Chapter 7

Get straight

A Hamiltonian system is said to be "integrable" if one can find a change of coordinates to an action-angle coordinate frame where the phase space dynamics is described by motion on circles, one circle for each degree of freedom. In the same spirit, a natural description of a hyperbolic, unstable flow would be attained if one found a change of coordinates into a frame where the stable/unstable manifolds are straight lines, and the flow is along hyperbolas. Achieving this globally for anything but a handful of contrived examples is too much to hope for. Still, as we shall now show, we can make some headway on straightening out the flow locally.

Even though such nonlinear coordinate transformations are very important, especially in celestial mechanics, we shall not necessarily use them much in what follows, so you can safely skip this chapter on the first reading. Except, perhaps, you might want to convince yourself that cycle stabilities are indeed metric invariants of flows (sect. 8.5), and you might like transformations that turn a Keplerian ellipse into a harmonic oscillator (example 7.2) and regularize the 2-body Coulomb collisions (sect. 7.3) in classical helium.

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7.1 Changing coordinates

Problems are handed down to us in many shapes and forms, and they are not always expressed in the most convenient way. In order to simplify a given problem, one may stretch, rotate, bend and mix the coordinates, but in doing so, the vector field will also change. The vector field lives in a (hyper)plane tangent to phase space and changing the coordinates of phase space affects the coordinates of the tangent space as well, in a way that we will now describe.

Denote by h the *conjugation function* which maps the coordinates of the

initial phase space $\mathcal{M}$ into the reparametrized phase space $\mathcal{M}' = h(\mathcal{M})$, with a point $x \in \mathcal{M}$ related to a point $y \in \mathcal{M}'$ by $y = h(x)$. The change of coordinates must be one-to-one and span both $\mathcal{M}$ and $\mathcal{M}'$, so given any point y we can go back to $x = h^{-1}(y)$. For smooth flows the reparametrized dynamics should support the same number of derivatives as the initial one. If h is a (piecewise) analytic function, we refer to h as a *smooth conjugacy*.

The evolution rule $g^t(y_0)$ on $\mathcal{M}'$ can be computed from the evolution rule $f^t(x_0)$ on $\mathcal{M}$ by taking the initial point $y_0 \in \mathcal{M}'$, going back to $\mathcal{M}$, evolving, and then mapping the final point $x(t)$ back to $\mathcal{M}'$:

$$y(t) = g^t(y_0) = h \circ f^t \circ h^{-1}(y_0)\,. \tag{7.1}$$

Here "$\circ$" stands for functional composition $h \circ f(x) = h(f(x))$, so (7.1) is a shorthand for $y(t) = h(f^t(h^{-1}(y_0)))$.

The vector field $\dot{x} = v(x)$ in $\mathcal{M}$, locally tangent to the flow f^t, is related to the flow by differentiation (2.4) along the trajectory. The vector field $\dot{y} = w(y)$ in $\mathcal{M}'$, locally tangent to g^t follows by the chain rule:

$$\begin{aligned} w(y) &= \frac{dg^t}{dt}(y)\Big|_{t=0} = \frac{d}{dt}\left(h \circ f^t \circ h^{-1}(y)\right)\Big|_{t=0} \\ &= h'(h^{-1}(y))v(h^{-1}(y)) = h'(x)v(x)\,. \end{aligned} \tag{7.2}$$

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With the indices reinstated, this stands for

$$w_i(y) = \frac{\partial h_i(x)}{\partial x_j} v_j(x)\,, \qquad y_i = h_i(x)\,. \tag{7.3}$$

Imagine that the phase space is a rubber sheet with the flow lines drawn on it. A coordinate change h corresponds to pulling and tugging on the rubber sheet smoothly, without cutting, glueing, or self-intersections of the distorted rubber sheet. Trajectories that are closed loops in $\mathcal{M}$ will remain closed loops in the new manifold $\mathcal{M}'$, but their shapes will change. Globally h deforms the rubber sheet in a highly nonlinear manner, but locally it simply rescales and shears the tangent field by $\partial_j h_i$, hence the simple transformation law (7.2) for the velocity fields.

The time itself is a parametrization of points along flow lines, and it can also be reparametrized, $s = s(t)$, with the attendent modification of (7.2). An example is the 2-body collision regularization of the helium Hamiltonian (5.6), to be undertaken in sect. 7.3 below.

7.2 Rectification of flows

A profitable way to exploit invariance of dynamics under smooth conjugacies is to use it to pick out the simplest possible representative of an

equivalence class. In general and globally these are just words, as we have no clue how to pick such "canonical" representative, but for smooth flows we can always do it localy and for sufficiently short time, by appealing to the *rectification theorem*, a fundamental theorem of ordinary differential equations. The theorem assures us that there exists a solution (at least for a short time interval) and what the solution looks like. The rectification theorem holds in the neighborhood of points of the vector field $v(x)$ that are not singular, that is, everywhere except for the equilibrium points (2.7), and points at which v is infinite. According to the theorem, in a small neighborhood of a non-singular point there exists a change of coordinates $y = h(x)$ such that $\dot{x} = v(x)$ in the new coordinates takes the standard form

$$\begin{aligned} \dot{y}_1 &= 1 \\ \dot{y}_2 = \dot{y}_3 &= \cdots = \dot{y}_d = 0\,, \end{aligned} \tag{7.4}$$

with unit velocity flow along y_1, and no flow along any of the remaining directions.

Example 7.1 Harmonic oscillator, rectified: *As a simple example of global rectification of a flow consider the harmonic oscillator*

$$\dot{q} = p\,, \qquad \dot{p} = -q\,. \tag{7.5}$$

The trajectories $x(t) = (q(t), p(t))$ just go around the origin, so a fair guess is that the system would have a simpler representation in polar coordinates $y = (r, \theta)$:

$$h^{-1} : \left\{ \begin{array}{rcl} q &=& h_1^{-1}(r,\theta) = r\cos\theta \\ p &=& h_2^{-1}(r,\theta) = r\sin\theta \end{array} \right. . \tag{7.6}$$

The Jacobian matrix of the transformation is

$$h' = \begin{bmatrix} \cos\theta & \sin\theta \\ -\dfrac{\sin\theta}{r} & -\dfrac{\cos\theta}{r} \end{bmatrix} \tag{7.7}$$

resulting in (7.2) of rectified form

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$$\dot{r} = 0\,, \qquad \dot{\theta} = -1\,. \tag{7.8}$$

In the new coordinates the radial coordinate r is constant, and the angular coordinate θ wraps around a cylinder with constant angular velocity. There is a subtle point in this change of coordinates: the domain of the map h^{-1} is not the plane $\mathbb{R}^2$, but rather the plane minus the origin. We had mapped a plane into a cylinder, and coordinate transformations should not change the topology of the space in which the dynamics takes place; the coordinate transformation is not defined on the equilibrium point $x = (0, 0)$, or $r = 0$.

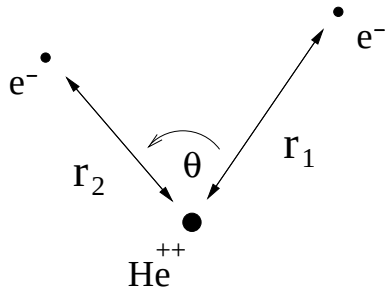

Figure 7.1: Coordinates for the helium three body problem in the plane.

7.3 Classical dynamics of collinear helium

(G. Tanner)

So far much has been said about 1-dimensional maps, game of pinball and other curious but rather idealized dynamical systems. If you have become impatient and started wondering what good are the methods learned so far in solving real life physical problems, good news are here. We will apply here concepts of nonlinear dynamics to nothing less than the helium, a dreaded three-body Coulomb problem.

Can we really jump from three static disks directly to three charged particles moving under the influence of their mutually attracting or repelling forces? It turns out, we can, but we have to do it with care. The full problem is indeed not accessible in all its detail, but we are able to analyze a somewhat simpler subsystem – collinear helium. This system plays an important role in the classical and quantum dynamics of the full three-body problem.

The classical helium system consists of two electrons of mass m_e and charge $-e$ moving about a positively charged nucleus of mass m_{he} and charge $+2e$.

The helium electron-nucleus mass ratio $m_{he}/m_e = 1836$ is so large that we may work in the infinite nucleus mass approximation $m_{he} = \infty$, fixing the nucleus at the origin. Finite nucleus mass effects can be taken into account without any substantial difficulty. We are now left with two electrons moving in three spatial dimensions around the origin. The total angular momentum of the combined electron system is still conserved. In the special case of angular momentum $L = 0$, the electrons move in a fixed plane containing the nucleus. The three body problem can then be written in terms of three independent coordinates only, the electron-nucleus distances r_1 and r_2 and the inter-electron angle Θ, see figure 7.1.

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This looks like something we can lay our hands on; the problem has been reduced to three degrees of freedom, six phase space coordinates in all, and the total energy is conserved. But let us go one step further; the electrons are attracted by the nucleus but repelled by each other. They will tend to stay as far away from each other as possible, preferably on opposite sides of the nucleus. It is thus worth having a closer look at the situation where the three particles are all on a line with the nucleus being

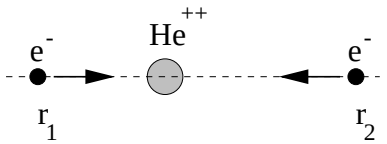

Figure 7.2: Collinear helium, with the two electrons on opposite sides of the nucleus.

somewhere between the two electrons. If we, in addition, let the electrons have momenta pointing towards the nucleus as in figure 7.2, then there is no force acting on the electrons perpendicular to the common interparticle axis. That is, if we start the classical system on the dynamical subspace $\Theta = \pi$, $\frac{d}{dt}\Theta = 0$, the three particles will remain in this *collinear configuration* for all times.

7.3.1 Scaling

In what follows we will restrict the dynamics to this collinear subspace. It is a system of two degrees of freedom with the Hamiltonian

$$H = \frac{1}{2m_e}\left(p_1^2 + p_2^2\right) - \frac{2e^2}{r_1} - \frac{2e^2}{r_2} + \frac{e^2}{r_1 + r_2} = E\,, \tag{7.9}$$

where E is the total energy. As the dynamics is restricted to the fixed energy shell, the four phase space coordinates are not independent; the energy shell dependence can be made explicit by writing $(r_1, r_2, p_1, p_2) \to (r_1(E), r_2(E), p_1(E), p_2(E))$.

We will first consider the dependence of the dynamics on the energy E. A simple analysis of potential versus kinetic energy tells us that if the energy is positive both electrons can escape to $r_i \to \infty$, $i = 1, 2$. More interestingly, a single electron can still escape even if E is negative, carrying away an unlimited amount of kinetic energy, as the total energy of the remaining inner electron has no lower bound. Not only that, but one electron *will* escape eventually for almost all starting conditions. The overall dynamics thus depends critically on whether $E > 0$ or $E < 0$. But how does the dynamics change otherwise with varying energy? Fortunately, not at all. Helium dynamics remains invariant under a change of energy up to a simple scaling transformation; a solution of the equations of motion at a fixed energy $E_0 = -1$ can be transformed into a solution at an arbitrary energy $E < 0$ by scaling the coordinates as

$$r_i(E) = \frac{e^2}{(-E)}\, r_i, \quad p_i(E) = \sqrt{-m_e E}\, p_i, \quad i = 1, 2\,,$$

together with a time transformation $t(E) = e^2 m_e^{1/2} (-E)^{-3/2}\, t$. We include the electron mass and charge in the scaling transformation in order to obtain a non–dimensionalized Hamiltonian of the form

$$H = \frac{p_1^2}{2} + \frac{p_2^2}{2} - \frac{2}{r_1} - \frac{2}{r_2} + \frac{1}{r_1 + r_2} = -1\,. \tag{7.10}$$

The case of negative energies chosen here is the most interesting one for us. It exhibits chaos, unstable periodic orbits and is responsible for the bound states and resonances of the quantum problem treated in sect. 34.5.

7.3.2 Regularization of two–body collisions

Next, we have a closer look at the singularities in the Hamiltonian (7.10). Whenever two bodies come close to each other, accelerations become large, numerical routines require lots of small steps, and numerical precision suffers. No numerical routine will get us through the singularity itself, and in collinear helium electrons have no option but to collide with the nucleus. Hence a *regularization* of the differential equations of motions is a necessary prerequisite to any numerical work on such problems, both in celestial mechanics (where a spaceship executes close approaches both at the start and its destiantion) and in quantum mechanics (where much of semiclassical physics is dominated by returning classical orbits that probe the quantum wave function at the nucleus).

There is a fundamental difference between two–body collisions $r_1 = 0$ or $r_2 = 0$, and the triple collision $r_1 = r_2 = 0$. Two–body collisions can be regularized, with the singularities in equations of motion removed by a suitable coordinate transformation together with a time transformation preserving the Hamiltonian structure of the equations. Such regularization is not possible for the triple collision, and solutions of the differential equations can not be continued through the singularity at the origin. As we shall see, the chaos in collinear helium originates from this singularity of triple collisions.

A regularization of the two–body collisions is achieved by means of the Kustaanheimo–Stiefel (KS) transformation, which consists of a coordinate dependent time transformation which stretches the time scale near the origin, and a canonical transformation of the phase space coordinates. In order to motivate the method, we apply it first to the 1-dimensional Kepler problem

☞ remark 34.1

$$H = \frac{1}{2}p^2 - \frac{2}{x} = E\,. \tag{7.11}$$

Example 7.2 Keplerian ellipse, rectified: *To warm up, consider the $E = 0$ case, starting at $x = 0$ at $t = 0$. Even though the equations of motion are singular at the intial point, we can immediately integrate*

$$\frac{1}{2}\dot{x}^2 - \frac{2}{x} = 0$$

by means of separation of variables

$$\sqrt{x}dx = \sqrt{2}dt\,, \qquad x = (3t)^{\frac{2}{3}}\,, \tag{7.12}$$

and observe that the solution is not singular. The aim of regularization is to compensate for the infinite acceleration at the origin by introducing a fictitious time, in terms of which the passage through the origin is smooth.

A time transformation $dt = f(q,p)d\tau$ for a system described by a Hamiltonian $H(q,p) = E$ leaves the Hamiltonian structure of the equations of motion unaltered, if the Hamiltonian itself is transformed into $\mathcal{H}(q,p) = f(q,p)(H(q,p) - E)$. For the 1–dimensional Coulomb problem with (7.11) we choose the time transformation $dt = xd\tau$ which lifts the $|x| \to 0$ singularity in (7.11) and leads to a new Hamiltonian

$$\mathcal{H} = \frac{1}{2}xp^2 - 2 - Ex = 0. \tag{7.13}$$

The solution (7.12) is now parametrized by the fictitous time $d\tau$ through a pair of equations

$$x = \tau^2\,, \qquad t = \frac{1}{3}\tau^3\,.$$

The equations of motion are, however, still singular as $x \to 0$:

$$\frac{d^2x}{d\tau^2} = -\frac{1}{2x}\frac{dx}{d\tau} + xE\,.$$

Appearance of the square root in (7.12) now suggests a canonical transformation of form

$$x = Q^2\,, \quad p = \frac{P}{2Q} \tag{7.14}$$

which maps the Kepler problem into that of a harmonic oscillator with Hamiltonian

$$H(Q,P) = \frac{1}{8}P^2 - EQ^2 = 2, \tag{7.15}$$

with all singularities completely removed.

We now apply this method to collinear helium. The basic idea is that one seeks a higher-dimensional generalization of the "square root removal" trick (7.14), by introducing a new vector Q with property $r = |Q|^2$. In this simple 1-dimensional example the KS transformation can be implemented by

$$r_1 = Q_1^2\,, \qquad r_2 = Q_2^2\,, \qquad p_1 = \frac{P_1}{2Q_1}\,, \qquad p_2 = \frac{P_2}{2Q_2} \tag{7.16}$$

and reparametrization of time by $d\tau = dt/r_1r_2$. The singular behavior in the original momenta at r_1 or $r_2 = 0$ is again compensated by stretching the time scale at these points. The Hamiltonian structure of the equations of motions with respect to the new time τ is conserved, if we consider the Hamiltonian

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$$H_{ko} = \frac{1}{8}(Q_2^2P_1^2 + Q_1^2P_2^2) - 2R_{12}^2 + Q_1^2Q_2^2(-E + 1/R_{12}^2) = 0 \tag{7.17}$$

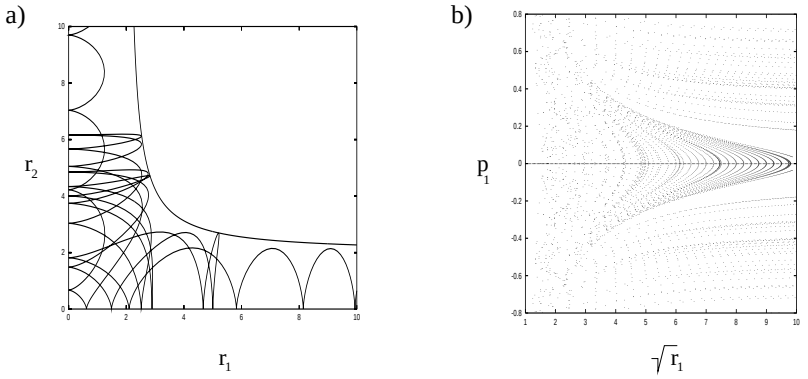

Figure 7.3: (a) A typical trajectory in the r_1 – r_2 plane; the trajectory enters here along the r_1 axis and escapes to infinity along the r_2 axis; (b) Poincaré map (r_2=0) for collinear helium. Strong chaos prevails for small r_1 near the nucleus.

with $R_{12} = (Q_1^2 + Q_2^2)^{1/2}$, and we will take $E = -1$ in what follows. The equations of motion now have the form

$$\dot{P}_1 = 2Q_1\left[2 - \frac{P_2^2}{8} - Q_2^2\left(1 + \frac{Q_2^2}{R_{12}^4}\right)\right]; \qquad \dot{Q}_1 = \frac{1}{4}P_1 Q_2^2 \tag{7.18}$$
$$\dot{P}_2 = 2Q_2\left[2 - \frac{P_1^2}{8} - Q_1^2\left(1 + \frac{Q_1^2}{R_{12}^4}\right)\right]; \qquad \dot{Q}_2 = \frac{1}{4}P_2 Q_1^2.$$

Individual electron–nucleus collisions at $r_1 = Q_1^2 = 0$ or $r_2 = Q_2^2 = 0$ no longer pose a problem to a numerical integration routine. The equations (7.18) are singular only at the triple collision $R_{12} = 0$, that is, when both electrons hit the nucleus at the same time.

The new coordinates and the Hamiltonian (7.17) are very useful when calculating trajectories for collinear helium; they are, however, less intuitive as a visualization of the three-body dynamics. We will therefore refer to the old coordinates r_1, r_2 when discussing the dynamics and the periodic orbits.

To summarize, we have brought a 3-body problem into a form where the 2-body collisions have been transformed away, and the phase space trajectories computable numerically. To appreciate the full beauty of what has been attained, you have to fast-forward to chapter 34; we are already "almost" ready to quantize helium by semiclassical methods.

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7.4 Rectification of maps

In sect. 7.2 we had argued that nonlinear coordinate transformations can be profitably employed to simplify the representation of a flow. We

shall now apply the same idea to nonlinear maps, and determine a smooth nonlinear change of coordinates that flattens out the vicinity of a fixed point and makes the map *linear* in an open neighborhood. In its simplest form the idea can be implemented only for an isolated nondegenerate fixed point (otherwise are needed in the normal form expansion around the point), and only in a finite neigborhood of a point, as the conjugating function in general has a finite radius of convergence. In sect. 8.4 we will extend the method to periodic orbits.

7.4.1 Rectification of a fixed point in one dimension

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Consider a 1-dimensional map $x_{n+1} = f(x_n)$ with a fixed point at $x = 0$, with stability $\Lambda = f'(0)$. If $|\Lambda| \neq 1$, one can determine term-by-term the power series for a smooth conjugation $h(x)$ centered at the fixed point, $h(0) = 0$, that flattens out the neighborhood of the fixed point

$$f(x) = h^{-1}(\Lambda h(x)) \tag{7.19}$$

and replaces the nonlinear map $f(x)$ by a *linear* map $y_{n+1} = \Lambda y_n$.

To compute the conjugation h we use the functional equation $h^{-1}(\Lambda x) = f(h^{-1}(x))$ and the expansions

$$\begin{aligned} f(x) &= \Lambda x + x^2 f_2 + x^3 f_3 + \dots \\ h^{-1}(x) &= x + x^2 h_2 + x^3 h_3 + \dots \ . \end{aligned} \tag{7.20}$$

Equating the coefficients of x^k on both sides of the functional equation yields h_k order by order as a function of f_2, $f_3, \dots$. If $h(x)$ is a conjugation, so is any scaling $h(bx)$ of the function for a real number b. Hence the value of $h'(0)$ is not determined by the functional equation (7.19); it is convenient to set $h'(0) = 1$.

The algebra is not particularly illuminating and best left to computers. In any case, for the time being we will not use much beyond the first, linear term in these expansions.

Here we assume $\Lambda \neq 1$. If the fixed point has first $k-1$ derivatives vanishing, the conjugacy is to the kth *normal form*.

In several dimensions, Λ is replaced by the Jacobian matrix, and one has to check that the eigenvalues $\mathbf{J}$ are non-resonant, that is, there is no integer linear relation between the stability exponents (8.4).

Commentary

Remark 7.1 Rectification of maps. The methods outlined above are standard in the analysis of fixed points and construction of normal forms for bifurcations,

see for example ref. [1.14, 7.2, 7.4, 7.5, 7.6, 7.7, 7.8, 7.9, 3.6]. The geometry underlying such methods is pretty, and we enjoyed reading, for example, Percival and Richards [7.10], chaps. 2 and 4 of Ozorio de Almeida's monograph [7.11], and, as always, Arnol'd [7.1].

Recursive formulas for evaluation of derivatives needed to evaluate (7.20) are given, for example, in Appendix A of ref. [9.5]).

Résumé

Dynamics $(\mathcal{M}, f)$ is invariant under the group of all smooth conjugacies

$$(\mathcal{M}, f) \;\to\; (\mathcal{M}', g) = (h(\mathcal{M}), h \circ f \circ h^{-1})\,.$$

This invariance can be used to (i) find a simplified representation for the flow and (ii) identify a set of invariants, numbers computed within a particular choice of $(\mathcal{M}, f)$, but invariant under all $\mathcal{M} \to h(\mathcal{M})$ smooth conjugacies.

The $2D$-dimensional phase space of an integrable Hamiltonian system of D degrees of freedom is fully foliated by D-tori. In the same spirit, for a uniformly hyperbolic, chaotic dynamical system one would like to change into a coordinate frame where the stable/unstable manifolds form a set of transversally interesecting hyper-planes, with the flow everywhere locally hyperbolic. That cannot be achieved in general: Fully globally integrable and fully globally chaotic flows are a very small subset of all possible flows, a "set of measure zero" in the world of all dynamical systems.

What we *really* care about is developping invariant notions of what a given dynamical system is. The totality of smooth one-to-one nonlinear coordinate transformations h which map all trajectories of a given dynamical system $(\mathcal{M}, f^t)$ onto all trajectories of dynamical systems $(\mathcal{M}', g^t)$ gives us a huge equivalence class, much larger than the equivalence classes familiar from the theory of linear transformations, such as the rotation group $O(d)$ or the Galilean group of all rotations and translations in $\mathbb{R}^d$. In the theory of Lie groups, the full invariant specification of an object is given by a finite set of Casimir invariants. What a good full set of invariants for a group of general nonlinear smooth conjugacies might be is not known, but the set of all periodic orbits and their stability eigenvalues will turn out to be a good start.

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