Chapter 2

N-Body Problems with $2 \leq N \leq 100$

2.1. Introduction

In general, we will wish to consider N-body problems in which N may be relatively large and relatively small. N-body problems with $2 \leq N \leq 100$ will be considered to be *small* and we will begin with these. For $N = 2$, and under important restrictions, it may be possible to solve related problems in closed form. This is the case, for example, in astromechanics (van de Kamp (1964)). Inclusion of various important constraints, however, then demands numerical methodology.

Now, if N is small, we would like to do a very good job in solving the N-body problem. By this we mean that we would like not only to solve the problem with accuracy, but we would also like to preserve numerically any basic physical invariants of the system. To do this in detail, we concentrate theoretically and computationally on the 3-body problem, because it contains *all* the difficulties of the general N-body problem. The entire discussion extends in a natural way to the general N-body problem, and, in particular, to the more simplistic 2-body problem.

For $i = 1, 2, 3$, let P_i of mass m_i be at $\vec{r}_i = (x_i, y_i, z_i)$ at time t. Let the positive distance between P_i and P_j, $i \neq j$, be $r_{ij} = r_{ji}$. Let $\phi = \phi_{ij} = \phi(r_{ij})$, given in ergs, be a potential for the pair P_i, P_j. Then the force on P_i due to P_j is

$$\vec{F}_i = -\frac{\partial \phi}{\partial r_{ij}} \frac{\vec{r}_i - \vec{r}_j}{r_{ij}},$$

and in this section we assume Newtonian dynamical differential equations for the 3-body problem, and these are

$$m_i \frac{d^2 \vec{r}_i}{dt^2} = -\frac{\partial \phi}{\partial r_{ij}} \frac{\vec{r}_i - \vec{r}_j}{r_{ij}} - \frac{\partial \phi}{\partial r_{ik}} \frac{\vec{r}_i - \vec{r}_k}{r_{ik}}, \quad i = 1, 2, 3 \tag{2.1}$$

where $i = 1$ implies $j = 2, k = 3$; $i = 2$ implies $j = 1, k = 3$; $i = 3$ implies $j = 1, k = 2$.

The following summary theorem incorporates several well known results.

Theorem 2.1. (Goldstein (1980)) *System* (2.1) *conserves energy, linear momentum, and angular momentum. It is also covariant under translation, rotation, and uniform relative motion of coordinate frames.*

2.2. Numerical Methodology

In general, (2.1) will be nonlinear and will require numerical methodology. In order to solve an initial value problem for (2.1) numerically, we first rewrite it as the equivalent first order system

$$\frac{d\vec{r}_i}{dt} = \vec{v}_i, \quad i = 1, 2, 3 \tag{2.2}$$

$$m_i \frac{d\vec{v}_i}{dt} = -\frac{\partial \phi}{\partial r_{ij}} \frac{\vec{r}_i - \vec{r}_j}{r_{ij}} - \frac{\partial \phi}{\partial r_{ik}} \frac{\vec{r}_i - \vec{r}_k}{r_{ik}}, \quad i = 1, 2, 3. \tag{2.3}$$

Our numerical formulation now proceeds as follows. For $\Delta t > 0$, let $t_n = n(\Delta t), n = 0, 1, 2, \ldots$. At time t_n, let P_i be at $\vec{r}_{i,n} = (x_{i,n}, y_{i,n}, z_{i,n})$ with velocity $\vec{v}_{i,n} = (v_{i,x,n}, v_{i,y,n}, v_{i,z,n})$. Denote the distances $\|P_1P_2\|$, $\|P_1P_3\|$, $\|P_2P_3\|$ by $r_{12,n}$, $r_{13,n}$, $r_{23,n}$, respectively. Differential equations (2.2) and (2.3) are now approximated, respectively, by the difference equations

$$\frac{\vec{r}_{i,n+1} - \vec{r}_{i,n}}{\Delta t} = \frac{\vec{v}_{i,n+1} + \vec{v}_{i,n}}{2} \tag{2.4}$$

$$\begin{aligned} m_i \frac{\vec{v}_{i,n+1} - \vec{v}_{i,n}}{\Delta t} = & -\frac{\phi(r_{ij,n+1}) - \phi(r_{ij,n})}{r_{ij,n+1} - r_{ij,n}} \frac{\vec{r}_{i,n+1} + \vec{r}_{i,n} - \vec{r}_{j,n+1} - \vec{r}_{j,n}}{r_{ij,n+1} + r_{ij,n}} \\ & - \frac{\phi(r_{ik,n+1}) - \phi(r_{ik,n})}{r_{ik,n+1} - r_{ik,n}} \frac{\vec{r}_{i,n+1} + \vec{r}_{i,n} - \vec{r}_{k,n+1} - \vec{r}_{k,n}}{r_{ik,n+1} + r_{ik,n}}. \end{aligned} \tag{2.5}$$

Note that the force is approximated, not the potential. We take the very same potential as in continuum mechanics, the significance of which will be seen shortly. Consistency follows immediately as $\Delta t \to 0$. Also note that, for the present, we assume in (2.5) that $r_{lm,n+1} \neq r_{lm,n}$, for any choices of l, m.

System (2.4), (2.5) consists of 18 implicit equations for the unknowns $x_{i,n+1}$, $y_{i,n+1}, z_{i,n+1}, v_{i,x,n+1}, v_{i,y,n+1}, v_{i,z,n+1}$ in the 18 knowns $x_{i,n}$, $y_{i,n}$, $z_{i,n}$, $v_{i,x,n}$, $v_{i,y,n}$, $v_{i,z,n}$ and is solvable readily by Newton's method, as described in Appendix II.

2.3. Conservation Laws

Because of its physical significance, let us show now that the numerical solution generated by (2.4) and (2.5) conserves the same energy, linear momentum, and angular momentum as does (2.1).

Consider first energy conservation. Define

$$W_N = \sum_{n=0}^{N-1} \left\{ \sum_{i=1}^{3} m_i(\vec{r}_{i,n+1} - \vec{r}_{i,n}) \cdot (\vec{v}_{i,n+1} - \vec{v}_{i,n})/\Delta t \right\}. \tag{2.6}$$

Note immediately relative to (2.6) that, since we are considering specifically the three-body problem, the symbol N in summation (2.6) is, in this section only, a numerical time index. Then insertion of (2.4) into (2.6) and simplification yields

$$\begin{aligned} W_N = & \frac{1}{2}m_1(v_{1,N})^2 + \frac{1}{2}m_2(v_{2,N})^2 + \frac{1}{2}m_3(v_{3,N})^2 \\ & - \frac{1}{2}m_1(v_{1,0})^2 - \frac{1}{2}m_2(v_{2,0})^2 - \frac{1}{2}m_3(v_{3,0})^2, \end{aligned}$$

so that

$$W_N = K_N - K_0. \tag{2.7}$$

Insertion of (2.5) into (2.6) implies, with some tedious algebraic manipulation,

$$W_N = \sum_{n=0}^{N-1} (-\phi_{12,n+1} - \phi_{13,n+1} - \phi_{23,n+1} + \phi_{12,n} + \phi_{13,n} + \phi_{23,n})$$

so that

$$W_N = -\phi_N + \phi_0. \tag{2.8}$$

Elimination of W_N between (2.7) and (2.8) then yields conservation of energy, that is,

$$K_N + \phi_N = K_0 + \phi_0, \quad N = 1, 2, 3, \ldots.$$

Moreover, since K_0 and ϕ_0 depend only on initial data, it follows that K_0 and ϕ_0 are the same in both the continuous and the discrete cases, so that the energy conserved by the numerical method is exactly that of the continuous system. Note, in addition, that the proof is independent of Δt. Thus, we have proved the following theorem.

Theorem 2.2. *Independently of Δt, the numerical method of Section 2.2 is energy conserving, that is,*

$$K_N + \phi_N = K_0 + \phi_0, \quad N = 1, 2, 3, \ldots.$$

To show the conservation of linear momentum, we proceed as follows. The linear momentum $\vec{M}_i(t_n) = \vec{M}_{i,n}$ of P_i at t_n is defined to be the vector

$$\vec{M}_{i,n} = m_i(v_{i,n,x}, v_{i,n,y}, v_{i,n,z}). \tag{2.9}$$

The linear momentum $\vec{M}_n$ of the three-body system at time t_n is defined to be the vector

$$\vec{M}_n = \sum_{i=1}^{3} \vec{M}_{i,n}. \tag{2.10}$$

Now, from (2.5),

$$m_1(\vec{v}_{1,n+1} - \vec{v}_{1,n}) + m_2(\vec{v}_{2,n+1} - \vec{v}_{2,n}) + m_3(\vec{v}_{3,n+1} - \vec{v}_{3,n}) \equiv \vec{0}.$$

Thus, for $n = 0, 1, 2, \ldots,$

$$m_1(v_{1,n+1,x} - v_{1,n,x}) + m_2(v_{2,n+1,x} - v_{2,n,x}) + m_3(v_{3,n+1,x} - v_{3,n,x}) = 0. \tag{2.11}$$

Summing both sides of (2.11) from $n = 0$ to $n = N - 1$ implies

$$m_1 v_{1,N,x} + m_2 v_{2,N,x} + m_3 v_{3,N,x} = C_1, \quad N \geq 1 \tag{2.12}$$

in which

$$m_1 v_{1,0,x} + m_2 v_{2,0,x} + m_3 v_{3,0,x} = C_1. \tag{2.13}$$

Similarly,

$$m_1 v_{1,N,y} + m_2 v_{2,N,y} + m_3 v_{3,N,y} = C_2 \tag{2.14}$$

$$m_1 v_{1,N,z} + m_2 v_{2,N,z} + m_3 v_{3,N,z} = C_3 \tag{2.15}$$

in which

$$m_1 v_{1,0,y} + m_2 v_{2,0,y} + m_3 v_{3,0,y} = C_2 \tag{2.16}$$

$$m_1 v_{1,0,z} + m_2 v_{2,0,z} + m_3 v_{3,0,z} = C_3. \tag{2.17}$$

Thus,

$$\vec{M}_n = \sum_{i=1}^{3} \vec{M}_{i,n} = (C_1, C_2, C_3) = \vec{M}_0, \quad n = 1, 2, 3, \ldots,$$

which is the classical law of conservation of linear momentum. Note that $\vec{M}_0$ depends only on the initial data. Thus we have the following theorem.

Theorem 2.3. *Independently of* Δt*, the numerical method of Section* 2.2 *conserves linear momentum, that is,*

$$\vec{M}_n = \vec{M}_0, \quad n = 1, 2, 3, \ldots.$$

To show the conservation of angular momentum, we proceed as follows. The angular momentum $\vec{L}_{i,n}$ of P_i at t_n is defined to be the cross product vector

$$\vec{L}_{i,n} = m_i(\vec{r}_{i,n} \times \vec{v}_{i,n}). \tag{2.18}$$

The angular momentum of a three-body system at t_n is defined to be the vector

$$\vec{L}_n = \sum_{i=1}^{3} \vec{L}_{i,n}. \tag{2.19}$$

It then follows readily that

$$\begin{aligned}
&\vec{L}_{i,n+1} - \vec{L}_{i,n} \\
&\quad = m_i(\vec{r}_{i,n+1} + \vec{r}_{i,n}) \times (\vec{v}_{i,n+1} - \vec{v}_{i,n}) \\
&\quad = m_i \Bigg[(\vec{r}_{i,n+1} - \vec{r}_{i,n}) \times \frac{1}{2}(\vec{v}_{i,n+1} + \vec{v}_{i,n}) \\
&\qquad\qquad + \frac{1}{2}(\vec{r}_{i,n+1} + \vec{r}_{i,n}) \times (\vec{v}_{i,n+1} - \vec{v}_{i,n})\Bigg] \\
&\quad = m_i \left[(\vec{r}_{i,n+1} - \vec{r}_{i,n}) \times \frac{1}{\Delta t}(\vec{r}_{i,n+1} - \vec{r}_{i,n}) + \frac{1}{2}(\vec{r}_{i,n+1} + \vec{r}_{i,n}) \times \vec{a}_{i,n}\Delta t\right] \\
&\quad = \frac{1}{2}(\Delta t)(\vec{r}_{i,n+1} + \vec{r}_{i,n}) \times \vec{F}_{i,n}.
\end{aligned}$$

For notational simplicity, set

$$\vec{T}_{i,n} = \frac{1}{2}(\vec{r}_{i,n+1} + \vec{r}_{i,n}) \times \vec{F}_{i,n}.$$

It follows readily, with some algebraic manipulation, that

$$\vec{T}_n = \vec{T}_{1,n} + \vec{T}_{2,n} + \vec{T}_{3,n} = 0.$$

Thus, one finds

$$\vec{L}_{n+1} - \vec{L}_n = \vec{0}, \quad n = 0, 1, 2, 3, \ldots,$$

so that

$$\vec{L}_n = \vec{L}_0, \quad n = 1, 2, 3, \ldots,$$

which implies, independently of Δt, the conservation of angular momentum. Note again that $\vec{L}_0$ depends only on the initial data. Thus the following theorem has been proved.

Theorem 2.4. *Independently of* Δt, *the numerical method of Section* 2.2 *conserves angular momentum, that is*

$$\vec{L}_n = \vec{L}_0, \quad n = 1, 2, 3, \ldots.$$

2.4. Covariance

We begin the discussion of Newtonian covariance by stating the basic concepts. When a dynamical equation is structurally invariant under a transformation, the equation is said to be *covariant or symmetric*. The transformations we will consider are the basic ones, namely, translation, rotation, and uniform relative motion. We will concentrate on two dimensional systems, because the related techniques and results extend directly to three dimensions. A general Newtonian force will be considered. Finally, we will concentrate on the motion of a single particle P of mass m, with extension to the N-body problem following in a natural way. And though the assumptions just made may seem to be excessive, it will be seen shortly that they render the required mathematical methodology readily transparent.

Suppose now that a particle P of mass m is in motion in the XY plane and that for $\Delta t > 0$ its motion from given initial data is determined by a force $\vec{F}(t_n) = \vec{F}_n = (F_{n,x},\ F_{n,y})$ and by the dynamical difference equations

$$F_{n,x} = m(v_{n+1,x} - v_{n,x})/(\Delta t) \tag{2.20}$$

$$F_{n,y} = m(v_{n+1,y} - v_{n,y})/(\Delta t). \tag{2.21}$$

The fundamental problem that we now consider is as follows. Let $x = f_1(x^*, y^*), y = f_2(x^*, y^*)$ be a change of coordinates. Under this transformation, let $F_{n,x} = F^*_{n,x^*}, F_{n,y} = F^*_{n,y^*}$. Then we will want to prove that in the X^*Y^* system the dynamical equations of motion are

$$F^*_{n,x^*} = m(v_{n+1,x^*} - v_{n,x^*})/(\Delta t) \tag{2.22}$$

$$F^*_{n,y^*} = m(v_{n+1,y^*} - v_{n,y^*})/(\Delta t), \tag{2.23}$$

which will establish covariance.

In consistency with (2.4), we assume that

$$\frac{x_{n+1} - x_n}{\Delta t} = \frac{v_{n+1,x} + v_{n,x}}{2}, \quad \frac{x^*_{n+1} - x^*_n}{\Delta t} = \frac{v_{n+1,x^*} + v_{n,x^*}}{2} \tag{2.24}$$

$$\frac{y_{n+1} - y_n}{\Delta t} = \frac{v_{n+1,y} + v_{n,y}}{2}, \quad \frac{y^*_{n+1} - y^*_n}{\Delta t} = \frac{v_{n+1,y^*} + v_{n,y^*}}{2}. \tag{2.25}$$

Relative to (2.24) and (2.25), the following lemma will be of value.

Lemma 2.1. *Equations* (2.24) *and* (2.25) *imply*

$$v_{1,x} = \frac{2}{\Delta t}(x_1 - x_0) - v_{0,x}; \quad v_{1,x^*} = \frac{2}{\Delta t}(x^*_1 - x^*_0) - v_{0,x^*} \tag{2.26}$$

$$v_{1,y} = \frac{2}{\Delta t}(y_1 - y_0) - v_{0,y}; \quad v_{1,y^*} = \frac{2}{\Delta t}(y^*_1 - y^*_0) - v_{0,y^*} \tag{2.27}$$

$$v_{n,x} = \frac{2}{\Delta t}\left[x_n + (-1)^n x_0 + 2\sum_{j=1}^{n-1}(-1)^j x_{n-j}\right] + (-1)^n v_{0,x}, \quad n \ge 2 \tag{2.28}$$

$$v_{n,x^*} = \frac{2}{\Delta t}\left[x^*_n + (-1)^n x^*_0 + 2\sum_{j=1}^{n-1}(-1)^j x^*_{n-j}\right] + (-1)^n v_{0,x^*}, \quad n \ge 2 \tag{2.29}$$

$$v_{n,y} = \frac{2}{\Delta t}\left[y_n + (-1)^n y_0 + 2\sum_{j=1}^{n-1}(-1)^j y_{n-j}\right] + (-1)^n v_{0,y}, \quad n \ge 2 \tag{2.30}$$

$$v_{n,y^*} = \frac{2}{\Delta t}\left[y^*_n + (-1)^n y^*_0 + 2\sum_{j=1}^{n-1}(-1)^j y^*_{n-j}\right] + (-1)^n v_{0,y^*}, \quad n \ge 2. \tag{2.31}$$

Proof. Equations (2.26) follow directly from (2.24) with $n = 0$. Equations (2.27) follow directly from (2.25) with $n = 0$. Equations (2.28)–(2.31) follow readily by mathematical induction. □

Theorem 2.5. *Equations* (2.20) and (2.21) *are covariant relative to the translation*

$$x^* = x - a, \quad y^* = y - b; \quad a, b \text{ constants}.$$

Proof. Define $v_{0,x} = v_{0,x^*}, v_{0,y} = v_{0,y^*}$. Then, from (2.26) in Lemma 2.1,

$$v_{1,x} = \frac{2}{\Delta t}\big[(x_1^* + a) - (x_0^* + a)\big] - v_{0,x^*} = v_{1,x^*}.$$

Similarly,

$$v_{1,y} = v_{1,y^*}$$

For $n > 1$, (2.28) and (2.29) in Lemma 2.1 yield

$$v_{n,x} = \frac{2}{\Delta t}\left[(x_n^* + a) + (-1)^n(x_0^* + a) + 2\sum_{j=1}^{n-1}(-1)^j(x_{n-j}^* + a)\right] + (-1)^n v_{0,x^*}. \tag{2.32}$$

However, by the lemma, for n both odd and even, (2.32) implies

$$v_{n,x} = v_{n,x^*}.$$

Similarly,

$$v_{n,y} = v_{n,y^*}.$$

Thus, for all $n = 0, 1, 2, 3, \ldots$

$$v_{n,x} = v_{n,x^*},$$
$$v_{n,y} = v_{n,y^*}.$$

Thus,

$$F_{n,x^*}^* = F_{n,x} = m\frac{v_{n+1,x} - v_{n,x}}{\Delta t} = m\frac{v_{n+1,x^*} - v_{n,x^*}}{\Delta t}.$$

Similarly,

$$F_{n,y^*}^* = m\frac{v_{n+1,y^*} - v_{n,y^*}}{\Delta t},$$

and the theorem is proved. □

Theorem 2.6. *Under the rotation*

$$\begin{cases} x^* &= x\cos\theta + y\sin\theta \\ y^* &= y\cos\theta - x\sin\theta \end{cases} \tag{2.33}$$

where θ *is the smallest positive angle measured counterclockwise from the* X *to the* X^* *axis, Eqs.* (2.20), (2.21) *are covariant.*

Proof. The proof follows along the same lines as that of Theorem 2.5 after one defines

$$\begin{cases} v_{0,x^*} &= v_{0,x}\cos\theta + v_{0,y}\sin\theta \\ v_{0,y^*} &= v_{0,y}\cos\theta - v_{0,x}\sin\theta \end{cases} \tag{2.34}$$

and notes that

$$\begin{cases} F^*_{n,x^*} &= F_{n,x}\cos\theta + F_{n,y}\sin\theta \\ F^*_{n,y^*} &= F_{n,y}\cos\theta - F_{n,x}\sin\theta \end{cases}. \tag{2.35}$$

□

Theorem 2.7. *Under relative uniform motion of coordinate systems, Eqs.* (2.20), (2.21) *are covariant.*

Proof. Consider first motion in one dimension. Assume then that the X and X^* axes are in relative motion defined by

$$x^*_n = x_n - ct_n, \quad n = 0, 1, 2, 3, \ldots, \tag{2.36}$$

in which c is a positive constant. If $v_{0,x}$ is the initial velocity of P along the X axis, define v_{0,x^*} along the X^* axis by

$$v_{0,x^*} = v_{0,x} - c. \tag{2.37}$$

Hence, for $n = 1$,

$$v_{1,x} = \frac{2}{\Delta t}\left[(x^*_1 + ct_1) - (x^*_0 + ct_0)\right] - v_{0,x} = v_{1,x^*} + c. \tag{2.38}$$

For $n > 1$,

$$\begin{aligned} v_{n,x} = {} & \frac{2}{\Delta t}\left\{x^*_n + (-1)^n x^*_0 + 2\sum_{j=1}^{n-1}(-1)^j x^*_{n-j}\right\} + (-1)^n v_{0,x} \\ & + \frac{2c}{\Delta t}\left\{t_n + (-1)^n t_0 + 2\sum_{j=1}^{n-1}(-1)^j t_{n-j}\right\}. \end{aligned}$$

But, it follows readily that

$$t_n + (-1)^n t_0 + 2\sum_{j=1}^{n-1}(-1)^j t_{n-j} = \begin{cases} 0, & n \text{ even} \\ \Delta t, & n \text{ odd} \end{cases}.$$

Thus, with the aid of the lemma, it follows that for both n odd and even,

$$v_{n,x} = v_{n,x^*} + c.$$

Thus for all $n = 0, 1, 2, 3, \ldots,$

$$F^*_{n,x^*} = F_{n,x} = m\frac{v_{n+1,x^*} + c - v_{n,x^*} - c}{\Delta t} = m\frac{v_{n+1,x^*} - v_{n,x^*}}{\Delta t}. \tag{2.39}$$

Under the assumption that

$$y^* = y - dt_n$$

in which d is a constant, one finds similarly that

$$F^*_{n,y^*} = m\frac{v_{n+1,y^*} - v_{n,y^*}}{\Delta t}, \tag{2.40}$$

and the covariance is established. □

2.5. Perihelion Motion

In this section and in the next two sections, we show how to apply conservative methodology to problems in physics. As a first application, let us examine a planar 3-body problem in which the force of interaction is gravitation. In such problems conservation of energy, linear momentum, and angular momentum are basic.

Let $P_i, i = 1, 2, 3$, be three bodies, with respective masses m_i, in motion in the XY plane, in which the force of interaction is gravitation. The force $\vec{F}_{i,j}$ between any two of the bodies will have magnitude $F_{i,j} = G\frac{m_i m_j}{r^2_{ij}}$, in which $G = (6.67)10^{-8}$, and r_{ij} is the distance between the bodies. For initial data, let us choose

$$
\begin{array}{lll}
m_1 = (6.67)^{-1}10^8 & m_2 = (6.67)^{-1}10^6 & m_3 = (6.67)^{-1}10^5 \\
x_{1,0} = 0.0 & x_{2,0} = 0.5 & x_{3,0} = -1.0 \\
y_{1,0} = 0.0 & y_{2,0} = 0.0 & y_{3,0} = 8.0 \\
v_{1,0,x} = 0.0 & v_{2,0,x} = 0.0 & v_{3,0,x} = 0.0 \\
v_{1,0,y} = 0.0 & v_{2,0,y} = 1.63 & v_{3,0,y} = -3.75.
\end{array}
$$

The differential equations of motion for this system are

$$
\begin{aligned}
m_1\ddot{x}_1 &= -\frac{Gm_1m_2}{r_{12}^2}\frac{x_1 - x_2}{r_{12}} - \frac{Gm_1m_3}{r_{13}^2}\frac{x_1 - x_3}{r_{13}} \\
m_1\ddot{y}_1 &= -\frac{Gm_1m_2}{r_{12}^2}\frac{y_1 - y_2}{r_{12}} - \frac{Gm_1m_3}{r_{13}^2}\frac{y_1 - y_3}{r_{13}} \\
m_2\ddot{x}_2 &= -\frac{Gm_1m_2}{r_{12}^2}\frac{x_2 - x_1}{r_{12}} - \frac{Gm_2m_3}{r_{23}^2}\frac{x_2 - x_3}{r_{23}} \\
m_2\ddot{y}_2 &= -\frac{Gm_1m_2}{r_{12}^2}\frac{y_2 - y_1}{r_{12}} - \frac{Gm_2m_3}{r_{23}^2}\frac{y_2 - y_3}{r_{23}} \\
m_3\ddot{x}_3 &= -\frac{Gm_1m_3}{r_{13}^2}\frac{x_3 - x_1}{r_{13}} - \frac{Gm_2m_3}{r_{23}^2}\frac{x_3 - x_2}{r_{23}} \\
m_3\ddot{y}_3 &= -\frac{Gm_1m_3}{r_{13}^2}\frac{y_3 - y_1}{r_{13}} - \frac{Gm_2m_3}{r_{23}^2}\frac{y_3 - y_2}{r_{23}},
\end{aligned}
$$

in which

$$r_{ij}^2 = (x_i - x_j)^2 + (y_i - y_j)^2.$$

For $\Delta t = 0.001$, and $i = 1, 2, 3;\ n = 0, 1, 2, \ldots,$ we approximate the solution of this system with the following form of the recursion formulas, which is most convenient for Newtonian iteration, since the denominators in the iteration formulas are all unity:

$$
\begin{aligned}
x_{i,n+1} - x_{i,n} - \frac{1}{2}(\Delta t)(v_{i,n+1,x} + v_{i,n,x}) &= 0 \\
y_{i,n+1} - y_{i,n} - \frac{1}{2}(\Delta t)(v_{i,n+1,y} + v_{i,n,y}) &= 0 \\
v_{i,n+1,x} - v_{i,n,x} - \frac{\Delta t}{m_i}F_{i,n,x} &= 0 \\
v_{i,n+1,y} - v_{i,n,y} - \frac{\Delta t}{m_i}F_{i,n,y} &= 0,
\end{aligned}
$$

in which the F's are given by

$$F_{1,n,x} = -\frac{Gm_1m_2[(x_{1,n+1}+x_{1,n})-(x_{2,n+1}+x_{2,n})]}{r_{12,n}r_{12,n+1}[r_{12,n}+r_{12,n+1}]} - \frac{Gm_1m_3[(x_{1,n+1}+x_{1,n})-(x_{3,n+1}+x_{3,n})]}{r_{13,n}r_{13,n+1}[r_{13,n}+r_{13,n+1}]}$$

$$F_{1,n,y} = -\frac{Gm_1m_2[(y_{1,n+1}+y_{1,n})-(y_{2,n+1}+y_{2,n})]}{r_{12,n}r_{12,n+1}[r_{12,n}+r_{12,n+1}]} - \frac{Gm_1m_3[(y_{1,n+1}+y_{1,n})-(y_{3,n+1}+y_{3,n})]}{r_{13,n}r_{13,n+1}[r_{13,n}+r_{13,n+1}]}$$

$$F_{2,n,x} = -\frac{Gm_1m_2[(x_{2,n+1}+x_{2,n})-(x_{1,n+1}+x_{1,n})]}{r_{12,n}r_{12,n+1}[r_{12,n}+r_{12,n+1}]} - \frac{Gm_2m_3[(x_{2,n+1}+x_{2,n})-(x_{3,n+1}+x_{3,n})]}{r_{23,n}r_{23,n+1}[r_{23,n}+r_{23,n+1}]}$$

$$F_{2,n,y} = -\frac{Gm_1m_2[(y_{2,n+1}+y_{2,n})-(y_{1,n+1}+y_{1,n})]}{r_{12,n}r_{12,n+1}[r_{12,n}+r_{12,n+1}]} - \frac{Gm_2m_3[(y_{2,n+1}+y_{2,n})-(y_{3,n+1}+y_{3,n})]}{r_{23,n}r_{23,n+1}[r_{23,n}+r_{23,n+1}]}$$

$$F_{3,n,x} = -\frac{Gm_1m_3[(x_{3,n+1}+x_{3,n})-(x_{1,n+1}+x_{1,n})]}{r_{13,n}r_{13,n+1}[r_{13,n}+r_{13,n+1}]} - \frac{Gm_2m_3[(x_{3,n+1}+x_{3,n})-(x_{2,n+1}+x_{2,n})]}{r_{23,n}r_{23,n+1}[r_{23,n}+r_{23,n+1}]}$$

$$F_{3,n,y} = -\frac{Gm_1m_3[(y_{3,n+1}+y_{3,n})-(y_{1,n+1}+y_{1,n})]}{r_{13,n}r_{13,n+1}[r_{13,n}+r_{13,n+1}]} - \frac{Gm_2m_3[(y_{3,n+1}+y_{3,n})-(y_{2,n+1}+y_{2,n})]}{r_{23,n}r_{23,n+1}[r_{23,n}+r_{23,n+1}]},$$

and

$$r_{ij,m}^2 = (x_{i,m}-x_{j,m})^2 + (y_{i,m}-y_{j,m})^2; \quad m = n, n+1.$$

In the absence of P_3, the motion of P_2 relative to P_1 is the periodic orbit shown in Figure 2.1, for which the period is $\tau = 3.901$. If the major axis of motion is the line of greatest distance between any two points of an orbit, and if the length of the major axis is defined to be $2a$, the major axis of P_2's motion relative to P_1 lies on the X axis and $a = 0.730$.

The initial data for P_3 were chosen so that this body begins its motion relatively far from both P_1 and P_2, arrives in the vicinity of $(-1, 0)$ almost simultaneously with P_2 and then proceeds past $(-1, 0)$ at a relatively

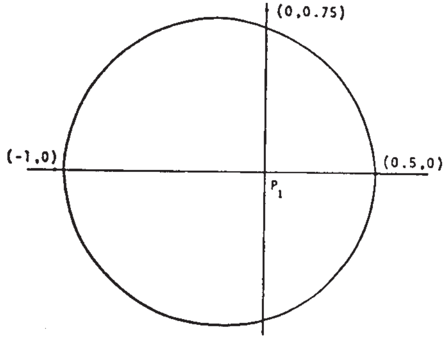

Figure 2.1. A periodic orbit.

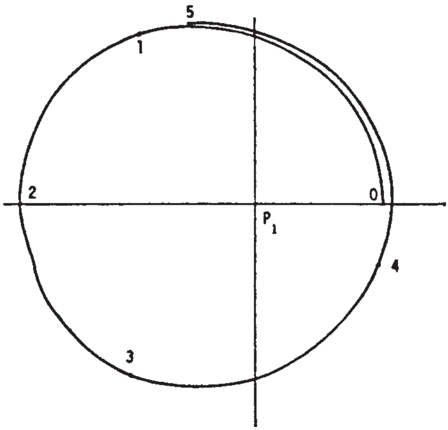

Figure 2.2. Orbit deflection.

high speed, assuring only a short period of strong gravitational attraction. Particles P_2 and P_3 come closest in the third quadrant at t_{2125}, when P_2 is at $(-0.9296, -0.1108)$ and P_3 is at $(-0.9325, -0.1012)$. The effect of the interaction is to deflect P_2 outward, as is seen clearly in Figure 2.2, where the motion of P_2 relative to P_1 has been plotted from t_0 to t_{5000}, with the integer labels $n = 0, 1, 2, 3, 4, 5$, marking the positions t_{1000n}. After having been deflected, P_2 goes into the new orbit about P_1 which is shown in Figure 2.3. The end points of the new major axis are (0.4943, 0.1664) and $(-0.9105, -0.3075)$, so that $a = 0.74135$. The new period is $\tau = 3.9905$.

Now, the *perihelion* point is the position of P_2 which is closest to P_1 during the orbit. Since P_2 has been deflected into a new orbit, its perihelion point has moved. The perihelion motion is measured by the angle

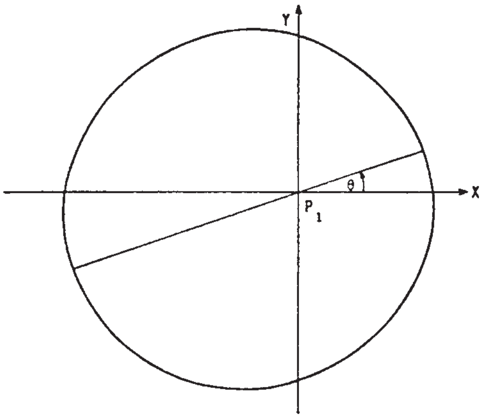

Figure 2.3. Positive perihelion motion.

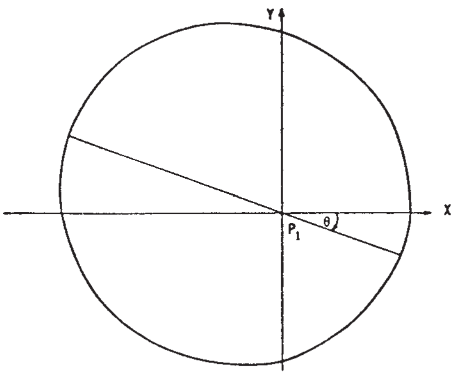

Figure 2.4. Negative perihelion motion.

of inclination θ of the new major axis with the X axis. and is given by $\tan\theta = 0.34$. The perihelion motion of this example is positive.

If we now change the initial data of P_3 to $x_{3,0} = -0.5$, $y_{3,0} = 8.0$, $v_{3,0,x} = -0.25$, $v_{3,0,y} = -4.00$, then the strongest gravitational effect between P_2 and P_3 occurs in the second quadrant at t_{1966} when P_2 is at $(-0.94582, 0.01950)$ and P_3 is at $(-0.94418, 0.01796)$. P_2 is then perturbed into the new orbit shown in Figure 2.4. The end points of the new major axis are $(0.50724, -0.18349)$ and $(-0.92692, 0.33474)$, so that $a = 0.76246$. The new period is $\tau = 4.162$. The resulting perihelion motion is now negative, since the angle θ of the new major axis with the X axis is given by $\tan\theta = -0.36$.

From the above and similar examples, it follows that the major axis of P_2 is deflected in the same direction as is P_2. In actual planetary motions, for example, in a Sun–Mercury–Venus system, where the mass of the sun is distinctly dominant, it would appear that when Mercury and Venus are relatively close in the first or third quadrants, the perihelion motion of Mercury should be perturbed a small amount in the positive angular direction, while relative closeness in the second or fourth quadrants should result in a small negative angular perturbation. All such possibilities can occur for the motions of Mercury and Venus. Thus, the perihelion motion of Mercury should be a complex, nonlinear, oscillatory motion. This conclusion was verified on the computer with ten full orbits of Mercury.

2.6. The Fundamental Problem of Electrostatics

The fundamental problem of electrostatics is a conservative problem which is described as follows. Given m electric charges $q_1, q_2, \ldots, q_m$, called the *source charges*, and n electric charges $Q_1, Q_2, \ldots, Q_n$, called the *test charges*, calculate the trajectories of $Q_1, Q_2, \ldots, Q_n$ from given initial data if the positions of the source charges are fixed (Griffiths (1981)). The fundamental problem is a *discrete* problem and has all the inherent difficulties of an n-body problem when $n \geq 3$. The classical way to avoid these difficulties is to consider special classes of problems in which the source charges are distributed continuously, thus allowing the introduction of integrals, fields, Gauss's law, Laplace's equation, and Poisson's equation. In this section we will show how to solve the fundamental problem when m and n are finite. We will use Coulomb's law in the following way. If two particles P_1, P_2 have respective charges e_1, e_2, then a potential ϕ defined by them is taken to be $e_1 e_2 / r_{12}$, in which r_{12} is the distance between them.

For convenience we now let the test charges be $Q_1, Q_2, \ldots, Q_n$ and let the source charges be $q_{n+1}, q_{n+2}, \ldots, q_N$, in which $N = n + m$. Then the motion of the test charges is determined by (2.4), (2.5).

As an example let us consider the following. Let Q_1, Q_2, Q_3 be electrons and let q_1 be a positron which is fixed at the origin $(0, 0, 0)$ of xyz space. The mass of each particle is $(9.1085)10^{-28}$ g. The charge of each of Q_1, Q_2, Q_3 is $-(4.8028)10^{-10}$ esu, while the charge of q_1 is $(4.8028)10^{-10}$ esu. The transformations

$$\boldsymbol{R} = (X, Y, Z) = 10^{12}(x, y, z) = 10^{12}\boldsymbol{r} \tag{2.41}$$

$$T = 10^{22}t \tag{2.42}$$

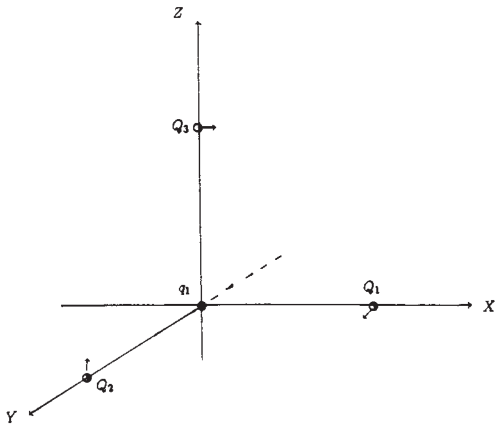

Figure 2.5. Initial data.

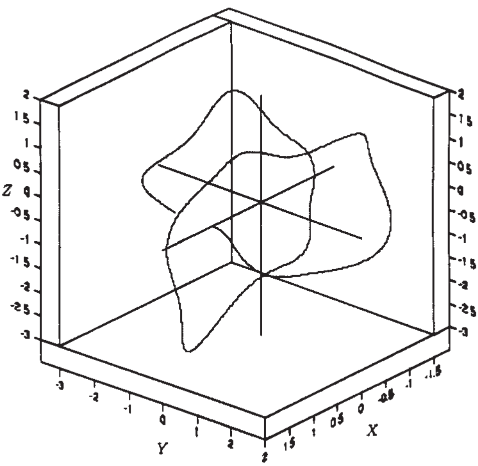

Figure 2.6. Motion of Q_1.

are introduced for the actual calculations. In the XYZ variables, the initial positions of Q_1, Q_2, Q_3 are taken to be $(1,0,0), (0,1,0), (0,0,1)$, respectively. The initial velocities of Q_1, Q_2, Q_3 are taken to be $(0,1,0), (0,0,1), (1,0,0)$, respectively. These initial data are shown in Figure 2.5. The initial energy is $-(6.606)10^{-8}$ erg. Finally, let $\Delta T = 0.00001$.

Figures 2.6–2.8 show the complex motions of Q_1, Q_2, Q_3, respectively, every 5000 time steps over 5000000 time steps. The trajectories are complex

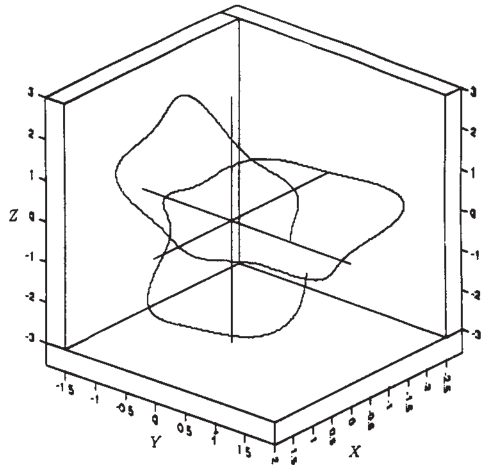

Figure 2.7. Motion of Q_2.

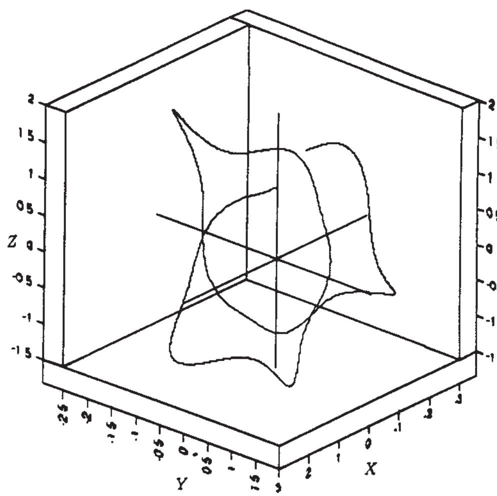

Figure 2.8. Motion of Q_3.

three dimensional motions, which are not available analytically. In all cases, one finds that $|X_i| < 3, |Y_i| < 3, |Z_i| < 3, i = 1, 2, 3$ and that each X, Y, Z takes on both positive and negative values. The three electrons are usually well separated, as is shown typically in Table 2.1, while the system is held together by the single positron at the origin. The entries in the

Table 2.1. Positions of Q_1, Q_2, Q_3.

T	Q	X	Y	Z
1000000	Q_1	−0.7091	2.4993	0.6711
	Q_2	0.6711	−0.7091	2.4993
	Q_3	2.4993	0.6711	−0.7091
2000000	Q_1	1.2035	−0.9622	−0.2833
	Q_2	−0.2833	1.2035	−0.9622
	Q_3	−0.9622	−0.2833	1.2035
3000000	Q_1	1.6067	1.3750	−0.9647
	Q_2	−0.9647	1.6067	1.3750
	Q_3	1.3750	−0.9647	1.6067
4000000	Q_1	−0.4644	−1.7039	1.4298
	Q_2	1.4297	−0.4644	−1.7039
	Q_3	−1.7039	1.4296	−0.4644
5000000	Q_1	1.5599	−0.2895	0.4383
	Q_2	0.4354	1.5472	−0.2751
	Q_3	−0.2727	0.4340	1.5471

table indicate that, to four decimal places, there may be some symmetry in the three trajectories due to the special initial conditions of the problem. However, this is revealed to be false at the times $T = 4000000, 5000000$. Thereafter, the system becomes physically unstable as Q_2 begins to oscillate around the positron, thus negating the effect of the positron on Q_1 and Q_3. Replacement of the positron by a fixed positive charge three times that of the positron yields a physically stable system with electron trajectories as complex as those shown in Figures 2.6–2.8.

2.7. The Calogero Hamiltonian System

Thus far we have emphasized a Newtonian formulation of the N-body problem. However, a more general formulation would use Hamiltonians. In this section we will discuss a Calogero Hamiltonian system and in the next we will discuss a Toda Hamiltonian system.

A Calogero Hamiltonian system (Calogero (1975), Marsden (1981)) is a system of N particles on a line with Hamiltonian

$$H = \frac{1}{2}\sum_{i=1}^{N} p_i^2 + \sum_{\substack{i \neq j \\ i,j=1}}^{N} \frac{1}{(q_i - q_j)^2}. \tag{2.43}$$

For (2.43),

$$\sum_{i=1}^{N} p_i \tag{2.44}$$

is a system invariant.

We will show how to reformulate particle interactions characterized by (2.43) by means of difference equations so that (2.43) and (2.44) continue to remain system invariants.

For clarity and intuition, let us begin with a two-particle Calogero system whose Hamiltonian is

$$H = \frac{1}{2}\sum_{i=1}^{2} p_i^2 + \frac{2}{(q_1 - q_2)^2}, \quad q_1 \neq q_2. \tag{2.45}$$

Let $\Delta t > 0$, and $t_k = k\Delta t, k = 0, 1, 2, \ldots$. Denote p_1, p_2, q_1, q_2 at time t_k by $p_{1,k}, p_{2,k}, q_{1,k}, q_{2,k}$, respectively. For $i = 1, 2$ and $k = 0, 1, 2, \ldots$, define

$$\frac{p_{i,k+1} + p_{i,k}}{2} = \frac{q_{i,k+1} - q_{i,k}}{\Delta t} \tag{2.46}$$

$$\frac{p_{i,k+1} - p_{i,k}}{\Delta t} = F_{i,k}, \tag{2.47}$$

where

$$F_{1,k} = 2\frac{q_{1,k+1} + q_{1,k} - q_{2,k+1} - q_{2,k}}{(q_{1,k} - q_{2,k})^2(q_{1,k+1} - q_{2,k+1})^2}, \quad q_{1,k} \neq q_{2,k}, \quad k = 0, 1, 2, \ldots, \tag{2.48}$$

$$F_{2,k} = -F_{1,k}. \tag{2.49}$$

Theorem 2.8. *Given $p_{1,0}, p_{2,0}, q_{1,0}, q_{2,0}$, then* (2.47)–(2.49) *imply the invariance of $p_{1,k} + p_{2,k}$, that is,*

$$p_{1,k} + p_{2,k} \equiv p_{1,0} + p_{2,0}, \quad k = 0, 1, 2, \ldots. \tag{2.50}$$

Proof. From (2.47)–(2.49)

$$p_{1,k+1} = p_{1,k} + (\Delta t)F_{1,k},$$
$$p_{2,k+1} = p_{2,k} - (\Delta t)F_{1,k}.$$

Hence, for $k = 0, 1, 2, \ldots$,

$$p_{1,k+1} + p_{2,k+1} = p_{1,k} + p_{2,k},$$

which implies (2.50). □

Theorem 2.9. *Difference formulas* (2.46)–(2.49) *imply the invariance of Hamiltonian* (2.45) *for given* $p_{1,0}, p_{2,0}, q_{1,0}, q_{2,0}$, *that is, for* $k = 0, 1, 2, \ldots,$

$$\frac{1}{2}\left(p_{1,k}^2 + p_{2,k}^2\right) + \frac{1}{(q_{1,k} - q_{2,k})^2} \equiv \frac{1}{2}\left(p_{1,0}^2 + p_{2,0}^2\right) + \frac{2}{(q_{1,0} - q_{2,0})^2}. \tag{2.51}$$

Proof. Let

$$W_n = \sum_{k=0}^{n-1} \left[(q_{1,k+1} - q_{1,k})F_{1,k} + (q_{2,k+1} - q_{2,k})F_{2,k}\right]. \tag{2.52}$$

Then, from (2.46) and (2.47),

$$\begin{aligned} W_n &= \sum_{k=0}^{n-1} \left[(q_{1,k+1} - q_{1,k})\frac{p_{1,k+1} - p_{1,k}}{\Delta t} + (q_{2,k+1} - q_{2,k})\frac{p_{2,k+1} - p_{2,k}}{\Delta t}\right] \\ &= \sum_{k=0}^{n-1} \left[\frac{q_{1,k+1} - q_{1,k}}{\Delta t}(p_{1,k+1} - p_{1,k}) + \frac{q_{2,k+1} - q_{2,k}}{\Delta t}(p_{2,k+1} - p_{2,k})\right] \\ &= \frac{1}{2}\sum_{k=0}^{n-1} \left[(p_{1,k+1}^2 - p_{1,k}^2) + (p_{2,k+1}^2 - p_{2,k}^2)\right] \end{aligned}$$

so that

$$W_n = \frac{1}{2}\left(p_{1,n}^2 + p_{2,n}^2\right) - \frac{1}{2}\left(p_{1,0}^2 - p_{2,0}^2\right). \tag{2.53}$$

However, Eqs. (2.48), (2.49), and (2.52) imply

$$\begin{aligned} W_n &= 2\sum_{k=0}^{n-1} \left[(q_{1,k+1} - q_{1,k})\frac{q_{1,k+1} + q_{1,k} - q_{2,k+1} - q_{2,k}}{(q_{1,k} - q_{2,k})^2(q_{1,k+1} - q_{2,k+1})^2}\right. \\ &\qquad \left. - (q_{2,k+1} - q_{2,k})\frac{q_{1,k+1} + q_{1,k} - q_{2,k+1} - q_{2,k}}{(q_{1,k} - q_{2,k})^2(q_{1,k+1} - q_{2,k+1})^2}\right] \\ &= 2\sum_{k=0}^{n-1} \frac{(q_{1,k+1} - q_{2,k+1})^2 - (q_{1,k} - q_{2,k})^2}{(q_{1,k} - q_{2,k})^2(q_{1,k+1} - q_{2,k+1})^2} \\ &= 2\sum_{k=0}^{n-1} \left[\frac{1}{(q_{1,k} - q_{2,k})^2} - \frac{1}{(q_{1,k+1} - q_{2,k+1})^2}\right], \end{aligned}$$

so that

$$W_n = \frac{2}{(q_{1,0} - q_{2,0})^2} - \frac{2}{(q_{1,n} - q_{2,n})^2}. \tag{2.54}$$

Elimination of W_n between (2.53) and (2.54) then yields (2.51) and the theorem is proved.

The extension to systems of N particles then follows directly from formulation (2.46)–(2.49), but with $i = 1, 2, \ldots, N$.

To implement the formulation practically, consider system (2.46)–(2.49) with the initial data $p_{1,0} = 1, p_{2,0} = -1, q_{1,0} = 1, q_{2,0} = -1$. Then the Newtonian iteration formulas for solving the system at t_{k+1} in terms of data at t_k are

$$q_{1,k+1}^{(n+1)} = q_{1,k} + \Delta t \left[\frac{p_{1,k+1}^{(n)} + p_{1,k}}{2} \right] \tag{2.55}$$

$$q_{2,k+1}^{(n+1)} = q_{2,k} + \Delta t \left[\frac{p_{2,k+1}^{(n)} + p_{2,k}}{2} \right] \tag{2.56}$$

$$p_{1,k+1}^{(n+1)} = p_{1,k} + 2\Delta t \left[\frac{q_{1,k+1}^{(n+1)} + q_{1,k} - q_{2,k+1}^{(n+1)} - q_{2,k}}{(q_{1,k} - q_{2,k})^2 \left(q_{1,k+1}^{(n+1)} - q_{2,k+1}^{(n+1)}\right)^2} \right] \tag{2.57}$$

$$p_{2,k+1}^{(n+1)} = p_{2,k} - 2\Delta t \left[\frac{q_{1,k+1}^{(n+1)} + q_{1,k} - q_{2,k+1}^{(n+1)} - q_{2,k}}{(q_{1,k} - q_{2,k})^2 \left(q_{1,k+1}^{(n+1)} - q_{2,k+1}^{(n+1)}\right)^2} \right]. \tag{2.58}$$

Calculation for 500000 steps with $\Delta t = 0.0001$ yields the typical results shown in Table 2.2 every 50000 time steps. The table shows clearly that both the Hamiltonian and $p_1 + p_2$ are conserved. In addition, it shows an increasingly repulsive effect which the particles exert on each other. □

Table 2.2. Calogero.

k	H	q_1	q_2	p_1	p_2
1	1.5	1.000000	−1.000000	1.000000	−1.000000
50000	1.5	6.964067	−6.964067	1.220529	−1.220529
100000	1.5	13.076572	−13.076572	1.223551	−1.223551
150000	1.5	19.196231	−19.196231	1.224191	−1.224191
200000	1.5	25.317857	−25.317857	1.224427	−1.224427
250000	1.5	31.440301	−31.440301	1.224539	−1.224539
300000	1.5	37.563163	−37.563163	1.224601	−1.224601
350000	1.5	43.686267	−43.686267	1.224638	−1.224638
400000	1.5	49.809524	−49.809524	1.224663	−1.224663
450000	1.5	55.932884	−55.932884	1.224680	−1.224680
500000	1.5	62.056317	−62.056317	1.224692	−1.224692

2.8. The Toda Hamiltonian System

A Toda Hamiltonian system (Toda (1967)) is a system of N particles on a line with Hamiltonian

$$H = \frac{1}{2}\sum_{i=1}^{N} p_i^2 + \sum_{i=1}^{N-1} \exp(q_i - q_{i+1}). \tag{2.59}$$

We will show how to reformulate particle interactions characterized by (2.59) by means of difference equations so that (2.44) and (2.59) remain system invariants. Formulas (2.46)–(2.49), for $N = 2$, need be modified only slightly, that is, (2.48) needs to be changed, and this is done as follows:

$$F_{1,k} = \begin{cases} -\frac{\exp(q_{1,k+1}-q_{2,k+1})-\exp(q_{1,k}-q_{2,k})}{(q_{1,k+1}-q_{2,k+1})-(q_{1,k}-q_{2,k})}; (q_{1,k+1} - q_{1,k}) - (q_{2,k+1} - q_{2,k}) \neq 0 \\ -\exp(q_{1,k} - q_{2,k}); (q_{1,k+1} - q_{1,k}) - (q_{2,k+1} - q_{2,k}) = 0. \end{cases} \tag{2.60}$$

Theorem 2.10. *Given* $p_{1,0}, p_{2,0}, q_{1,0}, q_{2,0}$, *then Eqs.* (2.46), (2.47), (2.49), (2.60) *imply*

$$p_{1,k} + p_{2,k} \equiv p_{1,0} + p_{2,0}, \quad k = 0, 1, 2, \ldots. \tag{2.61}$$

Proof. The proof is essentially identical to that of Theorem 2.8. □

Theorem 2.11. *Under the assumptions of Theorem* 2.10, *it follows for* $k = 0, 1, 2, \ldots,$ *that*

$$\frac{1}{2}\left(p_{1,k}^2 + p_{2,k}^2\right) + \exp(q_{1,k} - q_{2,k}) \equiv \frac{1}{2}\left(p_{1,0}^2 + p_{2,0}^2\right) + \exp(q_{1,0} - q_{2,0}). \tag{2.62}$$

Proof. Consider first the case $(q_{1,k+1} - q_{1,k}) - (q_{2,k+1} - q_{2,k}) \neq 0$. Recall also Eq. (2.52), that is,

$$W_n = \sum_{k=0}^{n-1} \left[(q_{1,k+1} - q_{1,k})F_{1,k} + (q_{2,k+1} - q_{2,k})F_{2,k}\right].$$

Thus, Eq. (2.53), that is

$$W_n = \frac{1}{2}\left(p_{1,n}^2 + p_{2,n}^2\right) - \frac{1}{2}\left(p_{1,0}^2 - p_{2,0}^2\right)$$

is again valid, using the same argument as used to derive (2.53).

Next, Eqs. (2.46), (2.47), (2.49), (2.52) and (2.60) imply

$$\begin{aligned} W_n &= \sum_{k=0}^{n-1} \left\{ (q_{1,k+1} - q_{1,k}) \left[-\frac{\exp(q_{1,k+1} - q_{2,k+1}) - \exp(q_{1,k} - q_{2,k})}{(q_{1,k+1} - q_{2,k+1}) - (q_{1,k} - q_{2,k})} \right] \right. \\ &\qquad \left. + (q_{2,k+1} - q_{2,k}) \left[\frac{\exp(q_{1,k+1} - q_{2,k+1}) - \exp(q_{1,k} - q_{2,k})}{(q_{1,k+1} - q_{2,k+1}) - (q_{1,k} - q_{2,k})} \right] \right\} \\ &= \sum_{k=0}^{n-1} \{ -[\exp(q_{1,k+1} - q_{2,k+1}) - \exp(q_{1,k} - q_{2,k})] \}, \end{aligned}$$

so that

$$W_n = \exp(q_{1,0} - q_{2,0}) - \exp(q_{1,n} - q_{2,n}). \tag{2.63}$$

Finally, elimination of W_n between Eqs. (2.53) and (2.63) yields (2.62).

In the second case, when $(q_{1,k+1} - q_{1,k}) - (q_{2,k+1} - q_{2,k}) = 0$, the corresponding summation term in (2.52) becomes simply

$$[(q_{1,k+1} - q_{1,k}) - (q_{2,k+1} - q_{2,k})][-\exp(q_{1,k} - q_{2,k})]$$

which is zero, and the theorem continues to be valid. □

Practical implementation uses formulas entirely analogous to (2.55)–(2.58), but which incorporate (2.60) for the Toda lattice. Calculation for 240000 steps with $\Delta t = 0.000001$ with initial data $q_{1,0} = 1$, $q_{2,0} = -1$, $p_{1,0} = 10$, $p_{2,0} = -10$ yields the results in Table 2.3. The second part of (2.60) is essential numerically at the turning point, which occurs between

Table 2.3. Toda.

k	H	q_1	q_2	p_1	p_2
1	107.39	1.000000	−1.000000	10.000000	−10.000000
20000	107.39	1.198295	−1.198295	9.818524	−9.818524
40000	107.39	1.392152	−1.392152	9.549895	−9.549895
60000	107.39	1.579463	−1.579463	9.156625	−9.156625
80000	107.39	1.757265	−1.757265	8.590050	−8.590050
100000	107.39	1.921525	−1.921525	7.792399	−7.792399
120000	107.39	2.067027	−2.067027	6.7051120	−6.7051120
140000	107.39	2.187513	−2.187513	5.286525	−5.286525
160000	107.39	2.276273	−2.276273	3.537755	−3.537755
180000	107.39	2.327260	−2.327260	1.526700	−1.526700
200000	107.39	2.336502	−2.336502	−0.609200	0.609200
220000	107.39	2.303235	−2.303235	−2.694399	2.694399
240000	107.39	2.230142	−2.230142	−4.569209	4.569209

$k = 180000$ and $k = 200000$. The table indicates clearly the invariance of both H and $p_1 + p_2$.

2.9. Remarks

In applying Newton's iteration formulas to the resulting algebraic or transcendental system of the method of Section 2.2, it is convenient to know how many solutions the system has. We now give an example to show that the solution need not be unique, and indeed has two solutions. Each problem one considers will require a related analysis.

Consider the initial value problem

$$\ddot{x} = x^2, \quad x(0) = 1, \quad \dot{x} = 1. \tag{2.64}$$

Choosing $\phi(x) = -\frac{1}{3}x^3$, the system to be solved is

$$x_{k+1} = x_k + \frac{1}{2}(\Delta t)(v_{k+1} + v_k) \tag{2.65}$$

$$v_{k+1} = v_k + \frac{1}{3}(\Delta t)\left(x_{k+1}^2 + x_{k+1}x_k + x_k^2\right). \tag{2.66}$$

Substitution of (2.66) into (2.65) yields

$$x_{k+1}^2 + \left(1 - \frac{6}{(\Delta t)^2}\right) x_{k+1} + \left(1 + \frac{6}{(\Delta t)^2} + \frac{6}{(\Delta t)}\right) = 0. \tag{2.67}$$

Since the initial conditions are given in (2.38), it follows from (2.67) that

$$x_1^2 + \left(1 - \frac{6}{(\Delta t)^2}\right) x_1 + \left(1 + \frac{6}{(\Delta t)^2} + \frac{6}{(\Delta t)}\right) = 0. \tag{2.68}$$

However, examination of the discriminant of (2.68) reveals that for $\Delta t < 0.79490525$, Eq. (2.68) has two real roots. Indeed, one must choose the negative sign in the quadratic formula to get the correct root. For $\Delta t = 0.01$, the correct physical approximation is $x_1 = 1.01005$, while the incorrect solution is $x_1 = 59998$.

Note also that if in (2.5) one would find that any $r_{lm,n+1} = r_{lm,n}$, then $\phi(r_{lm,n+1}) = \phi(r_{lm,n})$. In this case, the corresponding term in (2.6) need only be replaced by

$$-(r_{lm,n+1} - r_{lm,n}) \left. \frac{\partial \phi}{\partial r} \right|_{r=r_{lm,n}}$$

and the theorem will continue to be valid.

Note finally that conservative methodology will be applied again in Chapter 8.