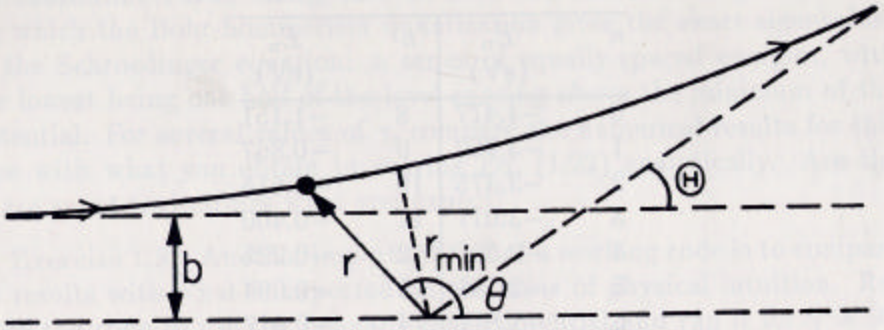

Figure I.1 Quantities involved in the scattering of a particle by a central potential.

vibrational state. Find the value of β appropriate for the H_2 molecule, modify the program above to use the Morse potential, and calculate the spectrum of vibrational states. Show that a much more reasonable number of levels is now obtained. Compare the energies with experiment and with those of the Lennard-Jones potential and interpret the latter differences.

Project I: Scattering by a central potential

In this project, we will investigate the classical scattering of a particle of mass m by a central potential, in particular the Lennard-Jones potential considered in Section 1.4 above. In a scattering event, the particle, with initial kinetic energy E and impact parameter b, approaches the potential from a large distance. It is deflected during its passage near the force center and eventually emerges with the same energy, but moving at an angle Θ with respect to its original direction. Since the potential depends upon only the distance of the particle from the force center, the angular momentum is conserved and the trajectory lies in a plane. The polar coordinates of the particle, (r, θ), are a convenient way to describe its motion, as shown in Figure I.1. (For details, see any textbook on classical mechanics, such as [Go80].)

Of basic interest is the deflection function, $\Theta(b)$, giving the final scattering angle, Θ, as a function of the impact parameter; this function also depends upon the incident energy. The differential cross section for scattering at an angle Θ, $d\sigma/d\Omega$, is an experimental observable that is

related to the deflection function by

$$\frac{d\sigma}{d\Omega} = \frac{b}{\sin\Theta}\left|\frac{db}{d\Theta}\right| . \qquad (I.1)$$

Thus, if $d\Theta/db = (db/d\Theta)^{-1}$ can be computed, then the cross section is known.

Expressions for the deflection function can be found analytically for only a very few potentials, so that numerical methods usually must be employed. One way to solve the problem would be to integrate the equations of motion in time (i.e., Newton's law relating the acceleration to the force) to find the trajectories corresponding to various impact parameters and then to tabulate the final directions of the motion (scattering angles). This would involve integrating four coupled first-order differential equations for two coordinates and their velocities in the scattering plane, as discussed in Section 2.5 below. However, since angular momentum is conserved, the evolution of θ is related directly to the radial motion, and the problem can be reduced to a one-dimensional one, which can be solved by quadrature. This latter approach, which is simpler and more accurate, is the one we will pursue here.

To derive an appropriate expression for Θ, we begin with the conservation of angular momentum, which implies that

$$L = mvb = mr^2\frac{d\theta}{dt} , \qquad (I.2)$$

is a constant of the motion. Here, $d\theta/dt$ is the angular velocity and v is the asymptotic velocity, related to the bombarding energy by $E = \frac{1}{2}mv^2$. The radial motion occurs in an effective potential that is the sum of V and the centrifugal potential, so that energy conservation implies

$$\frac{1}{2}m\left(\frac{dr}{dt}\right)^2 + \frac{L^2}{2mr^2} + V = E . \qquad (I.3)$$

If we use r as the independent variable in (I.2), rather than the time, we can write

$$\frac{d\theta}{dr} = \frac{d\theta}{dt}\left(\frac{dr}{dt}\right)^{-1} = \frac{bv}{r^2}\left(\frac{dr}{dt}\right)^{-1} , \qquad (I.4)$$

and solving (I.3) for dr/dt then yields

$$\frac{d\theta}{dr} = \pm\frac{b}{r^2}\left(1 - \frac{b^2}{r^2} - \frac{V}{E}\right)^{-1/2} . \qquad (I.5)$$

Recalling that $\theta = \pi$ when $r = \infty$ on the incoming branch of the trajectory and that θ is always decreasing, this equation can be integrated immediately to give the scattering angle,

$$\Theta = \pi - 2\int_{r_{\min}}^{\infty} \frac{b\,dr}{r^2}\left(1 - \frac{b^2}{r^2} - \frac{V}{E}\right)^{-1/2}, \qquad (I.6)$$

where $r_{\min}$ is the distance of closest approach (the turning point, determined by the outermost zero of the argument of the square root) and the factor of 2 in front of the integral accounts for the incoming and outgoing branches of the trajectory, which give equal contributions to the scattering angle.

One final transformation is useful before beginning a numerical calculation. Suppose that there exists a distance $r_{\max}$ beyond which we can safely neglect V. In this case, the integrand in (I.6) vanishes as r^{-2} for large r, so that numerical quadrature could be very inefficient. In fact, since the potential has no effect for $r > r_{\max}$, we would just be "wasting time" describing straight-line motion. To handle this situation efficiently, note that since $\Theta = 0$ when $V = 0$, Eq. (I.6) implies that

$$\pi = 2\int_{b}^{\infty} \frac{b\,dr}{r^2}\left(1 - \frac{b^2}{r^2}\right)^{-1/2}, \qquad (I.7)$$

which, when substituted into (I.6), results in

$$\Theta = 2b\left[\int_{b}^{r_{\max}} \frac{dr}{r^2}\left(1 - \frac{b^2}{r^2}\right)^{-1/2} - \int_{r_{\min}}^{r_{\max}} \frac{dr}{r^2}\left(1 - \frac{b^2}{r^2} - \frac{V}{E}\right)^{-1/2}\right]. \qquad (I.8)$$

The integrals here extend only to $r_{\max}$ since the integrands become equal when $r > r_{\max}$.

Our goal will be to study scattering by the Lennard-Jones potential (1.16), which we can safely set to zero beyond $r_{\max} = 3a$ if we are not interested in energies smaller than about

$$V(r = 3a) \approx 5 \times 10^{-3} V_0 .$$

The study is best done in the following sequence of steps:

Step 1 Before beginning *any* numerical computation, it is important to have some idea of what the results should look like. Sketch what you think the deflection function is at relatively low energies, $E \lesssim V_0$, where the peripheral collisions at large $b \leq r_{\max}$ will take place in a predominantly attractive potential and the more central collisions will "bounce" against the repulsive core. What happens at much higher energies, $E \gg V_0$, where the attractive pocket in V can be neglected? Note that for values of b where the deflection function has a maximum or a minimum, Eq. (I.1) shows that the cross section will be infinite, as occurs in the rainbow formed when light scatters from water drops.

Step 2 To have analytically soluble cases against which to test your program, calculate the deflection function for a square potential, where $V(r) = U_0$ for $r < r_{\max}$ and vanishes for $r > r_{\max}$. What happens when U_0 is negative? What happens when U_0 is positive and $E < U_0$? when $E > U_0$?

Step 3 Write a program that calculates, for a specified energy E, the deflection function by a numerical quadrature to evaluate both integrals in Eq. (I.8) at a number of equally spaced b values between 0 and $r_{\max}$. (Note that the singularities in the integrands require some special treatment.) Check that the program is working properly and is accurate by calculating deflection functions for the square-well potential discussed in Step 2. Compare the accuracy with that of an alternative procedure in which the first integral in (I.8) is evaluated analytically, rather than numerically.

Step 4 Use your program to calculate the deflection function for scattering from the Lennard-Jones potential at selected values of E ranging from $0.1\,V_0$ to $100\,V_0$. Reconcile your answers in Step 1 with the results you obtain. Calculate the differential cross section as a function of Θ at these energies.

Step 5 If your program is working correctly, you should observe, for energies $E \lesssim V_0$, a singularity in the deflection function where Θ appears to approach $-\infty$ at some critical value of b, b_{crit}, that depends on E. This singularity, which disappears when E becomes larger than about V_0, is characteristic of "orbiting." In this phenomenon, the integrand in Eq. (I.6) has a linear, rather than a square root, singularity at the turning point, so that the scattering angle becomes logarithmically infinite. That is, the effective potential,

$$V + E\left(\frac{b}{r}\right)^2 ,$$

has a parabolic maximum and, when $b = b_{\text{crit}}$, the peak of this parabola is equal to the incident energy. The trajectory thus spends a very long time at the radius where this parabola peaks and the particle spirals many times around the force center. By tracing b_{crit} as a function of energy

and by plotting a few of the effective potentials involved, convince yourself that this is indeed what's happening. Determine the maximum energy for which the Lennard-Jones potential exhibits orbiting, either by a solution of an appropriate set of equations involving V and its derivatives or by a systematic numerical investigation of the deflection function. If you pursue the latter approach, you might have to reconsider the treatment of the singularities in the numerical quadratures.

Chapter 2

Ordinary Differential Equations

Many of the laws of physics are most conveniently formulated in terms of differential equations. It is therefore not surprising that the numerical solution of differential equations is one of the most common tasks in modeling physical systems. The most general form of an ordinary differential equation is a set of M coupled first-order equations

$$\frac{d\mathbf{y}}{dx} = \mathbf{f}(x, \mathbf{y}) , \tag{2.1}$$

where x is the independent variable and $\mathbf{y}$ is a set of M dependent variables ($\mathbf{f}$ is thus an M-component vector). Differential equations of higher order can be written in this first-order form by introducing auxiliary functions. For example, the one-dimensional motion of a particle of mass m under a force field $F(z)$ is described by the second-order equation

$$m\frac{d^2z}{dt^2} = F(z) . \tag{2.2}$$

If we define the momentum

$$p(t) = m\frac{dz}{dt} ,$$

then (2.2) becomes the two coupled first-order (Hamilton's) equations

$$\frac{dz}{dt} = \frac{p}{m} \; ; \quad \frac{dp}{dt} = F(z) , \tag{2.3}$$

which are in the form of (2.1). It is therefore sufficient to consider in detail only methods for first-order equations. Since the matrix structure