Go with the flow

Poetry is what is lost in translation.
Robert Frost

(R. Mainieri, P. Cvitanović and E.A. Spiegel)

We start out with a recapitulation of the basic notions of dynamics. Our aim is narrow; we keep the exposition focused on prerequisites to the applications to be developed in this text. We assume that the reader is familiar with dynamics on the level of the introductory texts mentioned in Section ??, and concentrate here on developing intuition about what a dynamical system can do. It will be a coarse brush sketch—a full description of all possible behaviors of dynamical systems is beyond human ken. Anyway, for a novice there is no shortcut through this lengthy detour; a sophisticated traveler might prefer to skip this well-trodden territory and embark upon the journey at Chapter ??.

fast track:
Chapter ??, p. ??

2.1 Dynamical systems

In a dynamical system we observe the world as a function of time. We express our observations as numbers and record how they change with time; given sufficiently detailed information and understanding of the underlying natural laws, we see the future in the present as in a mirror. The motion of the planets against the celestial firmament provides an example. Against the daily motion of the stars from East to West, the planets distinguish themselves by moving among the fixed stars. Ancients discovered that by knowing a sequence of planet’s positions—latitudes and longitudes—its future position could be predicted.

For the solar system, tracking the latitude and longitude in the celestial sphere suffices to completely specify the planet’s apparent motion. All possible values for positions and velocities of the planets form the phase space of the system. More generally, a state of a physical system, at a given instant in time, can be represented by a single point in an abstract space called state space or phase space $\mathcal{M}$. As the system changes, so does the representative point in state space. We refer to the evolution of such points as dynamics, and the function $f^t$ which specifies where the representative point is at time $t$ as the evolution rule.

If there is a definite rule $f$ that tells us how this representative point
moves in $\mathcal{M}$, the system is said to be deterministic. For a deterministic
dynamical system, the evolution rule takes one point of the state space
and maps it into exactly one point. However, this is not always possible.
For example, knowing the temperature today is not enough to predict
the temperature tomorrow; knowing the value of a stock today will not
determine its value tomorrow. The state space can be enlarged, in the
hope that in a sufficiently large state space it is possible to determine an
evolution rule, so we imagine that knowing the state of the atmosphere,
measured over many points over the entire planet should be sufficient to
determine the temperature tomorrow. Even that is not quite true, and
we are less hopeful when it comes to stocks.

For a deterministic system almost every point has a unique future,
so trajectories cannot intersect. We say ‘almost’ because there might
exist a set of measure zero (tips of wedges, cusps, etc.) for which a
trajectory is not defined. We may think such sets a nuisance, but it is
quite the contrary—they will enable us to partition state space, so that
the dynamics can be better understood.

Locally, the state space $\mathcal{M}$ looks like $\mathbb{R}^d$, meaning that $d$ numbers
are sufficient to determine what will happen next. Globally, it may be a
more complicated manifold formed by patching together several pieces of
$\mathbb{R}^d$, forming a torus, a cylinder, or some other geometric object. When
we need to stress that the dimension $d$ of $\mathcal{M}$ is greater than one, we may
refer to the point $x \in \mathcal{M}$ as $x_i$ where $i = 1, 2, 3, \ldots, d$. The evolution
rule $f^t : \mathcal{M} \rightarrow \mathcal{M}$ tells us where a point $x$ is in $\mathcal{M}$ after a time interval
$t$.

The pair $(\mathcal{M}, f)$ constitute a dynamical system.

The dynamical systems we will be studying are smooth. This is
expressed mathematically by saying that the evolution rule $f^t$ can be
differentiated as many times as needed. Its action on a point $x$ is sometimes
indicated by $f(x, t)$ to remind us that $f$ is really a function of two
variables: the time and a point in state space. Note that time is relative
rather than absolute, so only the time interval is necessary. This follows
from the fact that a point in state space completely determines all fu-
ture evolution, and it is not necessary to know anything else. The time
parameter can be a real variable $(t \in \mathbb{R})$, in which case the evolution is
called a flow, or an integer $(t \in \mathbb{Z})$, in which case the evolution advances
in discrete steps in time, given by iteration of a map. Actually, the
evolution parameter need not be the physical time; for example, a time-
stationary solution of a partial differential equation is parametrized by
spatial variables. In such situations one talks of a ‘spatial profile’ rather
than a ‘flow’.

Nature provides us with innumerable dynamical systems. They man-
ifest themselves through their trajectories: given an initial point $x_0$, the
evolution rule traces out a sequence of points $x(t) = f^t(x_0)$, the trajec-
tory through the point $x_0 = x(0)$. A trajectory is parameterized
by the time $t$ and thus belongs to $(f^t(x_0), t) \in \mathcal{M} \times \mathbb{R}$. By extension,
we can also talk of the evolution of a region $\mathcal{M}_i$ of the state space: just
apply $f^t$ to every point in $\mathcal{M}_i$ to obtain a new region $f^t(\mathcal{M}_i)$, as in
Fig. 2.1.

Because $f^t$ is a single-valued function, any point of the trajectory can be used to label the trajectory. If we mark the trajectory by its initial point $x_0$, we are describing it in the Lagrangian coordinates. We can regard the transport of the material point at $t = 0$ to its current point $x(t) = f^t(x_0)$ as a coordinate transformation from the Lagrangian coordinates to the Eulerian coordinates.

The subset of points in $M$ that belong to the (possibly infinite) trajectory of a given point $x_0$ is called the orbit of $x_0$; we shall talk about forward orbits, backward orbits, periodic orbits, etc.. For a flow, an orbit is a smooth continuous curve; for a map, it is a sequence of points.

What are the possible trajectories? This is a grand question, and there are many answers, chapters to follow offering some. Here is the first attempt to classify all possible trajectories:

stationary: $f^t(x) = x$ for all $t$
periodic: $f^t(x) = f^{t+T_p}(x)$ for a given minimum period $T_p$
aperiodic: $f^t(x) \neq f^{t'}(x)$ for all $t \neq t'$

The ancients tried to make sense of all dynamics in terms of periodic motions; epicycles, integrable systems. The embarrassing truth is that for a generic dynamical systems almost all motions are aperiodic. So we refine the classification by dividing aperiodic motions into two subtypes: those that wander off, and those that keep coming back.

A point $x \in M$ is called a wandering point, if there exists an open neighborhood $M_0$ of $x$ to which the trajectory never returns

$$f^t(x) \notin M_0 \quad \text{for all} \quad t > t_{\min}. \quad (2.1)$$

In physics literature, the dynamics of such state is often referred to as transient.

A periodic orbit (or a cycle) corresponds to a trajectory that returns exactly to the initial point in a finite time. Periodic orbits form a very small subset of the state space, in the same sense that rational numbers are a set of zero measure on the unit interval.

Periodic orbits and stationary points are the simplest examples of ‘non-wandering’ invariant sets preserved by dynamics. Dynamics can also preserve higher-dimensional smooth compact invariant manifolds; most commonly encountered are the $M$-dimensional tori of Hamiltonian dynamics, with notion of periodic motion generalized to quasiperiodic (superposition of $M$ incommesurate frequencies) motion on a smooth torus, and families of solutions related by a continuous symmetry.

For times much longer than a typical ‘turnover’ time, it makes sense to relax the notion of exact (quasi)periodicity, and replace it by the notion of recurrence. A point is recurrent or non-wandering if for any open neighborhood $M_0$ of $x$ and any time $t_{\min}$ there exists a later time $t$, such that

$$f^t(x) \in M_0. \quad (2.2)$$

In other words, the trajectory of a non-wandering point reenters the neighborhood $M_0$ infinitely often. We shall denote by $\Omega$ the non-
wandering set of $f$, i.e., the union of all the non-wandering points of $\mathcal{M}$. The set $\Omega$, the non-wandering set of $f$, is the key to understanding the long-time behavior of a dynamical system; all calculations undertaken here will be carried out on non-wandering sets.

So much about individual trajectories. What about clouds of initial points? If there exists a connected state space volume that maps into itself under forward evolution (and you can prove that by the method of Lyapunov functionals, or several other methods available in the literature), the flow is globally contracting onto a subset of $\mathcal{M}$ which we shall refer to as the attractor. The attractor may be unique, or there can coexist any number of distinct attracting sets, each with its own basin of attraction, the set of all points that fall into the attractor under forward evolution. The attractor can be a fixed point, a periodic orbit, aperiodic, or any combination of the above. The most interesting case is that of an aperiodic recurrent attractor, to which we shall refer loosely as a strange attractor. We say ‘loosely’, as will soon become apparent that diagnosing and proving existence of a genuine, card-carrying strange attractor is a highly nontrivial undertaking.

Conversely, if we can enclose the non-wandering set $\Omega$ by a connected state space volume $M_0$ and then show that almost all points within $M_0$, but not in $\Omega$, eventually exit $M_0$, we refer to the non-wandering set $\Omega$ as a repeller. An example of a repeller is not hard to come by—the pinball game of Section 1.3 is a simple chaotic repeller.

It would seem, having said that the periodic points are so exceptional that almost all non-wandering points are aperiodic, that we have given up the ancients’ fixation on periodic motions. Nothing could be further from truth. As longer and longer cycles approximate more and more accurately finite segments of aperiodic trajectories, we shall establish control over non-wandering sets by defining them as the closures of the union of all periodic points.

Before we can work out an example of a non-wandering set and get a better grip on what chaotic motion might look like, we need to ponder flows in a little more depth.

2.2 Flows

There is no beauty without some strangeness.

William Blake

A flow is a continuous-time dynamical system. The evolution rule $f^t$ is a family of mappings of $\mathcal{M} \rightarrow \mathcal{M}$ parameterized by $t \in \mathbb{R}$. Because $t$ represents a time interval, any family of mappings that forms an evolution rule must satisfy:

(a) $f^0(x) = x$ (in 0 time there is no motion)

(b) $f^t(f^{t'}(x)) = f^{t+t'}(x)$ (the evolution law is the same at all times)

(c) the mapping $(x, t) \mapsto f^t(x)$ from $\mathcal{M} \times \mathbb{R}$ into $\mathcal{M}$ is continuous.
The family of mappings $f^t(x)$ thus forms a continuous (forward semi-) group. Why ‘semi’-group? It may fail to form a group if the dynamics is not reversible, and the rule $f^t(x)$ cannot be used to rerun the dynamics backwards in time, with negative $t$; with no reversibility, we cannot define the inverse $f^{-t}(f^t(x)) = f^0(x) = x$, in which case the family of mappings $f^t(x)$ does not form a group. In exceedingly many situations of interest—for times beyond the Lyapunov time, for asymptotic attractors, for dissipative partial differential equations, for systems with noise, for non-invertible maps—the dynamics cannot be run backwards in time, hence, the circumspect emphasis on semigroups. On the other hand, there are many settings of physical interest, where dynamics is reversible (such as finite-dimensional Hamiltonian flows), and where the family of evolution maps $f^t$ does form a group.

For infinitesimal times, flows can be defined by differential equations. We write a trajectory as

$$x(t + \tau) = f^{t+\tau}(x_0) = f(f(x_0, t), \tau)$$

(2.3)

and express the time derivative of a trajectory at point $x(t)$,

$$\frac{dx}{d\tau} \bigg|_{\tau=0} = \partial_x f(f(x_0, t), \tau) \bigg|_{\tau=0} = \dot{x}(t).$$

(2.4)

as the time derivative of the evolution rule, a vector evaluated at the same point. By considering all possible trajectories, we obtain the vector $\dot{x}(t)$ at any point $x \in \mathcal{M}$. This vector field is a (generalized) velocity field:

$$v(x) = \dot{x}(t).$$

(2.5)

Newton’s laws, Lagrange’s method, or Hamilton’s method are all familiar procedures for obtaining a set of differential equations for the vector field $v(x)$ that describes the evolution of a mechanical system. Equations of mechanics may appear different in form from (2.5), as they are often involve higher time derivatives, but an equation that is second or higher order in time can always be rewritten as a set of first order equations.

We are concerned here with a much larger world of general flows, mechanical or not, all defined by a time-independent vector field (2.5). At each point of the state space a vector indicates the local direction in which the orbit evolves. The length of the vector $|v(x)|$ is proportional to the speed at the point $x$, and the direction and length of $v(x)$ changes from point to point. When the state space is a complicated manifold embedded in $\mathbb{R}^d$, one can no longer think of the vector field as being embedded in the state space. Instead, we have to imagine that each point $x$ of state space has a different tangent plane $T_x\mathcal{M}$ attached to it. The vector field lives in the union of all these tangent planes, a space called the tangent bundle $T\mathcal{M}$.

**Example 2.1 A two-dimensional vector field $v(x)$:**

A simple example of a flow is afforded by the unforced Duffing system

$$\dot{x}(t) = y(t)$$

$$\dot{y}(t) = -0.15 y(t) + x(t) - x(t)^3$$

(2.6)
plotted in Fig. 2.2. The velocity vectors are drawn superimposed over the configuration coordinates \((x(t), y(t))\) of state space \(\mathcal{M}\), but they belong to a different space, the tangent bundle \(T\mathcal{M}\).

If \(v(x_q) = 0\), \(x_q\) is an equilibrium point (also referred to as a stationary, fixed, critical, stagnation point, zero of \(v\), or steady state), and the trajectory remains forever stuck at \(x_q\). Otherwise the trajectory passing through \(x_0\) at time \(t = 0\) can be obtained by integrating the equations (2.5):

\[
x(t) = f^t(x_0) = x_0 + \int_0^t d\tau \, v(x(\tau)), \quad x(0) = x_0.
\]

We shall consider here only autonomous flows, i.e., flows for which the velocity field \(v_i\) is stationary, not explicitly dependent on time. A non-autonomous system

\[
\frac{dy}{d\tau} = w(y, \tau),
\]

can always be converted into a system where time does not appear explicitly. To do so, extend (‘suspend’) state space to be \((d + 1)\)-dimensional by defining \(x = \{y, \tau\}\), with a stationary vector field

\[
v(x) = \begin{bmatrix} w(y, \tau) \\ 1 \end{bmatrix}.
\]

The new flow \(\dot{x} = v(x)\) is autonomous, and the trajectory \(y(\tau)\) can be read off \(x(t)\) by ignoring the last component of \(x\).

**Example 2.2 A flow with a strange attractor:**

The Duffing flow of Fig. 2.2 is bit of a bore–every trajectory ends up in one of the two attractive equilibrium points. Let’s construct a flow that does not die out, but exhibits a recurrent dynamics. Start with a harmonic oscillator

\[
\dot{x} = -y, \quad \dot{y} = x.
\]

The solutions are \(re^{it}, re^{-it}\), and the whole \(x-y\) plane rotates with constant angular velocity \(\dot{\theta} = 1\), period \(T = 2\pi\). Now make the system unstable by adding

\[
\dot{x} = -y, \quad \dot{y} = x + ay, \quad a > 0,
\]

or, in radial coordinates, \(\dot{r} = ar \sin^2 \theta, \quad \dot{\theta} = 1 + (a/2) \sin 2\theta\). The plane is still rotating with the same average angular velocity, but trajectories are now spiraling out. Any flow in the plane either escapes, falls into an attracting equilibrium point, or converges to a limit cycle. Richer dynamics requires at least one more dimension. In order to prevent the trajectory from escaping to \(\infty\), kick it into 3rd dimension when \(x\) reaches some value \(c\) by adding

\[
\dot{z} = b + z(x - c), \quad c > 0.
\]

As \(x\) crosses \(c\), \(z\) shoots upwards exponentially, \(z \simeq e^{(x-c)t}\). In order to bring it back, start decreasing \(x\) by modifying its equation to

\[
\dot{x} = -y - z.
\]
Large $z$ drives the trajectory toward $x = 0$; there the exponential contraction by $e^{-ct}$ kicks in, and the trajectory drops back toward the $x$-$y$ plane. This frequently studied example of an autonomous flow is called the Rössler system (for definitiveness we fix the parameters $a$, $b$, $c$ in what follows):

\[
\begin{align*}
\dot{x} &= -y - z \\
\dot{y} &= x + ay \\
\dot{z} &= b + z(x - c), \quad a = b = 0.2, \quad c = 5.7.
\end{align*}
\]

The system is as simple as they get—it would be linear, were it not for the sole bilinear term $xz$. Even for so ‘simple’ a system the nature of long-time solutions is far from obvious.

There are two repelling equilibrium points (2.7):

\[
\begin{align*}
(x^-, y^-, z^-) &= \left( 0.0070, -0.0351, 0.0351 \right) \\
(x^+, y^+, z^+) &= \left( 5.6929, -28.464, 28.464 \right)
\end{align*}
\]

One is close to the origin by construction—the other, some distance away, exists because the equilibrium condition has a 2nd-order nonlinearity.

To see what other solutions look like we need to resort to numerical integration. A typical numerically integrated long-time trajectory is sketched in Fig. 2.3. As we shall show in Section 4.1, for this flow any finite volume of initial conditions shrinks with time, so the flow is contracting. Trajectories that start out sufficiently close to the origin seem to converge to a strange attractor. We say ‘seem’ as there exists no proof that such an attractor is asymptotically aperiodic—it might well be that what we see is but a long transient on a way to an attractive periodic orbit. For now, accept that Fig. 2.3 and similar figures in what follows are examples of ‘strange attractors.’ (continued in Exercise 2.8 and Example 3.3) (Rytis Paskauskas)

### 2.3 Computing trajectories

On two occasions I have been asked [by members of Parliament], ‘Pray, Mr. Babbage, if you put into the machine wrong figures, will the right answers come out?’ I am not able rightly to apprehend the kind of confusion of ideas that could provoke such a question.

Charles Babbage

You have not learned dynamics unless you know how to integrate numerically whatever dynamical equations you face. Sooner or later, you need to implement some finite time-step prescription for integration of the equations of motion (2.5). The simplest is the Euler integrator which
advances the trajectory by $\delta \tau \times \text{velocity at each time step:}$

$$x_i \rightarrow x_i + v_i(x)\delta \tau .$$

(2.16)

This might suffice to get you started, but as soon as you need higher numerical accuracy, you will need something better. There are many excellent reference texts and computer programs that can help you learn how to solve differential equations numerically using sophisticated numerical tools, such as pseudo-spectral methods or implicit methods. If a ‘sophisticated’ integration routine takes days and gobbles up terabits of memory, you are using brain-damaged high level software. Try writing a few lines of your own Runge-Kutta code in some mundane everyday language. While you absolutely need to master the requisite numerical methods, this is neither the time nor the place to expound upon them; how you learn them is your business. And if you have developed some nice routines for solving problems in this text or can point another student to some, let us know.

**Summary**

Chaotic dynamics with a low-dimensional attractor can be visualized as a succession of nearly periodic but unstable motions. In the same spirit, turbulence in spatially extended systems can be described in terms of recurrent spatiotemporal patterns. Pictorially, dynamics drives a given spatially extended system through a repertoire of unstable patterns; as we watch a turbulent system evolve, every so often we catch a glimpse of a familiar pattern. For any finite spatial resolution and finite time the system follows approximately a pattern belonging to a finite repertoire of possible patterns, and the long-term dynamics can be thought of as a walk through the space of such patterns. Recasting this image into mathematics is the subject of this book.

**Further reading**

*Model ODE and PDE systems.* The Duffing system (2.6) arises in the study of electronic circuits [2]. Rössler system was introduced in Ref. [3] as a simplified set of equations describing no particular physical system, but capturing the essence of chaos in a simplest imaginable smooth flow. Otto Rössler, a man of classical education, was inspired in this quest by that rarely cited grandfather of chaos, Anaxagoras (456 B.C.). This, and references to earlier work can be found in Refs. [5, 7, 8]. We recommend in particular the inimitable Abraham and Shaw illustrated classic [6] for its beautiful sketches of the Rössler and many other flows.

*Diagnosing chaos.* In Section 1.3.1 we have stated that a deterministic system exhibits ‘chaos’ if its dynamics is locally unstable (positive Lyapunov exponent) and globally mixing (positive entropy). In Section 2.6 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 [12] is useful for extracting quasi-periodic and weakly chaotic regions of state space in Hamiltonian dy-
Exercises

(2.1) **Trajectories do not intersect.** A trajectory in the state space $\mathcal{M}$ is the set of points one gets by evolving $x \in \mathcal{M}$ forwards and backwards in time:

$$C_x = \{ y \in \mathcal{M} : f^t(x) = y \text{ for } t \in \mathbb{R} \}.$$  

Show that if two trajectories intersect, then they are the same curve.

(2.2) **Evolution as a group.** The trajectory evolution $f^t$ is a one-parameter semigroup where

$$f^{t+s} = f^t \circ f^s.$$  

Show that it is a commutative semigroup. In this case, the commutative character of the (semi-)group of evolution functions comes from the commutative character of the time parameter under addition. Can you think of any other (semi-)group replacing time?

(2.3) **Almost ODE’s.**

(a) Consider the point $x$ on $\mathbb{R}$ evolving according $\dot{x} = e^t$. Is this an ordinary differential equation?

(b) Is $\dot{x} = x(x(t))$ an ordinary differential equation?

(c) What about $\dot{x} = x(t + 1)$?

(2.4) **All equilibrium points are fixed points.** Show that a point of a vector field $v$ where the velocity is zero is a fixed point of the dynamics $f^t$.

(2.5) **Gradient systems.** Gradient systems (or ‘potential problems’) are a simple class of dynamical systems for which the velocity field is given by the gradient of an auxiliary function, the ‘potential’ $\phi$

$$\dot{x} = -\nabla \phi(x)$$  

where $x \in \mathbb{R}^d$, and $\phi$ is a function from that space to the reals $\mathbb{R}$.

(a) Show that the velocity of the particle is in the direction of most rapid decrease of the function $\phi$.

(b) Show that all extrema of $\phi$ are fixed points of the flow.

(c) Show that it takes an infinite amount of time for the system to reach an equilibrium point.

(d) Show that there are no periodic orbits in gradient systems.

(2.6) **Runge-Kutta integration.** Implement the fourth-order Runge-Kutta integration formula (see, for example, Ref. [9]) for $\dot{x} = v(x)$:

$$
\begin{align*}
x_{n+1} &= x_n + \frac{k_1}{6} + \frac{k_2}{3} + \frac{k_3}{3} + \frac{k_4}{6} + O(\delta t^5) \\
k_1 &= \delta t v(x_n), \\
k_2 &= \delta t v(x_n + k_1/2) \\
k_3 &= \delta t v(x_n + k_2/2) \\
k_4 &= \delta t v(x_n + k_3).
\end{align*}
\tag{2.17}
$$

If you already know your Runge-Kutta, program what you believe to be a better numerical integration routine, and explain what is better about it.

(2.7) **Rössler system.** Use the result of Exercise 2.6 or some other integration routine to integrate numerically the Rössler system (2.14). Does the result look like a ‘strange attractor’?

(2.8) **Equilibria of the Rössler system.**

(a) Find all equilibrium points $(x^0, y^0, z^0)$ of the Rössler system (2.14). How many are there?

(b) Assume that $b = a$. As we shall see, some surprisingly large, adn surprisingly small numbers arise in this system. In order to understand their size, introduce parameters

$$\epsilon = a/c, \quad D = 1 - 4\epsilon^2, \quad p^\pm = (1 \pm \sqrt{D})/2.$$  

\tag{2.18}
(2.9) **Can you integrate me?** Integrating equations numerically is not for the faint of heart. It is not always possible to establish that a set of non-linear ordinary differential equations has a solution for all times and there are many cases were the solution only exists for a limited time interval, as, for example, for the equation $\dot{x} = x^2$, $x(0) = 1$.

(a) For what times do solutions of $\dot{x} = x(x(t))$ exist? Do you need a numerical routine to answer this question?

(b) Let’s test the integrator you wrote in Exercise 2.6. The equation $\ddot{x} = -x$ with initial conditions $x(0) = 2$ and $\dot{x} = 0$ has as solution $x(t) = e^{-t}(1 + e^{2t})$. Can your integrator reproduce this solution for the interval $t \in [0, 10]$? Check your solution by plotting the error as compared to the exact result.

(c) Now we will try something a little harder. The equation is going to be third order

$$\dddot{x} + 0.6 \ddot{x} + \dot{x} - |x| + 1 = 0,$$

which can be checked—numerically—to be chaotic. As initial conditions we will always use $\dddot{x}(0) = \ddot{x}(0) = \dot{x}(0) = 0$. Can you reproduce the result $x(12) = 0.8462071873$ (all digits are significant)? Even though the equation being integrated is chaotic, the time intervals are not long enough for the exponential separation of trajectories to be noticeable (the exponential growth factor is $\approx 2.4$).

(d) Determine the time interval for which the solution of $\dddot{x} = x^2$, $x(0) = 1$ exists.

**Classical collinear helium dynamics.** In order to apply periodic orbit theory to quantization of helium we shall need to compute classical periodic orbits of the helium system. In this exercise we commence their evaluation for the collinear helium atom (5.6)

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

The nuclear charge for helium is $Z = 2$. Collinear helium has only 3 degrees of freedom and the dynamics can be visualized as a motion in the $(r_1, r_2)$-plane. In $(r_1, r_2)$-coordinates the potential is singular for $r_i \rightarrow 0$ nucleur-electron collisions. These 2-body collisions can be regularized by rescaling the coordinates, with details given in Section 7.3. In the transformed coordinates $(x_1, x_2, p_1, p_2)$ the Hamiltonian equations of motion take the form

$$\dot{P}_1 = 2Q_1 \left[2 - \frac{P_2^2}{8} - Q_2^2(1 + \frac{Q_1^2}{R^2})\right],$$  

$$\dot{P}_2 = 2Q_2 \left[2 - \frac{P_1^2}{8} - Q_1^2(1 + \frac{Q_2^2}{R^2})\right],$$  

$$\dot{Q}_1 = \frac{1}{4} P_1 Q_2^2, \quad \dot{Q}_2 = \frac{1}{4} P_2 Q_1^2.$$  

(2.19)

where $R = (Q_1^2 + Q_2^2)^{1/2}$.

(a) Integrate the equations of motion by the fourth order Runge-Kutta computer routine of Exercise 2.6 (or whatever integration routine you like). A convenient way to visualize the 3-d state space orbit is by projecting it onto the 2-dimensional $(r_1(t), r_2(t))$ plane.

(continued as Exercise 3.4)
References