(x_0)$ . By elementary properties of determinants it follows from (8.6) that Hamiltonian flows are phase-space volume preserving,  $|\det J| = 1$ . The initial condition (4.10) for J is  $J^0 = 1$ , so one always has

$$\det J = +1. \tag{8.30}$$

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**Example 8.5.** Hamiltonian Hénon map, reversibility. By (4.45) the Hénon map (3.18) for b = -1 value is the simplest 2-dimensional orientation preserving areapreserving map, often studied to better understand topology and symmetries of Poincaré sections of 2 dof Hamiltonian flows. We find it convenient to multiply (3.19) 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

$$x_{i+1} + x_{i-1} = a - x_i^2, \quad i = 1, ..., n_p,$$
 (8.31)

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

$$x_{n+1} = a - x_n^2 - y_n$$
  

$$y_{n+1} = x_n.$$
 (8.32)

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.

exercise 9.7 click to return: p. 144

**Example 8.6. 2-dimensional symplectic maps.** In the 2-dimensional case the eigenvalues (5.5) depend only on tr  $M^t$ 

$$\Lambda_{1,2} = \frac{1}{2} \left( \text{tr} \, M^t \pm \sqrt{(\text{tr} \, M^t - 2)(\text{tr} \, M^t + 2)} \right). \tag{8.33}$$

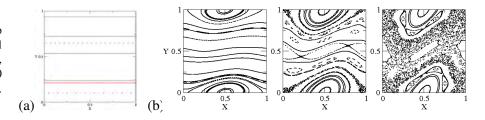
Greene's residue criterion states that the orbit is (i) elliptic if the *stability residue*  $|\text{tr } M^t|$  –  $2 \le 0$ , with complex eigenvalues  $\Lambda_1 = e^{i\theta t}$ ,  $\Lambda_2 = \Lambda_1^* = e^{-i\theta t}$ . If  $|\text{tr } M^t| - 2 > 0$ ,  $\lambda$  is real, and the trajectory is either

(ii) hyperbolic 
$$\Lambda_1 = e^{\lambda t}$$
,  $\Lambda_2 = e^{-\lambda t}$ , or (8.34)   
erse hyperbolic  $\Lambda_1 = -e^{\lambda t}$ ,  $\Lambda_2 = -e^{-\lambda t}$ . (8.35)

(iii) inverse hyperbolic 
$$\Lambda_1 = -e^{\lambda t}$$
,  $\Lambda_2 = -e^{-\lambda t}$ . (8.35)

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**Figure 8.5:** Phase portrait for the standard map for (a) k = 0: symbols denote periodic orbits, full lines represent quasiperiodic orbits. (b) k = 0.3, k = 0.85 and k = 1.4: each plot consists of 20 random initial conditions, each iterated 400 times.



**Example 8.7. Standard map.** Given a smooth function g(x), the map

$$x_{n+1} = x_n + y_{n+1} y_{n+1} = y_n + g(x_n)$$
(8.36)

is an area-preserving map. The corresponding nth iterate Jacobian matrix (4.21) is

$$M^{n}(x_{0}, y_{0}) = \prod_{k=n}^{1} \begin{bmatrix} 1 + g'(x_{k}) & 1 \\ g'(x_{k}) & 1 \end{bmatrix}.$$
 (8.37)

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 (8.36)  $mod\ 1$  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

$$x_{n+1} = x_n + y_0 = x_0 + (n+1)y_0 \mod 1$$
.

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 8.5 (a)).

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 8.5 (a), while, when k is sufficiently large, single trajectories wander erratically on a large fraction of the phase space, as in figure 8.5 (b).

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

Note that the map (8.36) provides a stroboscopic view of the flow generated by a (time-dependent) Hamiltonian

$$H(x, y; t) = \frac{1}{2}y^2 + G(x)\delta_1(t)$$
(8.38)

where  $\delta_1$  denotes the periodic delta function

$$\delta_1(t) = \sum_{m=-\infty}^{\infty} \delta(t-m) \tag{8.39}$$

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and

$$G'(x) = -g(x). (8.40)$$

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:

$$R_{P/Q} = \frac{1}{4} (2 - \operatorname{tr} M_{P/Q})$$
 (8.41)

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.

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.

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### **Exercises**

8.1. **Complex nonlinear Schrödinger equation.** Consider the complex nonlinear Schrödinger equation in one spatial dimension [17]:

$$i\frac{\partial \phi}{\partial t} + \frac{\partial^2 \phi}{\partial x^2} + \beta \phi |\phi|^2 = 0, \quad \beta \neq 0.$$

(a) Show that the function  $\psi: \mathbb{R} \to \mathbb{C}$  defining the traveling wave solution  $\phi(x,t) = \psi(x-ct)$  for c>0 satisfies a second-order complex differential equation equivalent to a Hamiltonian system in  $\mathbb{R}^4$  relative to the noncanonical symplectic form whose matrix is given by

$$w_c = \left[ \begin{array}{cccc} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -1 & 0 & 0 & -c \\ 0 & -1 & c & 0 \end{array} \right].$$

- (b) Analyze the equilibria of the resulting Hamiltonian system in  $\mathbb{R}^4$  and determine their linear stability properties.
- (c) Let  $\psi(s) = e^{ics/2}a(s)$  for a real function a(s) and determine a second order equation for a(s). Show

- that the resulting equation is Hamiltonian and has heteroclinic orbits for  $\beta$  < 0. Find them.
- (d) Find 'soliton' solutions for the complex nonlinear Schrödinger equation.

(Luz V. Vela-Arevalo)

- 8.2. **Symplectic** *vs.* **Hamiltonian matrices.** In the language of group theory, symplectic matrices form the symplectic Lie group Sp(d), while the Hamiltonian matrices form the symplectic Lie algebra sp(d), or the algebra of generators of infinitesimal symplectic transformations. This exercise illustrates the relation between the two:
  - (a) Show that if a constant matrix A satisfy the Hamiltonian matrix condition (8.9), then  $J(t) = \exp(tA)$ ,  $t \in \mathbb{R}$ , satisfies the symplectic condition (8.6), i.e., J(t) is a symplectic matrix.
  - (b) Show that if matrices  $\mathbf{T}_a$  satisfy the Hamiltonian matrix condition (8.9), then  $g(\phi) = \exp(\phi \cdot \mathbf{T})$ ,  $\phi \in \mathbb{R}^N$ , satisfies the symplectic condition (8.6), i.e.,  $g(\phi)$  is a symplectic matrix.

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(A few hints: (i) expand  $\exp(A)$ ,  $A = \phi \cdot \mathbf{T}$ , as a power series in A. Or, (ii) use the linearized evolution equation (8.13).

#### 8.3. When is a linear transformation canonical?

- (a) Let *A* be a  $[n \times n]$  invertible matrix. Show that the map  $\phi : \mathbb{R}^{2n} \to \mathbb{R}^{2n}$  given by  $(\mathbf{q}, \mathbf{p}) \mapsto (A\mathbf{q}, (A^{-1})^{\mathsf{T}}\mathbf{p})$  is a canonical transformation.
- (b) If **R** is a rotation in  $\mathbb{R}^3$ , show that the map  $(\mathbf{q}, \mathbf{p}) \mapsto (\mathbf{R} \mathbf{q}, \mathbf{R} \mathbf{p})$  is a canonical transformation.

(Luz V. Vela-Arevalo)

- 8.4. **Determinants of symplectic matrices.** Show that the determinant of a symplectic matrix is +1, by going through the following steps:
  - (a) use (8.21) to prove that for eigenvalue pairs each member has the same multiplicity (the same holds for quartet members),
  - (b) prove that the *joint* multiplicity of  $\lambda = \pm 1$  is even,
  - (c) show that the multiplicities of  $\lambda = 1$  and  $\lambda = -1$  cannot be both odd. Hint: write

$$P(\lambda) = (\lambda - 1)^{2m+1} (\lambda + 1)^{2l+1} Q(\lambda)$$

and show that Q(1) = 0.

8.5. **Cherry's example.** What follows refs. [2, 20] is mostly a reading exercise, about a Hamiltonian system that is *linearly stable* but *nonlinearly unstable*. Consider the Hamiltonian system on  $\mathbb{R}^4$  given by

$$H = \frac{1}{2}(q_1^2 + p_1^2) - (q_2^2 + p_2^2) + \frac{1}{2}p_2(p_1^2 - q_1^2) - q_1q_2p_1.$$

- (a) Show that this system has an equilibrium at the origin, which is linearly stable. (The linearized system consists of two uncoupled oscillators with frequencies in ratios 2:1).
- (b) Convince yourself that the following is a family of solutions parameterize by a constant  $\tau$ :

$$q_1 = -\sqrt{2} \frac{\cos(t-\tau)}{t-\tau}, \quad q_2 = \frac{\cos 2(t-\tau)}{t-\tau},$$
  
$$p_1 = \sqrt{2} \frac{\sin(t-\tau)}{t-\tau}, \quad p_2 = \frac{\sin 2(t-\tau)}{t-\tau}.$$

These solutions clearly blow up in a finite time; however they start at t=0 at a distance  $\sqrt{3}/\tau$  from the origin, so by choosing  $\tau$  large, we can find solutions starting arbitrarily close to the origin, yet going to infinity in a finite time, so the origin is *nonlinearly unstable*.

(Luz V. Vela-Arevalo)