Chapter 4
The KEPLER Problem

4.1 Introduction

The KEPLER problem [1–6] is certainly one of the most important problems in the history of physics and natural sciences in general. We will study this problem for several reasons: (i) it is a nice demonstration of the applicability of the methods introduced in the previous chapters, (ii) important concepts of the numerical treatment of ordinary differential equations can be introduced quite naturally, and (iii) it allows to revisit some of the most important aspects of classical mechanics.

The KEPLER problem is a special case of the two-body problem which is discussed in Appendix A. Let us summarize the main results. We consider two point particles interacting via the rotationally symmetric two body potential U which is solely a function of the distance between the particles. The symmetries of this problem allow several simplifications: (i) The problem can be reduced to the two dimensional motion of a point particle with reduced mass m in the central potential U. (ii) By construction, the total energy E is conserved. (iii) The length ℓ of the angular momentum vector is also conserved because of the symmetry of the potential U. Due to this rotational symmetry it is a natural choice to describe the particle's motion in polar coordinates (ρ, φ).

The final differential equations which have to be solved are of the form

$$\dot{\varphi} = \frac{\ell}{m\rho^2} \,, \tag{4.1}$$

and

$$\dot{\rho} = \pm\sqrt{\frac{2}{m}\left[E - U(\rho) - \frac{\ell^2}{2m\rho^2}\right]} \,. \tag{4.2}$$

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Here, one usually defines the effective potential

$$U_{\text{eff}}(\rho) = U(\rho) + \frac{\ell^2}{2m\rho^2}, \tag{4.3}$$

as the sum of the interaction potential and the centrifugal barrier $U_{\text{mom}}(\rho) = \ell^2/2m\rho^2$. Equation (4.2) can be transformed into an implicit equation for ρ

$$t = t_0 \pm \int_{\rho_0}^{\rho} \mathrm{d}\rho' \left\{ \frac{2}{m} \left[E - U_{\text{eff}}(\rho') \right] \right\}^{-\frac{1}{2}}, \tag{4.4}$$

with $\rho_0 \equiv \rho(t_0)$ the initial condition at time t_0. Furthermore, the angle φ is related to the radius ρ by

$$\varphi = \varphi_0 \pm \int_{\rho_0}^{\rho} \mathrm{d}\rho' \frac{\ell}{m\rho'^2} \left\{ \frac{2}{m} \left[E - U_{\text{eff}}(\rho') \right] \right\}^{-\frac{1}{2}}, \tag{4.5}$$

with the initial condition $\varphi_0 \equiv \varphi(t_0)$.

The KEPLER problem is defined by the gravitational interaction potential

$$U(\rho) = -\frac{\alpha}{\rho}, \quad \alpha > 0. \tag{4.6}$$

For this case, we show in Fig. 4.1 schematically the effective potential (4.3) (solid black line), together with the gravitational potential $U(\rho)$ (dashed-dotted line) and the centrifugal barrier U_{mom} (dashed line). The gravitational potential (4.6) is now

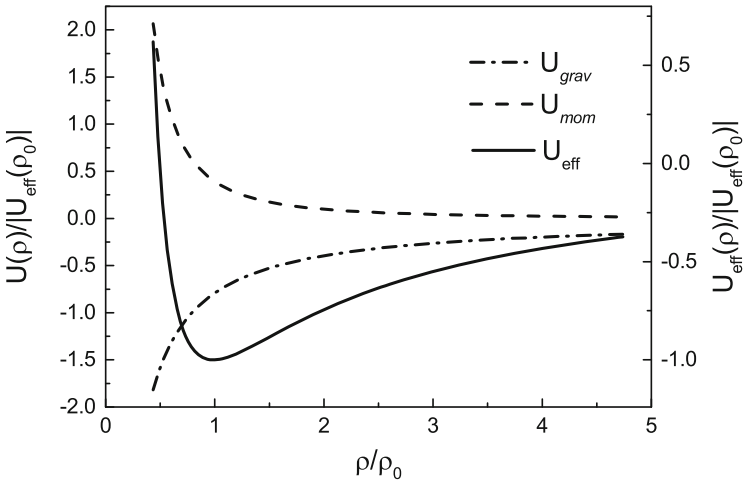

Fig. 4.1 Schematic illustration of the effective potential $U_{\text{eff}}(\rho)/U_{\text{eff}}(\rho_0)$ vs ρ/ρ_0 (*solid line, right hand scale*). Here, ρ_0 is the distance of the minimum in $U_{\text{eff}}(\rho)$. $U_{\text{grav}}(\rho)$ (*dashed-dotted line*) denotes the gravitational contribution while $U_{\text{mom}}(\rho)$ (*dashed line*) denotes the centrifugal barrier. Both potentials are normalized to $U_{\text{eff}}(\rho_0)$ (*Left hand scale applies*)

inserted into Eq. (4.5):

$$\varphi = \varphi_0 \pm \int_{\rho_0}^{\rho} \mathrm{d}\rho' \frac{\ell}{m\rho'^2} \left[\frac{2}{m} \left(E + \frac{\alpha}{\rho'} - \frac{\ell^2}{2m\rho'^2} \right) \right]^{-\frac{1}{2}} . \tag{4.7}$$

The substitution $u = 1/\rho$ simplifies Eq. (4.7) to

$$\varphi = \varphi_0 \mp \int_{u_1}^{u_2} \mathrm{d}u \left[\frac{2mE}{\ell^2} + \frac{2m\alpha}{\ell^2} u - u^2 \right]^{-\frac{1}{2}} , \tag{4.8}$$

where the integration boundaries u_1 and u_2 are $1/\rho_0$ and $1/\rho$, respectively. The integral can now be evaluated with the help of a simple substitution[1] and we obtain the angle φ as a function of ρ:

$$\varphi = \varphi_0 \pm \cos^{-1} \left(\frac{\frac{\ell}{\rho} - \frac{m\alpha}{\ell}}{\sqrt{2mE + \frac{m^2\alpha^2}{\ell^2}}} \right) + \text{const} . \tag{4.9}$$

This solution can conveniently be characterized by the introduction of two parameters, namely

$$a = \frac{\ell^2}{m\alpha} \tag{4.10}$$

and the *eccentricity* e

$$e = \sqrt{1 + \frac{2E\ell^2}{m\alpha^2}} . \tag{4.11}$$

Hence, by neglecting the integration constant and setting $\varphi_0 = 0$ we arrive at

$$\frac{a}{\rho} = 1 + e \cos(\varphi) \tag{4.12}$$

as the final form of Eq. (4.9). It describes for $e > 1$ a hyperbola, for $e = 1$ a parabola, and for $e < 1$ an ellipse. The case $e = 0$ is a special case of the ellipse and describes a circle with radius $\rho = a$. A more detailed discussion of this result, in particular the

[1] In particular, we substitute

$$w = \left(u - \frac{m\alpha}{\ell^2} \right) \left(\frac{2mE}{\ell^2} + \frac{m^2\alpha^2}{\ell^4} \right)^{-\frac{1}{2}} .$$

derivation of KEPLER's laws can be found in any textbook on classical mechanics [1–6]. We discuss now some numerical aspects.

4.2 Numerical Treatment

In the previous section we solved the KEPLER problem by evaluating the integrand (4.7) expressing the angle φ as a function of the radius ρ. However, in this section we aim at solving the integral equation (4.4) numerically with the help of the methods discussed in the previous chapter. Remember that Eq. (4.4) expresses the time t as a function of the radius ρ. This equation has to be inverted, in order to obtain $\rho(t)$, which, in turn, is then inserted into Eq. (4.1) in order to determine the angle $\varphi(t)$ as a function of time. This discussion will lead us in a natural way to the most common techniques applied to solve ordinary differential equations, which is of no surprise since Eq. (4.4) is the integral representation of Eq. (4.2).

We give a short outline of what we plan to do: We discretize the time axis in equally spaced time steps Δt, i.e. $t_n = t_0 + n\Delta t$. Accordingly, we define the radius ρ at time $t = t_n$ as $\rho(t_n) \equiv \rho_n$. We can use the methods introduced in Chap. 3 to approximate the integral (4.4) from some ρ_n to ρ_{n+1}. According to this chapter the absolute error introduced will behave like $\delta = |\rho_n - \rho_{n+1}|^K$ where the explicit value of K depends on the method used. However, since the radius ρ changes continuously with time t we know that for sufficiently small values of Δt the error δ will also become arbitrarily small. If we start from some initial values t_0 and ρ_0, we can successively calculate the values $\rho_1, \rho_2, \ldots$, by applying a small time step Δt.

Let us start by rewriting Eq. (4.4) as:

$$t - t_0 = \int_{\rho_0}^{\rho} \mathrm{d}\rho' f(\rho') \; . \tag{4.13}$$

As we discretized the time axis in equally spaced increments and defined $\rho_n \equiv \rho(t_n)$, we can rewrite (4.13) as

$$\Delta t = t_n - t_{n-1} = \int_{\rho_n}^{\rho_{n+1}} \mathrm{d}\rho' f(\rho') \; . \tag{4.14}$$

The forward rectangular rule, (3.9), results in the approximation

$$\Delta t = (\rho_{n+1} - \rho_n) f(\rho_n) \; . \tag{4.15}$$

We solve this equation for ρ_{n+1} and obtain

$$\rho_{n+1} = h(\rho_n)\Delta t + \rho_n \,, \tag{4.16}$$

where we defined

$$h(\rho) = \frac{1}{f(\rho)} = \sqrt{\frac{2}{m}\left[E - U_{\text{eff}}(\rho)\right]} \,, \tag{4.17}$$

following Eqs. (4.2) and (4.3). As Eq. (4.4) is the integral representation of the ordinary differential equation (4.2), approximation (4.16) corresponds to the approximation

$$D_+\rho_n = h(\rho_n) \,, \tag{4.18}$$

where $D_+\rho_n$ is the forward difference derivative (2.10a). Since the left hand side of the discretized differential equation (4.18) is independent of ρ_{n+1}, this method is referred to as an *explicit* method. In particular, consider an ordinary differential equation of the form

$$\dot{y} = F(y) \,. \tag{4.19}$$

Then the approximation method is referred to as an *explicit* EULER *method* if it is of the form

$$y_{n+1} = y_n + F(y_n)\Delta t \,. \tag{4.20}$$

Note that y might be a vector.

Let us use the backward rectangular rule (3.10) to solve Eq. (4.14). We obtain

$$t_{n+1} - t_n = (\rho_{n+1} - \rho_n) f(\rho_{n+1}) \,, \tag{4.21}$$

or equivalently

$$\rho_{n+1} = \rho_n + h(\rho_{n+1})\Delta t \,. \tag{4.22}$$

Again, this corresponds to an approximation of the differential equation (4.2) by

$$D_-\rho_{n+1} = h(\rho_{n+1}) \,, \tag{4.23}$$

where $D_-(\rho_{n+1})$ is the backward difference derivative (2.10b). In this case the quantity of interest ρ_{n+1} still appears in the argument of the function $h(\rho)$ and Eq. (4.22) is an *implicit* equation for ρ_{n+1} which has to be solved. In general, if the problem (4.19) is approximated by an algorithm of the form

$$y_{n+1} = y_n + F(y_{n+1})\Delta t \,, \tag{4.24}$$

it is referred to as an *implicit* EULER *method*. Note that the implicit equation (4.24) might be analytically unsolvable. Hence, one has to employ a numerical method to solve (4.24) which will also imply a numerical error. However, in the particular case of Eq. (4.22) we can solve it analytically since it is a fourth order polynomial in ρ_{n+1} of the form

$$\rho_{n+1}^4 - 2\rho_n\rho_{n+1}^3 + \left(\rho_n^2 - \frac{2E\Delta t^2}{m}\right)\rho_{n+1}^2 - \frac{2\alpha\Delta t^2}{m}\rho_{n+1} + \frac{\ell^2\Delta t^2}{m^2} = 0\,. \tag{4.25}$$

The solution of this equation is quite tedious and will not be discussed here, however, the method one employs is referred to as FERRARI's method [7].

A natural way to proceed is to regard the central rectangular rule (3.13) in a next step. Within this approximation we obtain for Eq. (4.13)

$$\Delta t = (\rho_{n+1} - \rho_n) f\left(\frac{\rho_{n+1} + \rho_n}{2}\right)\,, \tag{4.26}$$

which is equivalent to the implicit equation

$$\rho_{n+1} = \rho_n + h\left(\frac{\rho_{n+1} + \rho_n}{2}\right)\Delta t\,. \tag{4.27}$$

It can be written as an approximation to Eq. (4.2) with help of the central difference derivative $D_c\rho_{n+\frac{1}{2}}$:

$$D_c\rho_{n+\frac{1}{2}} = h\left(\frac{\rho_{n+1} + \rho_n}{2}\right)\,. \tag{4.28}$$

In general, for a problem of the form (4.19) a method of the form

$$y_{n+1} = y_n + F\left(\frac{y_{n+1} + y_n}{2}\right)\Delta t\,, \tag{4.29}$$

is referred to as the *implicit midpoint rule*. We note that this method might be more accurate since the error of the rectangular rule scales like $\mathcal{O}(\Delta t^2)$ while the error of the forward and backward rectangular rules scale like $\mathcal{O}(\Delta t)$. Nevertheless, in case of the KEPLER problem, one can solve the implicit equation (4.27) analytically for ρ_{n+1} which is certainly of advantage.

In this chapter the KEPLER problem was instrumental in introducing three common methods which can be employed to solve numerically ordinary differential equations of the form (4.19). More general and advanced methods to solve ordinary differential equations and a more systematic description of these methods will be offered in the next chapter.

However, let us discuss another point before proceeding to the chapter on the numerics of ordinary differential equations. As demonstrated in Sect. 1.3 the

approximation of the integral (4.4) involves a numerical error. What will be the consequence of this error? Since we demonstrated that the approximations we discussed result in a differential equation in finite difference form, i.e. Eqs. (4.18), (4.23), and (4.27), we know that the derivative $\dot{\rho}$ will exhibit an error. Consequently, energy conservation [see Appendix A, Eq. (A.27)] will be violated with the implication that deviations from the trajectory (4.12) can be expected. This is definitely not desirable.

A solution is provided by a special class of methods, known as *symplectic integrators*, which were specifically designed for such cases. They are based on a formulation of the problem using HAMILTON's equations of motion. (See, for instance, Refs. [1–5].) In the particular case of the KEPLER problem the HAMILTON function is equivalent to the total energy of the system and reads (in some scaled units):

$$H(p,q) = \frac{1}{2}\left(p_1^2 + p_2^2\right) - \frac{1}{\sqrt{q_1^2 + q_2^2}} \,. \tag{4.30}$$

Here $p = (p_1, p_2)$ are the generalized momentum coordinates of the point particle in the two-dimensional plane and (q_1, q_2) are the generalized position coordinates. From this HAMILTON's equations of motion

$$\begin{pmatrix} \dot{q} \\ \dot{p} \end{pmatrix} = \begin{pmatrix} \nabla_p H(p,q) \\ -\nabla_q H(p,q) \end{pmatrix} = \begin{pmatrix} a(q,p) \\ b(q,p) \end{pmatrix} \,, \tag{4.31}$$

follow, where the functions $a(q,p)$ and $b(q,p)$ have been introduced for a more convenient notation. Note that these functions are two dimensional vectors in the case of KEPLER's problem. The so called *symplectic* EULER *method* is given by

$$\begin{aligned} q_{n+1} &= q_n + a(q_n, p_{n+1})\Delta t \,, \\ p_{n+1} &= p_n + b(q_n, p_{n+1})\Delta t \,. \end{aligned} \tag{4.32}$$

Obviously, the first equation is explicit while the second is implicit. An alternative formulation reads

$$\begin{aligned} q_{n+1} &= q_n + a(q_{n+1}, p_n)\Delta t \,, \\ p_{n+1} &= p_n + b(q_{n+1}, p_n)\Delta t \,, \end{aligned} \tag{4.33}$$

where the first equation is implicit and the second equation is explicit. Of course, Eq. (4.31) may be solved with the help of the explicit EULER method (4.20), the implicit EULER method (4.24) or the implicit midpoint rule (4.29). The solution should be equivalent to solving Eq. (4.4) with the respective method and then calculating (4.1) successively. Again, a more systematic discussion of symplectic integrators can be found in the following chapters.

Let us conclude this chapter with a final remark. We decided to solve Eqs. (4.4) and (4.1) because we wanted to reproduce the dynamics of the system, i.e. we wanted to obtain $\rho(t)$ and $\varphi(t)$. This directed us to the numerical solution of two integrals. If we wanted to employ symplectic methods, which provide several advantages, we would have to solve four differential equations (4.31) instead of two integrals. Moreover, if we are not interested in the time evolution of the system but in the form of the trajectory in general, we could simply evaluate the integral (4.5) analytically or, if an analytical solution is not feasible for the potential $U(\rho)$ one is interested in, numerically. Methods to approximate such an integral were extensively discussed in Chap. 3.

Summary

KEPLER's two-body problem was used as an incentive to introduce intuitively numerical methods to solve ordinary first order differential equations. To serve this purpose the basic differential equations were transformed into integral form. These integrals were then solved with the help of the rules discussed in Sect. 3.2. Three basic methods have been identified, namely the *explicit* EULER method (based on the forward difference derivative), the *implicit* EULER method (based on the backward difference derivative), and the *explicit midpoint rule* (based on the central rectangular rule). Shortcomings of such methods have been discussed briefly as were remedies to overcome these.

Problems

1. Planetary-Orbits: Apply the methods of numerical integration to the integral (4.4) and compare it to the analytical result. Identify the three different cases of elliptic, parabolic or hyperbolic orbits by varying the initial conditions.
2. LENNARD-JONES Scattering: Consider the scattering of two point particles which interact via the LENNARD-JONES potential $U(r) = 4\sigma[(\varepsilon/r)^{12} - (\varepsilon/r)^6]$ with $\sigma, \varepsilon > 0$ (see Chapter 7). Calculate the orbit $\varphi(\rho)$.
3. Harmonic-Motion: Consider the motion of a point particle in the radial harmonic oscillator $U(\rho) = m\omega^2\rho^2/2$. According to BERTRAND's theorem (see Refs. [1–3]) the particle's trajectories should be closed orbits. Demonstrate this numerically as well as analytically.

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