Chapter 5: Integrating Regular and Chaotic Classical Orbits

We shall apply computational methods to a simple but interesting problem in classical mechanics: the relative motion of two atoms interacting via the Lennard-Jones 6-12 potential. The potential energy is

\[ V(r) = V_0 \left( \frac{\sigma}{r} \right)^{12} - 2 \left( \frac{\sigma}{r} \right)^6 \], \hspace{1cm} (1)\]

where \( r \) is the distance between the two atoms. You should use the graphic tools at your disposal to draw a graph of \( V(r) \) vs. \( r \). The potential energy has a minimum at \( r = \sigma \), and \( V_0 \) is the potential energy at the minimum relative to the potential energy as the atoms separate completely \( (r \to \infty) \). For \( r \gg \sigma \), there is an attractive force \( \propto r^{-7} \) between the atoms. This is the van der Waals attraction, which originates in the electrical polarizability of the atoms. For \( r \ll \sigma \), the atoms strongly repel one another. The precise form of the repulsive force, \( \propto r^{-13} \), is chosen for convenience, but the existence of some “hard core” repulsion is understood in terms of the Pauli exclusion principle. In mechanics we learn that we can separate the motion of the center of mass of a pair of particles from the relative motion. We are interested in the relative motion of masses \( m_1 \) and \( m_2 \), which is the same as the motion of one particle whose mass, \( m = m_1 m_2 / (m_1 + m_2) \), is the “reduced mass” of the pair:

\[ m \frac{d^2\mathbf{r}}{dt^2} = - \nabla V \], \hspace{1cm} (2)\]

where \( \mathbf{r} \) is the vector from one atom to the other and, for us, \( V \) is given by (1). We also learn that energy is conserved, so there is a constant \( E \) for which

\[ \frac{m|\dot{\mathbf{r}}|^2}{2} + V(r) = E \], \hspace{1cm} (3)\]

and, since the force is central, angular momentum is conserved, so there is a constant vector \( \mathbf{L} \) for which

\[ m\mathbf{r} \times \dot{\mathbf{r}} = \mathbf{L} \]. \hspace{1cm} (4)\]

Let’s simplify the equations by appropriate choice of units and coordinates: we choose the unit of length so that \( \sigma = 1 \). We choose the unit of mass so that \( m = 1 \). We choose the unit of time so that \( V_0 / m \sigma^2 = 1 \). We choose the coordinate system so that the direction of \( \mathbf{L} \) is the \( z \) axis. The motion is then confined to the \( x\)-\( y \) plane. The usual discussion in a mechanics course uses polar coordinates \( r, \phi \). With our conventions, a little algebra establishes

\[ \frac{\dot{r}^2}{2} + \frac{r^2 \dot{\phi}^2}{2} + V(r) = E \], \hspace{1cm} (5)\]

and

\[ r^2 \dot{\phi} = L \] \hspace{1cm} (6)\]

with

\[ V(r) = r^{-12} - 2r^{-6} \]. \hspace{1cm} (7)\]

We rewrite (6) as

\[ \dot{\phi} = \frac{L}{r^2} \] \hspace{1cm} (8)\]

Dr. Donald Fredkin wrote the original version of this chapter for an undergraduate version of this course, which we taught together at the University of California, San Diego, in 1996. I adapt it here with his permission.
5. Classical Mechanics

and substitute (8) into (5) to obtain

\[
\frac{\dot{r}^2}{2} + V_{\text{eff}}(r) = E ,
\]

with

\[
V_{\text{eff}}(r) = V(r) + \frac{L^2}{2r^2} = r^{-12} - 2r^{-6} + \frac{L^2}{2r^2} .
\]

Equation (9) is energy conservation for one-dimensional motion in the “effective potential” \(V_{\text{eff}}(r)\) given by (10). We start with this one-dimensional radial problem.

1. Turning points: finding zeroes of a function

For sufficiently small angular momentum \(L\), there is a range of energy \(E\) such that there are exactly two values of \(r\) for which \(V_{\text{eff}}(r) = E\), and therefore, by (9) \(\dot{r} = 0\). These special values, which we denote \(r_p\) (for periapsis, the closest approach) and \(r_a\) (for apoapsis, the furthest distance apart), with \(r_p < r_a\), are called turning points. Our first task is to write a function \texttt{turn} to compute the turning points. The prototype for \texttt{turn} is

```c
typedef struct pair {
    double a, b;
} pair;

/* Return the turning points for the radial motion with energy E and angular
momentum L in a Lennard-Jones potential. If the combination (E, L) is not
possible, return a negative value for a. Otherwise, 0 < a < b.
*/
pair turn(double E, double L);
```

The function \texttt{turn} has to find zeroes of \(E - V_{\text{eff}}(r)\). There is one rule to be remembered about one-dimensional zero finding: to find a zero of \(F(x)\), first find a bracketing interval \(a < x < b\) such that \(F(a)\) and \(F(b)\) have opposite signs, and then keep making the interval shorter while maintaining the bracketing property. Once a bracketing interval is established, there are excellent general-purpose algorithms for refining the bracketing interval.

Here is one strategy for finding the turning points: there is a critical value \(L_c\) of the angular momentum such that no bounded orbits exist for \(L \geq L_c\) (see the figure). You should compute the exact value of \(L_c\) for which there is a horizontal inflection point and the radial distance \(r_c\) at which that inflection point occurs. Now, if \(L < L_c\), we can find a minimum of \(V_{\text{eff}}(r)\) at \(r_{\text{min}}\) and a maximum of \(V_{\text{eff}}(r)\) at \(r_{\text{max}}\) (see the figure for \(L = 1.1\)). These extrema, \(r_{\text{min}}\) and \(r_{\text{max}}\), can be determined by applying a standard zero-finding function, which you will write, to \(V'_{\text{eff}}(r)\) as soon as bracketing intervals are available. For \(r_{\text{min}}\), a bracketing interval is given by \(r_1 < r_{\text{min}} < r_c\) for any \(r_1 < r_c\) at which \(V_{\text{eff}}\) has a negative slope; such an \(r_1\) can always be found by starting with the trial value \(r_1 = r_c\) and successively halving \(r_1\). Similarly, for \(r_{\text{max}}\), a bracketing interval is given by \(r_c < r_{\text{max}} < r_2\); for \(r_2 > r_c\) and \(V'_{\text{eff}}(r_2) < 0\); such an \(r_2\) can always be found by starting with the trial value \(r_2 = r_c\) and successively doubling \(r_2\). Now a bounded orbit exists if and only if \(V_{\text{eff}}(r_{\text{min}}) < E < V_{\text{eff}}(r_{\text{max}})\). Further, \(r_{\text{min}} < r_a < r_{\text{max}}\) brackets the apoapsis \(r_a\), and a bracketing interval \(r_0 < r_p < r_{\text{min}}\) can be readily found for the periapsis; we leave it to you to determine a suitable \(r_0\). Now write the function \texttt{turn}. Test it by linking it to the given main program.
5. Classical Mechanics

The one-dimensional effective potential (10) for angular momentum less than, equal to, and greater than the critical value. Note that the latter two have no potential well in which the system can orbit. For 
\( L < L_c \), \( V_{\text{eff}} \) has a minimum at \( r_{\text{min}} \) and a local maximum at \( r_{\text{max}} \); if the total energy \( E \) satisfies \( V_{\text{eff}}(r_{\text{min}}) < E < V_{\text{eff}}(r_{\text{max}}) \), then the orbital distance \( r \) will vary between periapsis \( r_p \) and apoapsis \( r_a \).

/* tstturn.c (header comments elided) */
#include <stdio.h>
#include <stdlib.h>
#include "turn.h"
int main(int argc, char **argv) {
    double E, L; /* energy and angular momentum */
    pair tp; /* turning points */
    if (argc != 3) {
        fprintf(stderr, "usage: %s E L\n", argv[0]);
        return 1;
    }
    E = atof(argv[1]);
    L = atof(argv[2]);
    tp = turn(E, L);
    if (tp.a > 0)
        printf("periapsis = %g\napoapsis = %g\n", tp.a, tp.b);
    else
        printf("no bounded orbit exists\n");
    return 0;
}

2. Radial period: numerical integration

From (9) we have
\[
\dot{r} = \pm \sqrt{2(E - V_{\text{eff}}(r))},
\] (11)
or
\[ dt = \pm \frac{dr}{\sqrt{2(E - V_{\text{eff}}(r))}} , \] (12)
where the sign is + when \( r \) is increasing and − when it is decreasing. The time to complete one cycle of the radial motion, with \( r \) varying from \( r_p \) to \( r_a \) and back to \( r_p \), is, therefore,
\[ T_r = \sqrt{2} \int_{r_p}^{r_a} \frac{dr}{\sqrt{E - V_{\text{eff}}(r)}} . \] (13)

Our next task is to write a function `period` to compute \( T_r \). The prototype for `period` is

```c
/* Return the period for the radial motion with energy E and angular momentum * L in a Lennard-Jones potential. If the combination (E, L) is not possible, * return a negative value. */
double period(double E, double L);
```

The function `period` should use `turn` to find \( r_p \) and \( r_a \) and then evaluate the integral (13) numerically to some reasonable precision. There are many ways to evaluate integrals numerically, and it does not usually matter much which method is chosen unless the program is going to evaluate thousands of integrals. However, there is a special problem here: the integrand diverges at the end points, although the integral does exist. Numerical integration methods that evaluate the integrand at the end points, or too close to them, are likely to fail. (Worse, the program might try to evaluate a square root of a negative number, because \( r_p \) and \( r_a \) are known only approximately.) Part of the solution is to use a so-called “open” formula, which does not evaluate the integrand at the end points. This, alone, does not sufficiently avoid the singularity at the end points, but there is a nice variation of Gaussian integration called the Gauss-Chebyshev formula, which computes
\[ \int_{-1}^{1} \frac{F(x)}{\sqrt{1 - x^2}} \approx C_n \sum_{k=0}^{n-1} F(\xi_k) \] (14)
for suitable coefficient \( C_n \) and evaluation points \( \xi_0 \ldots \xi_{n-1} \), which can be found in reference books or computed.\(^2\) Let us rewrite (13) in the form
\[ T_r = \int_{r_p}^{r_a} F(r) \frac{dr}{\sqrt{(r - r_p)(r_a - r)}} \] (15)
with
\[ F(r) = \frac{\sqrt{2(r - r_p)(r_a - r)}}{\sqrt{E - V_{\text{eff}}(r)}} . \] (16)
Note that \( F(r) \) is regular at the end points. To apply (14) to (15), we make the change of integration variable
\[ r = r_p + \frac{r_a - r_p}{2}(\rho + 1) = r_p + \frac{r_a + r_p}{2} + \frac{r_a - r_p}{2}\rho . \] (17)
Then (15) becomes
\[ T_r = \int_{-1}^{1} F\left(\frac{r_a + r_p}{2} + \frac{r_a - r_p}{2}\rho\right) \frac{d\rho}{\sqrt{1 - \rho^2}} , \] (18)

\(^2\) See, for example, *Numerical Recipes* §4.5.
Now write period. Link it to the\texttt{tstperiod} driver given below, and test it; the driver lets you experiment with the quadrature order $n$ in (14) from the command line. You can compute $\lim_{E \to V_{\text{eff}}(r_{\text{min}})} T_r$ exactly, providing one check on your function period.

\begin{verbatim}
/* tstperiod.c */
#include <stdio.h>
#include <stdlib.h>
#include "period.h"

int main(int argc, char **argv)
{
    double E, L, Tr;    /* energy, ang mom, radial period */
    int n=10;            /* default quadrature order */
    if (argc != 3 || argc>4) { /* very simple argument parsing */
        fprintf(stderr, "usage: %s E L [n]\n", argv[0]);
        return 1;
    }
    E = atof(argv[1]);
    L = atof(argv[2]);
    if(argc==4)
        n = atoi(argv[3]);
    if ( (Tr = period(E, L, n)) < 0) {
        fprintf(stderr, "no bound orbit exists\n");
        exit(1);
    }
    printf("radial period = %g\n", Tr);
    return 0;
}
\end{verbatim}

3. Orbits: numerical solution of ordinary differential equations

The direct approach to the determination and study of orbits is numerical solution of (2). Most numerical methods for solution of ordinary differential equations are designed for systems of first-order equations, so we rewrite the second-order (2) as

\begin{equation}
\frac{dr}{dt} = v \\
\frac{dv}{dt} = - \nabla V .
\end{equation}

Defining the four-dimensional vector $u$ by

\begin{equation}
\begin{align*}
u_1 &= x \\
u_2 &= y \\
u_3 &= v_x \\
u_4 &= v_y
\end{align*}
\end{equation}
gives (19) the practical form
\begin{align}
\dot{u}_1 &= u_3 \\
\dot{u}_2 &= u_4 \\
\dot{u}_3 &= -\partial V / \partial u_1 \\
\dot{u}_4 &= -\partial V / \partial u_2
\end{align}
(21)

For the potential given in (1), equation (21) takes the definitive form
\begin{align}
\dot{u}_1 &= u_3 \\
\dot{u}_2 &= u_4 \\
\dot{u}_3 &= f u_1 \\
\dot{u}_4 &= f u_2
\end{align}
(22)
with the definitions
\begin{align}
f &= 12(r_{sq}^{-7} - r_{sq}^{-4}) \\
r_{sq} &= u_1^2 + u_2^2
\end{align}
(23)

Now write a program called orbit to compute \(N\) points on an orbit, starting at \(u = u(0)\) when \(t = 0\) and ending at \(t = T\). Use whatever method you like,\(^3\) but write the program so that you can invoke it with the command
\texttt{orbit x0 y0 vx0 vy0 T N}

The program should write one line to standard output for each of the \(N\) times, starting at \(t = 0\) and ending with \(t = T\). Each line should contain seven numbers, separated by white space: \(t\), \(x\), \(y\), \(vx\), \(vy\), \(E\), and \(L\), where \(E\) and \(L\) are the energy and angular momentum. Although these two quantities are conserved in nature, they might not be when you run your program because of numerical errors (and, possibly, because of programming errors). You will have to decide on appropriate error tolerances. If \(E\) and \(L\) are not constant to within the intended accuracy of your solution, something is wrong. Plot some orbits found with orbit. Be sure the scales on the \(x\) and \(y\) axes are the same, and plot \(y\) vs. \(x\). A good set of initial conditions for getting started is \(x = 1.1\), \(y = 0\), \(v_x = 0\), \(v_y = 0.1\). What other plots are interesting? This is the point at which you should make all your programming pay off in insight. Use your programs. Look at \(x\) as a function of \(t\), and make a spectral analysis using the fast Fourier transform. Recall the considerations that enter such an analysis: \(T\) determines the frequency resolution, \(N/T\) (the sampling rate) must be high enough to avoid aliasing, and windowing may be necessary to reduce leakage (but then resolution suffers). Make a semilogarithmic plot (the \(y\)-axis should be logarithmic) of the spectrum. What features do you see? Can you explain these features qualitatively? Can you explain them quantitatively using your earlier programs? Make a linear plot to see why we recommend a semilogarithmic plot.

4. Orbits: chaotic motion
Orbits in the Lennard-Jones potential (1) and the corresponding spectra are easy to understand, because the dynamics is “separable” in polar coordinates. Now let’s consider motion in the noncentral potential
\begin{equation}
V(x, y) = \frac{1}{2}x^2 + \frac{1}{2}y^2 + x^2y - \frac{1}{3}y^3 , \quad (24)
\end{equation}

\(^3\) We recommend using a serious multistep ODE solver. Since this problem is not “stiff” (see Numerical Recipes §16.6), an Adams method is appropriate. There are several good solvers available from Netlib and elsewhere. Most are written in Fortran, which is a nuisance. CVODE is written in C and pretty much represents the current state of the art.
which was introduced by Hénon and Heiles to model aspects of dynamics in globular clusters.\textsuperscript{4} The equations of motion are
\begin{equation}
\begin{aligned}
\dot{x} &= v_x \\
\dot{y} &= v_y \\
\dot{v}_x &= -x - 2xy \\
\dot{v}_y &= -y - x^2 + y^2 
\end{aligned}
\end{equation}

(25)

Make a copy of orbit.c, calling the copy hh.c. Edit hh.c so that it solves (25). Note that angular momentum is no longer conserved, so there is no point printing it on each line. Plot some orbits found with hh. In particular, look at the two sets of initial conditions
\begin{equation}
x = 0.1 \quad y = 0 \quad v_x = 0 \quad v_y = 0.1 \\
x = 0.8 \quad y = -0.5 \quad v_x = 0 \quad v_y = 0
\end{equation}

(26)

Plot the spectrum of $x(t)$ for each orbit that you study. See if you can correlate the character of the spectra with the appearance of the orbits. You should also look at plots of $x$ and $y$ vs. $t$. Which of these views of an orbit are most useful? Using appropriate plotting software,\textsuperscript{5} you might examine three-dimensional plots of $(x(t), y(t), t)$.

\textsuperscript{4} M. Hénon and C. Heiles, \textit{Astron. J.} \textbf{69} (1964) 73.
\textsuperscript{5} E.g., the supplied \texttt{plot3d} program or \texttt{gsplot} in Octave.