Chapter VII.
Non-Canonical Hamiltonian Systems

We discuss theoretical properties and the structure-preserving numerical treatment of Hamiltonian systems on manifolds and of the closely related class of Poisson systems. We present numerical integrators for problems from classical and quantum mechanics.

VII.1 Constrained Mechanical Systems

Constrained mechanical systems form an important class of differential equations on manifolds. Their numerical treatment has been extensively investigated in the context of differential-algebraic equations and is documented in monographs like that of Brenan, Campbell & Petzold (1996), Eich-Soellner & Führer (1998), Hairer, Lubich & Roche (1989), and Chap. VII of Hairer & Wanner (1996). We concentrate here on the symmetry and/or symplecticity of such numerical integrators.

VII.1.1 Introduction and Examples

Consider a mechanical system described by position coordinates \(q_1, \ldots, q_d\), and suppose that the motion is constrained to satisfy \(g(q) = 0\) where \(g : \mathbb{R}^d \to \mathbb{R}^m\) with \(m < d\). Let \(T(q, \dot{q}) = \frac{1}{2} \dot{q}^T M(q) \dot{q}\) be the kinetic energy of the system and \(U(q)\) its potential energy, and put

\[
L(q, \dot{q}) = T(q, \dot{q}) - U(q) - g(q)^T \lambda, \quad (1.1)
\]

where \(\lambda = (\lambda_1, \ldots, \lambda_m)^T\) consists of Lagrange multipliers. The Euler–Lagrange equation of the variational problem for \(\int_0^T L(q, \dot{q}) \, dt\) is then given by

\[
\frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}} \right) - \frac{\partial L}{\partial q} = 0.
\]

Written as a first order differential equation we get

\[
\begin{align*}
\dot{q} &= v \\
M(q) \dot{v} &= f(q, v) - G(q)^T \lambda \\
0 &= g(q),
\end{align*}
\]

where \(f(q, v) = -\frac{\partial}{\partial q}(M(q)v) + \nabla_q T(q, v) - \nabla_q U(q)\) and \(G(q) = \frac{\partial g}{\partial q}(q)\).
Example 1.1 (Spherical Pendulum). We denote by \( q_1, q_2, q_3 \) the Cartesian coordinates of a point with mass \( m \) that is connected with a massless rod of length \( \ell \) to the origin. The kinetic and potential energies are \( T = \frac{m}{2} (\dot{q}_1^2 + \dot{q}_2^2 + \dot{q}_3^2) \) and \( U = mgq_3 \), respectively, and the constraint is the fixed length of the rod. We thus get the system
\[
\begin{align*}
\dot{q}_1 &= v_1, & m \dot{v}_1 &= -2q_1 \lambda \\
\dot{q}_2 &= v_2, & m \dot{v}_2 &= -2q_2 \lambda \\
\dot{q}_3 &= v_3, & m \dot{v}_3 &= -mg - 2q_1 \lambda \\
0 &= q_1^2 + q_2^2 + q_3^2 - \ell^2.
\end{align*}
\]
(1.3)

The physical meaning of \( \lambda \) is the tension in the rod which maintains the constant distance of the mass point from the origin.

Existence and Uniqueness of the Solution. A standard approach for studying the existence of solutions of differential-algebraic equations is to differentiate the constraints until an ordinary differential equation is obtained. Differentiating the constraint in (1.2) twice with respect to time yields
\[
0 = G(q) v \quad \text{and} \quad 0 = g''(q)(v, v) + G(q) \dot{v}.
\]
(1.4)

The equation for \( \dot{v} \) in (1.2) together with the second relation of (1.4) constitute a linear system for \( \dot{v} \) and \( \lambda \),
\[
\begin{pmatrix}
M(q) & G(q)^T \\
G(q) & 0
\end{pmatrix}
\begin{pmatrix}
\dot{v} \\
\lambda
\end{pmatrix}
= \begin{pmatrix}
f(q, v) \\
g''(q)(v, v)
\end{pmatrix}.
\]
(1.5)

Throughout this chapter we require the matrix appearing in (1.5) to be invertible for \( q \) close to the solution we are looking for. This then allows us to express \( \dot{v} \) and \( \lambda \) as functions of \((q, v)\). Notice that the matrix in (1.5) is invertible when \( G(q) \) has full rank and \( M(q) \) is invertible on \( \ker G(q) = \{ h \mid G(q)h = 0 \} \).

We are now able to discuss the existence of a solution of (1.2). First of all, observe that the initial values \( q_0, v_0, \lambda_0 \) cannot be arbitrarily chosen. They have to satisfy the first relation of (1.4) and \( \lambda_0 = \lambda(q_0, v_0) \), where \( \lambda(q, v) \) is obtained from (1.5). In the case that \( q_0, v_0, \lambda_0 \) satisfy these conditions, we call them consistent initial values. Furthermore, every solution of (1.2) has to satisfy
\[
\dot{q} = v, \quad \dot{v} = \dot{v}(q, v),
\]
(1.6)

where \( \dot{v}(q, v) \) is the function obtained from (1.5). It is known from standard theory of ordinary differential equations that (1.6) has locally a unique solution. This solution \((q(t), v(t))\) together with \( \lambda(t) := \lambda(q(t), v(t)) \) satisfies (1.5) by construction, and hence also the two differential equations of (1.2). Integrating the second relation of (1.4) twice and using the fact that the integration constants vanish for consistent initial values, proves also the remaining relation \( 0 = g(q) \) for this solution.
Formulation as a Differential Equation on a Manifold. We denote by
\[ \mathcal{Q} = \{ q \colon g(q) = 0 \} \] (1.7)
the configuration manifold, on which the positions \( q \) are constrained to lie. The tangent space at \( q \in \mathcal{Q} \) is \( T_q \mathcal{Q} = \{ v \colon G(q)v = 0 \} \). The equations (1.6) define thus a differential equation on the manifold
\[ T \mathcal{Q} = \{ (q, v) \colon q \in \mathcal{Q}, v \in T_q \mathcal{Q} \} = \{ (q, v) \colon g(q) = 0, G(q)v = 0 \}, \] (1.8)
the tangent bundle of \( \mathcal{Q} \). Indeed, we have just shown that for initial values \((q_0, v_0) \in T \mathcal{Q} \) (i.e., consistent initial values) the problems (1.6) and (1.2) are equivalent, so that the solutions of (1.6) stay on \( T \mathcal{Q} \).

Reversibility. The system (1.2) and the corresponding differential equation (1.6) are reversible with respect to the involution \((q, v) \mapsto (q, -v)\), if \( f(q, v) = f(q, -v) \). This follows at once from Example V.1.3, because the solution \( \tilde{v}(q, v) \) of (1.5) satisfies \( \tilde{v}(q, -v) = \tilde{v}(q, v) \).

For the numerical solution of differential-algebraic equations “index reduction” is a very popular technique. This means that instead of directly treating the problem (1.2) one numerically solves the differential equation (1.6) on the manifold \( \mathcal{M} \). Projection methods (Sect. IV.4) as well as methods based on local coordinates (Sect. IV.5) are much in use. If one is interested in a correct simulation of the reversible structure of the problem, the symmetric methods of Sect. V.4 can be applied. Here we do not repeat these approaches for this particular situation, instead we concentrate on the symplectic integration of constrained systems.

VII.1.2 Hamiltonian Formulation

In Sect. VI.1 we have seen that, for unconstrained mechanical systems, the equations of motion become more structured if we use the momentum coordinates \( p = \frac{\partial L}{\partial \dot{q}} = M(q)\dot{q} \) in place of the velocity coordinates \( v = \dot{q} \). Let us do the same for the constrained system (1.2). As in the proof of Theorem VI.1.3 we obtain the equivalent system
\[
\begin{align*}
\dot{q} &= H_p(p, q) \\
\dot{p} &= -H_q(p, q) - G(q)^T \lambda \\
0 &= g(q),
\end{align*}
\] (1.9)
where
\[ H(p, q) = \frac{1}{2} p^T M(q)^{-1} p + U(q) \] (1.10)
is the total energy of the system; \( H_p \) and \( H_q \) denote the column vectors of partial derivatives. Differentiating the constraint in (1.9) twice with respect to time, we get
\[
0 = G(q)H_p(p, q),
\] (1.11)
\[
0 = \frac{\partial}{\partial q} \left( G(q)H_p(p, q) \right) H_p(p, q) - G(q)H_{pp}(p, q) \left( H_q(p, q) + G(q)^T \lambda \right),
\] (1.12)
and assuming the matrix

\[ G(q)H_{pp}(p, q)G(q)^T \]

is invertible,

\[ (1.13) \]

equation (1.12) permits us to express \( \lambda \) in terms of \( (p, q) \).

**Formulation as a Differential Equation on a Manifold.** Inserting the so-obtained function \( \lambda(p, q) \) into (1.9) gives a differential equation for \( (p, q) \) on the manifold

\[ \mathcal{M} = \{(p, q); g(q) = 0, G(q)H_{p}(p, q) = 0\}. \]

(1.14)

As we will now see, this manifold has a differential-geometric interpretation as the cotangent bundle of the configuration manifold \( Q = \{q; g(q) = 0\} \). The Lagrangian for a fixed \( q \in Q \) is a function on the tangent space \( T_q Q \), i.e., \( L(q, \cdot) : T_q Q \to \mathbb{R} \). Its (Fréchet) derivative evaluated at \( \dot{q} \in T_q Q \) is therefore a linear mapping \( d_q L(q, \dot{q}) : T_q Q \to \mathbb{R} \), or in other terms, \( d_q L(q, \dot{q}) \) is in the cotangent space \( T_{\dot{q}}^* Q \). Since the duality is such that \( (d_q L(q, \dot{q}), v) = d_q L(q, \dot{q})v \) for \( v \in T_q Q \), condition (1.13) ensures that the Legendre transform \( \dot{q} \mapsto p = d_q L(q, \dot{q}) \) is an invertible transformation between \( T_q Q \) and \( T_{\dot{q}}^* Q \). We can therefore consider \( T_{\dot{q}}^* Q \) as a subspace of \( \mathbb{R}^d \) if every \( p \in T_{\dot{q}}^* Q \) is identified with \( \frac{dL}{dq}(q, \dot{q})^T = M(q)\dot{q} \in \mathbb{R}^d \) for the unique \( \dot{q} \in T_q Q \) for which \( p = d_q L(q, \dot{q}) \) holds. With this identification,

\[ T_{\dot{q}}^* Q = \{M(q)\dot{q}; \dot{q} \in T_q Q\}, \]

and the duality is given by \( (p, v) = p^Tv \) for \( p \in T_{\dot{q}}^* Q \) and \( v \in T_q Q \). We thus have \( p = M(q)\dot{q} \in T_{\dot{q}}^* Q \) if and only if \( \dot{q} = M(q)^{-1}p = H_{p}(p, q) \in T_q Q \). Since the tangent space at \( q \in Q \) is \( T_q Q = \{\dot{q}; G(q)\dot{q} = 0\} \), we obtain that

\[ p \in T_{\dot{q}}^* Q \quad \text{if and only if} \quad G(q)H_{p}(p, q) = 0. \]

Denoting by \( T^* Q = \{(p, q); q \in Q, p \in T_{\dot{q}}^* Q\} \) the **cotangent bundle** of \( Q \), we thus see that the constraint manifold \( \mathcal{M} \) of (1.14) equals

\[ \mathcal{M} = T^* Q. \]

(1.15)

The constrained Hamiltonian system (1.9) with Hamiltonian (1.10) can thus be viewed as a differential equation on the cotangent bundle \( T^* Q \) of the configuration manifold \( Q \).

In the following we consider the system (1.9)–(1.12) with (1.13) where \( H(p, q) \) is an arbitrary smooth function. The constraint manifold is then still given by (1.14). The existence and uniqueness of the solution of (1.9) can be discussed as before.

**Reversibility.** It is readily checked that the system (1.9) is reversible if \( H(-p, q) = H(p, q) \). This is always satisfied for a Hamiltonian (1.10).

**Preservation of the Hamiltonian.** Differentiation of \( H(p(t), q(t)) \) with respect to time yields

\[ -H_p^TH_q - H_p^T G^T \lambda + H_q^TH_p \]
with all expressions evaluated at \((p(t), q(t))\). The first and the last terms cancel, and the central term vanishes because \(GH_p = 0\) on the solution manifold. Consequently, the Hamiltonian \(H(p, q)\) is constant along solutions of (1.9).

**Symplecticity of the Flow.** Since the flow of the system (1.9) is a transformation on \(\mathcal{M}\), its derivative is a mapping between the corresponding tangent spaces. In agreement with Definition VI.2.2 we call a map \(\varphi : \mathcal{M} \to \mathcal{M}\) symplectic if, for every \(x = (p, q) \in \mathcal{M}\),

\[
\xi_1^T \varphi'(x)^T J \varphi'(x) \xi_2 = \xi_1^T J \xi_2 \quad \text{for all} \quad \xi_1, \xi_2 \in T_x \mathcal{M}.
\] (1.16)

If \(\varphi\) is actually defined and continuously differentiable in an open subset of \(\mathbb{R}^{2d}\) that contains \(\mathcal{M}\), then \(\varphi'(x)\) in the above formula is just the usual Jacobian matrix. Otherwise, some care is necessary in the interpretation of (1.16): \(\varphi'(x)\) is the tangent map given by the directional derivative \(\varphi'(x)\xi := (d/d\tau)\big|_{\tau=0} \varphi(x(\tau))\) for \(\xi \in T_x \mathcal{M}\), where \(x\) is a path on \(\mathcal{M}\) with \(x(0) = x, x'(0) = \xi\). The expression \(\xi_1^T \varphi'(x)^T\) in (1.16) should then be interpreted as \((\varphi'(x)\xi_1)^T\).

**Theorem 1.2.** Let \(H(p, q)\) and \(g(q)\) be twice continuously differentiable. The flow \(\varphi_t : \mathcal{M} \to \mathcal{M}\) of the system (1.9) is then a symplectic transformation on \(\mathcal{M}\), i.e., it satisfies (1.16).

**Proof.** We let \(x = (p, q)\), so that the system (1.9) becomes \(\dot{x} = J^{-1}(\nabla H(x) + \sum_{i=1}^{m} \lambda_i(x) \nabla g_i(x))\), where \(\lambda_i(x)\) and \(g_i(x)\) are the components of \(\lambda(x)\) and \(g(x)\), and \(\lambda(x)\) is the function obtained from (1.12). The variational equation of this system, satisfied by the directional derivative \(\Psi = \varphi'_t(x_0)\xi\), with \(x_0 = (p_0, q_0)\), reads

\[
\dot{\Psi} = J^{-1} \left( \nabla^2 H(x) + \sum_{i=1}^{m} \lambda_i(x) \nabla^2 g_i(x) + \sum_{i=1}^{m} \nabla g_i(x) \nabla \lambda_i(x) \right)^T \Psi.
\]

A direct computation, analogous to that in the proof of Theorem VI.2.4, yields for \(\xi_1, \xi_2 \in T_x \mathcal{M}\)

\[
\frac{d}{dt} \left( \xi_1^T \varphi'_t(x_0)^T J \varphi'_t(x_0) \xi_2 \right) = \ldots = \sum_{i=1}^{m} \xi_1^T \varphi'_t(x_0)^T \nabla g_i(x) \nabla \lambda_i(x) \varphi'_t(x_0) \xi_2 - \sum_{i=1}^{m} \xi_1^T \varphi'_t(x_0)^T \nabla \lambda_i(x) \nabla g_i(x) \varphi'_t(x_0) \xi_2. \quad (1.17)
\]

Since \(g_i(\varphi_t(x_0)) = 0\) for \(x_0 \in \mathcal{M}\), we have \(\nabla g_i(x)^T \varphi'_t(x_0) \xi_2 = 0\) and the same for \(\xi_1\), so that the expression in (1.17) vanishes. This proves the symplecticity of the flow on \(\mathcal{M}\). \(\square\)

Differentiating the constraint in (1.9) twice and solving for the Lagrange multiplier from (1.12) (this procedure is known as “index reduction” of the differential-algebraic system) yields the differential equation

\[
\dot{q} = H_p(p, q), \quad \dot{p} = -H_q(p, q) - G(q)^T \lambda(p, q), \quad (1.18)
\]
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Fig. 1.1. Numerical solution of the symplectic Euler method applied to (1.18) with $H(p, q) = \frac{1}{2}(p_1^2 + p_2^2 + p_3^2) + q_3, g(q) = q_1^2 + q_2^2 + q_3^2 - 1$ (spherical pendulum); initial value $q_0 = (0, \sin(0.1), -\cos(0.1)), p_0 = (0.06, 0, 0)$, step size $h = 0.003$ for method ‘sE’ (without projection) and $h = 0.03$ for method ‘sEproj’ (with projection).

where $\lambda(p, q)$ is obtained from (1.12). If we solve this system with the symplectic Euler method (implicit in $p$, explicit in $q$), the qualitative behaviour of the numerical solution is not correct. As was observed by Leimkuhler & Reich (1994), there is a linear error growth in the Hamiltonian and also a drift from the manifold $M$ (method ‘sE’ in Fig. 1.1). The explanation for this behaviour is the fact that (1.18) is no longer a Hamiltonian system. If we combine the symplectic Euler applied to (1.18) with an orthogonal projection onto $M$ (method ‘sEproj’), the result improves considerably but the linear error growth in the Hamiltonian is not eliminated. This numerical experiment illustrates that “index reduction” is not compatible with symplectic integration.

VII.1.3 A Symplectic First Order Method

We extend the symplectic Euler method to Hamiltonian systems with constraints. We integrate the $p$-variable by the implicit and the $q$-variable by the explicit Euler method. This gives

$$
\begin{align*}
\dot{p}_{n+1} &= p_n - h \left( H_q(\hat{p}_{n+1}, q_n) + G(q_n)^T \lambda_{n+1} \right) \\
q_{n+1} &= q_n + h H_p(\hat{p}_{n+1}, q_n) \\
0 &= g(q_{n+1}).
\end{align*}
$$

The numerical approximation $(\hat{p}_{n+1}, q_{n+1})$ satisfies the constraint $g(q) = 0$, but not $G(q)H_p(p, q) = 0$. To get an approximation $(p_{n+1}, q_{n+1}) \in M$, we append the projection

$$
\begin{align*}
p_{n+1} &= \hat{p}_{n+1} - h G(q_{n+1})^T \mu_{n+1} \\
0 &= G(q_{n+1})H_p(p_{n+1}, q_{n+1}).
\end{align*}
$$

Let us discuss some basic properties of this method.

Existence and Uniqueness of the Numerical Solution. Inserting the definition of $q_{n+1}$ from the second line of (1.19) into $0 = g(q_{n+1})$ gives a nonlinear system for $\hat{p}_{n+1}$ and $h\lambda_{n+1}$. Due to the factor $h$ in front of $H_p(\hat{p}_{n+1}, q_n)$, the implicit function theorem cannot be directly applied to prove existence and uniqueness of the numerical solution. We therefore write this equation as
0 = g(q_{n+1}) = g(q_n) + \int_0^1 G(q_n + \tau (q_{n+1} - q_n))(q_{n+1} - q_n) \, d\tau.

We now use \( g(q_n) = 0 \), insert the definition of \( q_{n+1} \) from the second line of (1.19) and divide by \( h \). Together with the first line of (1.19) this yields the system

\[
F(p_{n+1}, h\lambda_{n+1}, h) = 0
\]

with

\[
F(p, \nu, h) = \left( p - p_n + h H_q(p, q_n) + G(q_n)^T \nu, \int_0^1 G(q_n + \tau h H_p(p, q_n) H_p(p, q_n) \, d\tau \right).
\]

Since \((p_n, q_n) \in \mathcal{M}\) with \( \mathcal{M} \) from (1.14), we have \( F(p_n, 0, 0) = 0 \). Furthermore,

\[
\frac{\partial F}{\partial (p, \nu)}(p_n, 0, 0) = \left( \begin{array}{cc} I & G(q_n)^T \\ G(q_n) H_{pp}(p_n, q_n) & 0 \end{array} \right),
\]

and this matrix is invertible by (1.13). Consequently, an application of the implicit function theorem proves that the numerical solution \((\hat{p}_{n+1}, h\lambda_{n+1})\) (and hence also \(q_{n+1}\)) exists and is locally unique for sufficiently small \( h \).

The projection step (1.20) constitutes a nonlinear system for \( p_{n+1} \) and \( h\mu_{n+1} \), to which the implicit function theorem can be directly applied.

**Convergence of Order 1.** The above use of the implicit function theorem yields the rough estimates

\[
\hat{p}_{n+1} = p_n + \mathcal{O}(h), \quad h\lambda_{n+1} = \mathcal{O}(h), \quad h\mu_{n+1} = \mathcal{O}(h),
\]

which, together with the equations (1.19) and (1.20), give

\[
q_{n+1} = q(t_{n+1}) + \mathcal{O}(h^2), \quad p_{n+1} = p(t_{n+1}) - G(q(t_{n+1}))^T \nu + \mathcal{O}(h^2),
\]

where \((p(t), q(t))\) is the solution of (1.9) passing through \((p_n, q_n) \in \mathcal{M}\) at \( t = t_n \).

Inserting these relations into the second equation of (1.20) we get

\[
0 = G(q(t)) H_p(p(t), q(t)) + G(q(t)) H_{pp}(p(t), q(t)) G(q(t))^T \nu + \mathcal{O}(h^2)
\]

at \( t = t_{n+1} \). Since \( G(q(t)) H_p(p(t), q(t)) = 0 \), it follows from (1.13) that \( \nu = O(h^2) \). The local error is therefore of size \( O(h^2) \).

The convergence proof now follows standard arguments, because the method is a mapping \( \Phi_h : \mathcal{M} \rightarrow \mathcal{M} \) on the solution manifold. We consider the solutions \((p_n(t), q_n(t))\) of (1.9) passing through the numerical values \((p_n, q_n) \in \mathcal{M}\) at \( t = t_n \), we estimate the difference of two successive solutions in terms of the local error at \( t_n \), and we sum up the propagated errors (see Fig. 3.2 of Sect. II.3 in Hairer, Nørsett & Wanner (1993)). This proves that the global error satisfies \( p_n - p(t_n) = \mathcal{O}(h) \) and \( q_n - q(t_n) = \mathcal{O}(h) \) as long as \( t_n = nh \leq \text{Const.} \).
Symplecticity. We first study the mapping \( (p_n, q_n) \mapsto (\tilde{p}_{n+1}, q_{n+1}) \) defined by (1.19), and we consider \( \lambda_{n+1} \) as a function of \( (p_n, q_n) \). Differentiation with respect to \( (p_n, q_n) \) yields

\[
\begin{pmatrix}
I + hH_{qp}^T & 0 \\
-hH_{pp} & I
\end{pmatrix}
\begin{pmatrix}
\frac{\partial (\tilde{p}_{n+1}, q_{n+1})}{\partial (p_n, q_n)}
\end{pmatrix}
= \begin{pmatrix}
I - hG^T \lambda_p & S - hG^T \lambda_q \\
0 & I + hH_{qp}
\end{pmatrix}, \tag{1.21}
\]

where \( S = -hH_{qq} - h\lambda^T \gamma_{qq} \) is a symmetric matrix, the expressions \( H_{qp}, H_{pp}, H_{qq}, G \) are evaluated at \( (\tilde{p}_{n+1}, q_n) \), and \( \lambda, \lambda_p, \lambda_q \) at \( (p_n, q_n) \). A computation, identical to that of the proof of Theorem VI.3.3, yields

\[
\begin{pmatrix}
\frac{\partial (\tilde{p}_{n+1}, q_{n+1})}{\partial (p_n, q_n)}
\end{pmatrix}^T
J \begin{pmatrix}
\frac{\partial (\tilde{p}_{n+1}, q_{n+1})}{\partial (p_n, q_n)}
\end{pmatrix}
= \begin{pmatrix}
0 & I - h\lambda_p^T G \\
-I + hG^T \lambda_p & h(G^T \lambda_q - \lambda_q^T G)
\end{pmatrix}.
\]

We multiply this relation from the left by \( \xi_1 \in T_{(p_n, q_n)}M \) and from the right by \( \xi_2 \in T_{(\tilde{p}_{n+1}, q_n)}M \). With the partitioning \( \xi = (\xi_p, \xi_q) \) we have \( G(q_n)\xi_{3,j} = 0 \) for \( j = 1, 2 \) so that the expression reduces to \( \xi_1^T J \xi_2 \). This proves the symplecticity condition (1.16) for the mapping \( (p_n, q_n) \mapsto (\tilde{p}_{n+1}, q_{n+1}) \).

Similarly, the projection step \( (\tilde{p}_{n+1}, q_{n+1}) \mapsto (p_{n+1}, q_{n+1}) \) of (1.20) gives

\[
\frac{\partial (p_{n+1}, q_{n+1})}{\partial (\tilde{p}_{n+1}, q_{n+1})} = \begin{pmatrix}
I - hG^T \mu_p & S - hG^T \mu_q \\
0 & I
\end{pmatrix},
\]

where \( \mu_{n+1} \) of (1.20) is considered as a function of \( (\tilde{p}_{n+1}, q_{n+1}) \), and \( S = -h\mu^T \gamma_{qq} \). This is formally the same as (1.21) with \( H \equiv 0 \). Consequently, the symplecticity condition is also satisfied for this mapping. As a composition of two symplectic transformations, the numerical flow of our first order method is therefore also symplectic.

![Fig. 1.2. Spherical pendulum problem solved with the symplectic Euler method (1.19)-(1.20) and with the implicit Euler method; initial value \( q_0 = (\sin(1.3), 0, \cos(1.3)) \), \( p_0 = (3\cos(1.3), 6.5, -3\sin(1.3)) \), step size \( h = 0.01 \).](image)
Numerical Experiment. Consider the equations (1.3) for the spherical pendulum. For a mass $m = 1$ they coincide with the Hamiltonian formulation. Figure 1.2 (upper picture) shows the numerical solution (vertical coordinate $q_3$) over many periods obtained by method (1.19)-(1.20). We observe a regular qualitatively correct behaviour. For the implicit Euler method (i.e., the argument $q_n$ is replaced with $q_{n+1}$ in (1.19)) the numerical solution, obtained with the same step size and the same initial values, is less satisfactory. Already after one period the solution deteriorates and the pendulum loses energy.

VII.1.4 SHAKE and RATTLE

The numerical method (1.19)-(1.20) is only of order 1 and it is not symmetric. An algorithm that is of order 2, symmetric and symplectic was originally considered for separable Hamiltonians

$$H(p, q) = \frac{1}{2} p^T M^{-1} p + U(q)$$

(1.22)

with constant mass matrix $M$. Notice that in this case we are concerned with a second order differential equation $M\ddot{q} = -U_q(q) - G(q)^T \lambda$ with $g(q) = 0$.

SHAKE. Ryckaert, Ciccotti & Berendsen (1977) propose the method

$$q_{n+1} - 2q_n + q_{n-1} = -h^2 M^{-1} (U_q(q_n) + G(q_n)^T \lambda_n)$$

$$0 = g(q_{n+1})$$

(1.23)

for computations in molecular dynamics. It is a straightforward extension of the Störmer–Verlet scheme (I.1.15). The $p$-components, not used in the recursion, are approximated by $p_n = M(q_{n+1} - q_{n-1})/2h$.

RATTLE. The three-term recursion (1.23) may lead to an accumulation of round-off errors, and a reformulation as a one-step method is desirable. Using the same procedure as in (I.1.17) we formally get

$$p_{n+1/2} = p_n - \frac{h}{2} (U_q(q_n) + G(q_n)^T \lambda_n)$$

$$q_{n+1} = q_n + h M^{-1} p_{n+1/2}, \quad 0 = g(q_{n+1})$$

$$p_{n+1} = p_{n+1/2} - \frac{h}{2} (U_q(q_{n+1}) + G(q_{n+1})^T \lambda_{n+1})$$

(1.24)

The difficulty with this formulation is that $\lambda_{n+1}$ is not yet available at this step (it is computed together with $q_{n+2}$). As a remedy, Andersen (1983) suggests replacing the last line in (1.24) with a projection step similar to (1.20)

$$p_{n+1} = p_{n+1/2} - \frac{h}{2} (U_q(q_{n+1}) + G(q_{n+1})^T \mu_n)$$

$$0 = G(q_{n+1}) M^{-1} p_{n+1}.$$ 

(1.25)
This modification, called RATTLE, has the further advantage that the numerical approximation \((p_{n+1}, q_{n+1})\) lies on the solution manifold \(\mathcal{M}\). The symplecticity of this algorithm has been established by Leimkuhler & Skeel (1994).

**Extension to General Hamiltonians.** As observed independently by Jay (1994) and Reich (1993), the RATTLE algorithm can be extended to general Hamiltonians as follows: for consistent values \((p_n, q_n)\) define

\[
\begin{align*}
\dot{p}_{n+1/2} &= p_n - \frac{h}{2} \left( H_q(p_{n+1/2}, q_n) + G(q_n)^T \lambda_n \right) \\
\dot{q}_{n+1} &= q_n + \frac{h}{2} \left( H_p(p_{n+1/2}, q_n) + H_p(p_{n+1/2}, q_{n+1}) \right) \\
0 &= g(q_{n+1}) \\
\dot{p}_{n+1} &= p_{n+1/2} - \frac{h}{2} \left( H_q(p_{n+1/2}, q_{n+1}) + G(q_{n+1})^T \mu_n \right) \\
0 &= G(q_{n+1})H_p(p_{n+1}, q_{n+1}).
\end{align*}
\]

The first three equations of (1.26) are very similar to (1.19) and the last two equations to (1.20). The existence of (locally) unique solutions \((p_{n+1/2}, q_{n+1}, \lambda_n)\) and \((p_{n+1}, \mu_n)\) can therefore be proved in the same way. Notice also that this method gives a numerical solution that stays exactly on the solution manifold \(\mathcal{M}\).

**Theorem 1.3.** The numerical method (1.26) is symmetric, symplectic, and convergent of order two.

**Proof.** Although this theorem is the special case \(s = 2\) of Theorem 1.4, we outline its proof. We will see that the convergence result is easier to obtain for \(s = 2\) than for the general case.

If we add to (1.26) the consistency conditions \(g(q_n) = 0, G(q_n)H_p(p_n, q_n) = 0\) of the initial values, the symmetry of the method follows at once by exchanging \(h \leftrightarrow -h, p_{n+1} \leftrightarrow p_n, q_{n+1} \leftrightarrow q_n, \text{ and } \lambda_n \leftrightarrow \mu_n\). The symplecticity can be proved as for (1.19)-(1.20) by computing the derivative of \((p_{n+1}, q_{n+1})\) with respect to \((p_n, q_n)\), and by verifying the condition (1.16). This does not seem to be simpler than the symplecticity proof of Theorem 1.4.

The implicit function theorem applied to the two subsystems of (1.26) shows

\[
\begin{align*}
p_{n+1/2} &= p_n + \mathcal{O}(h), \quad h\lambda = \mathcal{O}(h), \quad p_{n+1} = p_{n+1/2} + \mathcal{O}(h), \quad h\mu = \mathcal{O}(h),
\end{align*}
\]

and, inserted into (1.26), yields

\[
\begin{align*}
q_{n+1} &= q(t_{n+1}) + \mathcal{O}(h^2), \quad p_{n+1} = p(t_{n+1}) - G(q(t_{n+1}))^T \nu + \mathcal{O}(h^2).
\end{align*}
\]

Convergence of order one follows therefore in the same way as for method (1.19)-(1.20). Since the order of a symmetric method is always even, this implies convergence of order two.

An easy way of obtaining high order methods for constrained Hamiltonian systems is by composition (Reich 1996a). Method (1.26) is an ideal candidate as basic integrator for compositions of the form (V.3.2). The resulting integrators are symmetric, symplectic, of high order, and yield a numerical solution that stays on the manifold \(\mathcal{M}\).
VII.1.5 The Lobatto IIIA - IIIB Pair

Another possibility for obtaining high order symplectic integrators for constrained Hamiltonian systems is by the use of partitioned Runge–Kutta or discontinuous collocation methods. We consider the system (1.9) and we search for polynomials $u(t)$ of degree $s$, $w(t)$ of degree $s - 1$, and $v(t)$ of degree $s - 2$ such that

$$u(t_n) = q_n, \quad v(t_n) = p_n - hb_1\delta(t_n)$$

(1.27)

with the defect

$$\delta(t) = \dot{v}(t) + H_q(v(t), u(t)) + G(u(t))^T w(t)$$

(1.28)

and, using the abbreviation $t_{n,i} = t_n + c_i h$,

$$\dot{u}(t_{n,i}) = H_p(v(t_{n,i}), u(t_{n,i})), \quad i = 1, \ldots, s$$

(1.29)

$$\dot{v}(t_{n,i}) = -H_q(v(t_{n,i}), u(t_{n,i})) - G(u(t_{n,i}))^T w(t_{n,i}), \quad i = 2, \ldots, s - 1$$

0 = $g(u(t_{n,i}))$, \quad $i = 1, \ldots, s$.

If these polynomials exist, the numerical solution is defined by

$$q_{n+1} = u(t_n + h), \quad p_{n+1} = v(t_n + h) - hb_1\delta(t_n + h)$$

$$0 = G(q_{n+1})H_p(p_{n+1}, q_{n+1}).$$

(1.30)

Why Discontinuous Collocation Based on Lobatto Quadrature? At a first glance (Theorem VI.4.2) it seems natural to consider collocation methods based on Gaussian quadrature for the entire system. This, however, has the disadvantage that the numerical solution does not satisfy $g(q_{n+1}) = 0$. To achieve this requirement, $t_n + h$ has to be one of the collocation points, i.e., we must have $c_s = 1$. Unfortunately, none of the collocation or discontinuous collocation methods with $c_s = 1$ is symplectic (see Exercise IV.6). We therefore turn our attention to partitioned methods, and we treat only the $q$-component by a collocation method satisfying $c_s = 1$. To satisfy the $s$ conditions $g(u(t_{n,i})) = 0$ of (1.29) there are only $s - 1$ free parameters $w(t_n), w(t_n + c_2 h), \ldots, w(t_n + c_s - 1 h)$ available. A remedy is to choose $c_1 = 0$ so that the first condition $g(u(t_n)) = 0$ is automatically verified. Encouraged by Theorem VI.4.5 we are thus led to consider the Lobatto nodes in the role of the $c_i$. The use of the partitioned Lobatto IIIA - IIIB pair for the treatment of constrained Hamiltonian systems has been suggested by Jay (1994, 1996).

Existence and Uniqueness of the Numerical Solution. The polynomial $u(t)$ of degree $s$ is uniquely determined by $u(t_n) = q_n$ and $\dot{u}(t_{n,i}) =: Q_i (i = 1, \ldots, s)$, the polynomial $v(t)$ of degree $s - 2$ is uniquely determined by $v(t_{n,i}) =: P_i (i = 1, \ldots, s - 1)$, and the polynomial $w(t)$ of degree $s - 1$ is uniquely determined by $hw(t_{n,i}) =: \Lambda_i (i = 1, \ldots, s)$. Notice that the value $\Lambda_s$ is only involved in (1.30) and not in (1.27)-(1.29). For the nonlinear system (1.27)-(1.29) we therefore consider
\[
X = (\dot{Q}_1, \ldots, \dot{Q}_s, P_1, \ldots, P_{s-1}, A_1, \ldots, A_{s-1})
\]
as independent variables, and we write the system as \(F(X, h) = 0\). The function \(F\) is composed of the \(s\) conditions for \(\dot{u}(t_n, i)\), of the definition of \(v(t_n)\) (divided by \(b_1\)) and the \(s - 2\) conditions for \(\dot{v}(t_n, i)\) (multiplied by \(h\)), and finally of the \(s - 1\) equations \(0 = g(u(t_n, i))\) for \(i = 2, \ldots, s\) (divided by \(h\)). Observe that \(0 = g(u(t_n))\) is automatically satisfied by the consistency of \((p_n, q_n)\). We note that \(P_s = v(t_n + h)\) and \(\dot{P}_i = hv(t_n, i)\) are linear combinations of \(F_1, \ldots, F_{s-1}\) with coefficients independent of the step size \(h\).

The function \(F(X, h)\) is well-defined for \(h\) in a neighbourhood of 0. For the first two blocks this is evident, for the last one it follows from the identity

\[
\frac{1}{h} g(u(t_n, i)) = \int_0^{\epsilon_n} G(u(t_n + \theta h)) \dot{u}(t_n + \theta h) d\theta
\]

using the fact that \(\dot{u}(t_n + \theta h)\) is a linear combination of \(\dot{Q}_i\) for \(i = 1, \ldots, s\). With the values

\[
X_0 = (H_p(p_n, q_n), \ldots, H_p(p_n, q_n), p_n, \ldots, p_n, 0, \ldots, 0)
\]
we have that \(F(X_0, 0) = 0\), because the values \((p_n, q_n)\) are assumed to be consistent. In view of an application of the implicit function theorem we compute

\[
\frac{\partial F}{\partial X}(X_0, 0) = \begin{pmatrix}
I \otimes I & -D \otimes H_{pp} & 0 \\
0 & B \otimes I & I \otimes G^T \\
A \otimes G & 0 & 0
\end{pmatrix}, \quad (1.31)
\]
where \(H_{pp}, G\) are evaluated at \((p_n, q_n)\), and \(A, B, D\) are matrices of dimension \((s - 1) \times s, (s - 1) \times (s - 1)\) and \(s \times (s - 1)\) respectively that depend only on the Lobatto quadrature and not on the differential equation. For example, the matrix \(B\) represents the linear mapping

\[
(P_1, \ldots, P_{s-1}) \mapsto (\dot{P}_1 + b_1^{-1} P_1, \dot{P}_2, \ldots, \dot{P}_{s-1}).
\]
This mapping is invertible, because the values on the right-hand side uniquely determine the polynomial \(v(t)\) of degree \(s - 2\).

Block Gaussian elimination then shows that (1.31) is invertible if and only if the matrix

\[
ADB^{-1} \otimes GH_{pp} G^T
\]
Because of (1.13) it remains to show that \(ADB^{-1}\) is invertible.

To achieve this without explicitly computing the matrices \(A, B, D\), we apply the method to the problem where \(p\) and \(q\) are of dimension one, \(H(p, q) = p^2/2\), and \(g(q) = q\). Assuming \(h = 1\) we get

\[
\begin{align*}
u(0) &= 0, & v(0) &= -b_1 (\dot{v}(0) + u(0)) \\
\dot{u}(c_i) &= v(c_i) & \text{for } i = 1, \ldots, s \\
\dot{v}(c_i) &= -w(c_i) & \text{for } i = 2, \ldots, s - 1 \\
0 &= u(c_i) & \text{for } i = 1, \ldots, s - 1
\end{align*}
\]
(1.32)
which is equivalent to
\[
\begin{pmatrix}
I & -D & 0 \\
0 & B & I \\
A & 0 & 0
\end{pmatrix}
\begin{pmatrix}
(\dot{u}(c_i))_{i=1}^s \\
(\dot{v}(c_i))_{i=1}^s \\
(\dot{w}(c_i))_{i=1}^s
\end{pmatrix}
= \begin{pmatrix}
0 \\
0 \\
0
\end{pmatrix},
\]
(1.33)
because \(H_{pp}(p,q) = 1\) and \(G(q) = 1\). Since \(u(t)\) is a polynomial of degree \(s\), the last equation of (1.32) implies that \(u(t) = C \prod_{j=1}^s (t - c_j)\). By the second relation the polynomial \(\dot{u}(t) - v(t)\), which is of degree \(s - 1\), vanishes at \(s\) points. Hence, \(v(t) = \dot{u}(t)\), which is possible only if \(C = 0\), because the degree of \(v(t)\) is \(s - 2\). Consequently, the linear system (1.33) has only the trivial solution, so that the matrix in (1.33) and hence also \(ADB^{-1}\) is invertible.

The implicit function theorem applied to \(F(X,h) = 0\) shows that the nonlinear system (1.27)-(1.30) possesses a locally unique solution for sufficiently small step sizes \(h\). Using the free parameter \(\lambda = hw(t_n + h)\), a further application of the implicit function theorem, this time to the small system (1.30), proves the existence and local uniqueness of \(p_{n+1}\).

**Theorem 1.4.** Let \((b_i, c_i)_{i=1}^s\) be the weights and nodes of the Lobatto quadrature (c.f. (II.1.17)). The method (1.27)-(1.29)-(1.30) is symmetric, symplectic, and super-convergent of order \(2s - 2\).

**Proof.** Symmetry. To the formulas (1.27)-(1.29)-(1.30) we add the consistency relations \(g(q_n) = 0, G(q_n)H_p(p_n, q_n) = 0\). Then we exchange \((t_n, p_n, q_n) \leftrightarrow (t_{n+1}, p_{n+1}, q_{n+1})\) and \(h \leftrightarrow -h\). Since \(b_1 = b_s\) and \(c_{s+1-i} = 1 - c_i\) for the Lobatto quadrature, the resulting formulas are equivalent to the original method (see also the proof of Theorem V.2.1).

**Symplecticity.** We fix \(\xi_1, \xi_2 \in T_{(p_n, q_n)} M\), we put \(x_n = (p_n, q_n)^T\), and we consider the bilinear mapping
\[
Q\left(\frac{\partial p_{n+1}}{\partial x_n}, \frac{\partial q_{n+1}}{\partial x_n}\right) = \xi_1^T \left(\frac{\partial p_{n+1}}{\partial x_n} \frac{\partial q_{n+1}}{\partial x_n} - \frac{\partial p_{n+1}}{\partial x_n} \frac{\partial q_{n+1}}{\partial x_n}\right) \xi_2.
\]
The symplecticity of the transformation \((p_n, q_n) \mapsto (p_{n+1}, q_{n+1})\) on the manifold \(M\) is then expressed by the relation
\[
Q\left(\frac{\partial p_{n+1}}{\partial x_n}, \frac{\partial q_{n+1}}{\partial x_n}\right) = Q\left(\frac{\partial p_n}{\partial x_n}, \frac{\partial q_n}{\partial x_n}\right).
\]
(1.34)
We now follow closely the proof of Theorem IV.2.3. We consider the polynomials \(u(t), v(t), w(t)\) of the method (1.27)-(1.29)-(1.30) as functions of \(t\) and \(x_n = (p_n, q_n)\), and we compute
\[
Q\left(\frac{\partial u(t_{n+1})}{\partial x_n}, \frac{\partial u(t_{n+1})}{\partial x_n}\right) = Q\left(\frac{\partial v(t_n)}{\partial x_n}, \frac{\partial u(t_n)}{\partial x_n}\right) = \int_{t_n}^{t_{n+1}} \frac{dQ}{dt} \left(\frac{\partial v(t)}{\partial x_n}, \frac{\partial u(t)}{\partial x_n}\right) dt.
\]
(1.35)
Since $u(t)$ is a polynomial of degree $s$ and $v(t)$ of degree $s - 2$, the integrand in (1.35) is a polynomial in $t$ of degree $2s - 3$. It is thus integrated without error by the Lobatto quadrature. By definition these polynomials satisfy the differential equation at the interior collocation points. Therefore, it follows from (1.17) that

$$\frac{dQ}{dt} \left( \frac{\partial v(t_{n,i})}{\partial x_n}, \frac{\partial u(t_{n,i})}{\partial x_n} \right) = 0 \quad \text{for } i = 2, \ldots, s - 1,$$

and that

$$\frac{dQ}{dt} \left( \frac{\partial v(t_{n,i})}{\partial x_n}, \frac{\partial u(t_{n,i})}{\partial x_n} \right) = \mathcal{Q} \left( \frac{\partial \delta(t_{n,i})}{\partial x_n}, \frac{\partial u(t_{n,i})}{\partial x_n} \right) \quad \text{for } i = 1 \text{ and } i = s.$$

Applying the Lobatto quadrature to the integral in (1.35) thus yields

$$hb_1 \mathcal{Q} \left( \frac{\partial \delta(t_{n,i})}{\partial x_n}, \frac{\partial u(t_{n,i})}{\partial x_n} \right) + hb_s \mathcal{Q} \left( \frac{\partial \delta(t_{n+1,i})}{\partial x_n}, \frac{\partial u(t_{n+1,i})}{\partial x_n} \right),$$

and the symplecticity relation (1.34) follows in the same way as in the proof of Theorem IV.2.3.

**Superconvergence.** This is the most difficult part of the proof. We remark that superconvergence of Runge–Kutta methods for differential-algebraic systems of index 3 has been conjectured by Hairer, Lubich & Roche (1989), and a first proof has been obtained by Jay (1993) for collocation methods. In his thesis Jay (1994) proves superconvergence for a more general class of methods, including the Lobatto IIIA - IIIB pair, using a ‘rooted-tree-type’ theory. A sketch of that very elaborate proof is published in Jay (1996). Using the idea of discontinuous collocation, the elegant proof for collocation methods can now be extended to cover the Lobatto IIIA - IIIB pair. In the following we explain how the local error can be estimated.

We consider the polynomials $u(t), v(t), w(t)$ defined in (1.27)-(1.29)-(1.30), and we define defects $\mu(t), \delta(t), \theta(t)$ as follows:

$$\dot{u}(t) = H_p(v(t), u(t)) + \mu(t)$$

$$\dot{v}(t) = -H_q(v(t), u(t)) - G(u(t))^T w(t) + \delta(t)$$

$$0 = g(u(t)) + \theta(t).$$

By definition of the method we have

$$\mu(t_{n+1,i}) = 0, \quad i = 1, \ldots, s$$

$$\delta(t_{n+1,i}) = 0, \quad i = 2, \ldots, s - 1$$

$$\theta(t_{n+1,i}) = 0, \quad i = 1, \ldots, s.$$ (1.37)

We let $q(t), p(t), \lambda(t)$ be the exact solution of (1.9) satisfying $q(t_n) = q_n, p(t_n) = p_n$, and we consider the differences

$$\Delta u(t) = u(t) - q(t), \quad \Delta v(t) = v(t) - p(t), \quad \Delta w(t) = w(t) - \lambda(t).$$
Subtracting (1.9) from (1.36) we get by linearization that

\[
\begin{align*}
\Delta u &= a_{11}(t)\Delta u + a_{12}(t)\Delta v + \mu(t) \\
\Delta v &= a_{21}(t)\Delta u + a_{22}(t)\Delta v + a_{23}(t)\Delta w + \delta(t),
\end{align*}
\]

(1.38)

where \(a_{12}(t) = H_{pp}(p(t), q(t))\), and where the other \(a_{ij}(t)\) are given by similar expressions. We have suppressed quadratic and higher order terms to keep the presentation as simple as possible. They do not influence the convergence result. To eliminate \(\Delta w\) in (1.38), we differentiate the algebraic relations in (1.9) and (1.36) twice, and we subtract them. This yields

\[
0 = F(t, \mu(t)) + b_1(t)\Delta u + b_2(t)\Delta v + B(t)\Delta w \\
+ G(u(t))H_{pp}(v(t), u(t))\delta(t) + G(u(t))\hat{\mu}(t) + \bar{\theta}(t),
\]

where \(F(t, \mu), B(t), b_1(t), b_2(t)\) are functions depending on \(p(t), q(t), \lambda(t), u(t), v(t), w(t)\), and where \(F(t, 0) = 0\) and \(B(t) \approx G(q_n)H_{pp}(p_n, q_n)G(q_n)^T\). Because of our assumption (1.13) we can extract \(\Delta w\) from this relation, and we insert it into (1.38). In this way we get a linear differential equation for \(\Delta u, \Delta v\), which can be solved by the ‘variation of constants’ formula. Using \(\Delta v(t_n) = 0\) (by (1.27)), the solution \(\Delta v(t_n + h)\) is seen to be of the form

\[
\begin{align*}
\Delta v(t_n + h) &= R_{22}(t_n + h, t_n)\Delta v(t_n) + \int_{t_n}^{t_n+h} \left( R_{21}(t_n + h, t)\mu(t) \\
&+ R_{22}(t_n + h, t)\left( \delta(t) + \tilde{F}(t, \mu(t)) + c_1(t)\hat{\mu}(t) \\
&+ C(t)\left( G(u(t))H_{pp}(v(t), u(t))\delta(t) + \bar{\theta}(t) \right) \right) \right) dt,
\end{align*}
\]

(1.39)

where \(R_{21}\) and \(R_{22}\) are the lower blocks of the resolvent, and \(\tilde{F}, c_1, C\) are functions as before. To prove that the local error of the \(p\)-component

\[
p_{n+1} - p(t_n + h) = \Delta v(t_n + h) - hb_1\delta(t_n + h)
\]

(1.40)

is of size \(O(h^{2s-1})\), we first integrate by parts those expressions in (1.39) which contain a derivative. For example,

\[
\int_{t_n}^{t_{n+1}} a(t)\hat{\mu}(t)\, dt = a(t)\mu(t)\bigg|_{t_n}^{t_{n+1}} - \int_{t_n}^{t_{n+1}} \dot{a}(t)\mu(t)\, dt = O(h^{2s-1}),
\]

because \(\mu(t_n) = \mu(t_n + h) = 0\) by (1.37) and an application of the Lobatto quadrature to the integral at the right-hand side gives zero as result with a quadrature error of size \(O(h^{2s-1})\). Similarly, integrating by parts twice yields

\[
\int_{t_n}^{t_{n+1}} a(t)\hat{\theta}(t)\, dt = a(t)\hat{\theta}(t)\bigg|_{t_n}^{t_{n+1}} - \dot{a}(t)\theta(t)\bigg|_{t_n}^{t_{n+1}} + \int_{t_n}^{t_{n+1}} \ddot{a}(t)\theta(t)\, dt
\]

\[
= a(t_{n+1})\hat{\theta}(t_{n+1}) - a(t_n)\hat{\theta}(t_n) + O(h^{2s-1}).
\]
To the other integrals in (1.39) we apply the Lobatto quadrature directly. Since $R_{22}(t_{n+1}, t_n)$ is the identity, this gives

$$p_{n+1} - p(t_{n+1}) = R_{22}(t_{n+1}, t_n) \left( \Delta v(t_n) + hb_1 \delta(t_n) \right) + \tilde{C}(t_{n+1}) \left( hb_1 G(u(t_{n+1})) H_{pp}(v(t_{n+1}), u(t_{n+1})) \delta(t_{n+1}) + \dot{\theta}(t_{n+1}) \right) + \tilde{C}(t_n) \left( hb_1 G(u(t_n)) H_{pp}(v(t_n), u(t_n)) \delta(t_n) - \dot{\theta}(t_n) \right) + O(h^{2s-1}),$$

where $\tilde{C}(t) = R(t_{n+1}, t) C(t)$. The term $\Delta v(t_n) + hb_1 \delta(t_n)$ vanishes by (1.27), and differentiation of the algebraic relation in (1.36) yields

$$0 = G(u(t)) \left( H_p(v(t), u(t)) + \mu(t) \right) + \dot{\theta}(t).$$

As a consequence of (1.27), (1.37) and the consistency of the initial values $(p_n, q_n)$, this gives

$$\dot{\theta}(t_n) = - G(q_n) H_p(p_n - hb_1 \delta(t_n), q_n) = hb_1 G(q_n) H_{pp}(p_n, q_n) \delta(t_n) + O(h^2 \delta(t_n)^2) = hb_1 G(u(t_n)) H_{pp}(v(t_n), u(t_n)) \delta(t_n) + O(h^2 \delta(t_n)^2).$$

Using (1.30) we get in the same way

$$\dot{\theta}(t_{n+1}) = - hb_1 G(u(t_{n+1})) H_{pp}(v(t_{n+1}), u(t_{n+1})) \delta(t_{n+1}) + O(h^2 \delta(t_{n+1})^2).$$

These estimates together show that the local error (1.41) is of size $O(h^{2s-1})$ + $O(h^2 \delta(t)^2)$. The defect $\delta(t)$ vanishes at $s - 2$ points in the interval $[t_n, t_{n+1}]$, so that $\delta(t) = O(h^{s-2})$ for $t \in [t_n, t_{n+1}]$ (for a rigorous proof of this statement one has to apply the techniques of the proof of Theorem II.1.5). Therefore we obtain

$$p_{n+1} - p(t_{n+1}) = O(h^{2s-2}),$$

and by the symmetry of the method also $O(h^{2s-2})$.

In analogy to (1.39), the variation of constants formula yields also an expression for the local error $q_{n+1} - q(t_{n+1}) = \Delta u(t_{n+1})$. One only has to replace $R_{21}$ and $R_{22}$ with the upper blocks $R_{11}$ and $R_{12}$ of the resolvent. Using $R_{12}(t_{n+1}, t_n) = 0$, we prove in the same way that the local error of the $q$-component is of size $O(h^{2s-1})$.

The estimation of the global error is obtained in the same way as for the first order method (1.19)-(1.20). Since the algorithm is a mapping $\Phi_h : \mathcal{M} \rightarrow \mathcal{M}$ on the solution manifold, it is not necessary to follow the technically difficult proofs in the context of differential-algebraic equations. Summing up the propagated local errors proves that the global error satisfies $p_n - p(t_n) = O(h^{2s-2})$ and $q_n - q(t_n) = O(h^{2s-2})$ as long as $t_n = nh \leq \text{Const.}$

### VII.1.6 Splitting Methods

When considering splitting methods for constrained mechanical systems, it should be borne in mind that such systems are differential equations on manifolds (see
Sect. VII.1.2). Splitting methods should therefore be based on a decomposition
\( f(y) = f^{[1]}(y) + f^{[2]}(y) \), where both \( f^{[1]}(y) \) are vector fields on the same manifold as \( f(y) \). Let us consider here the Hamiltonian system (1.9) with Hamiltonian
\[
H(p, q) = H^{[1]}(p, q) + H^{[2]}(p, q).
\]
(1.42)
The manifold for this differential equation is
\[
\mathcal{M} = \{ (p, q) \mid g(q) = 0, \ G(q)H_p(p, q) = 0 \}. \quad (1.43)
\]
Notice that (1.9), when \( H \) is simply replaced with \( H^{[i]} \), is not a good candidate for splitting methods: the existence of a solution is not guaranteed, and if the solution exists it need not stay on the manifold \( \mathcal{M} \). The following lemma indicates how splitting methods should be applied.

**Lemma 1.5.** Consider a Hamiltonian (1.42), a function \( g(q) \) with \( G(q) = g'(q) \), and let the manifold \( \mathcal{M} \) be given by (1.43). If (1.13) holds and if
\[
G(q)H_p^{[i]}(p, q) = 0 \quad \text{for all} \quad (p, q) \in \mathcal{M},
\]
then the system
\[
\begin{align*}
\dot{q} &= H_p^{[i]}(p, q) \\
\dot{p} &= -H_q^{[i]}(p, q) - G(q)^T \lambda \\
0 &= G(q)H_p(p, q)
\end{align*}
\]
(1.45)
defines a differential equation on the manifold \( \mathcal{M} \), and its flow is a symplectic transformation on \( \mathcal{M} \).

**Proof.** Differentiation of the algebraic relation in (1.45) with respect to time, and replacing \( \dot{q} \) and \( \dot{p} \) with their differential equations, yields an explicit relation for \( \lambda = \lambda(p, q) \) (as a consequence of (1.13)). Hence, a unique solution of (1.45) exists locally if \( G(q_0)H_p(p_0, q_0) = 0 \). The assumption (1.44) implies \( \frac{d}{dt} g(q(t)) = 0 \). This together with the algebraic relation of (1.45) guarantees that for \( (p_0, q_0) \in \mathcal{M} \) the solution stays on the manifold \( \mathcal{M} \). The symplecticity of the flow is proved as for Theorem 1.2.

Suppose now that the Hamiltonian \( H(p, q) \) of (1.9) can be split as in (1.42), where both \( H^{[i]}(p, q) \) satisfy (1.44). We denote by \( \varphi^{[i]}_t \) the flow of the system (1.45). If these flows can be computed analytically, the Lie-Trotter splitting \( \varphi^{[2]}_{t/2} \circ \varphi^{[1]}_{t/2} \) and the Strang splitting \( \varphi^{[1]}_{t/2} \circ \varphi^{[2]}_{t/2} \) yield first and second order numerical integrators, respectively. Considering more general compositions as in (II.5.6) and using the coefficients proposed in Sect. V.3, methods of high order are obtained. They give numerical approximations lying on the manifold \( \mathcal{M} \), and they are symplectic (also symmetric if the splitting is well chosen).
For the important special case where

\[ H(p, q) = T(p, q) + U(q) \]

is the sum of the kinetic and potential energies, both summands satisfy assumption (1.44). This gives a natural splitting that is often used in practice.

**Example 1.6 (Spherical Pendulum).** We normalize all constants to 1 (cf. Example 1.1) and we consider the problem (1.9) with

\[ H(p, q) = \frac{1}{2} (p_1^2 + p_2^2 + p_3^2) + q_3, \quad g(q) = \frac{1}{2} (q_1^2 + q_2^2 + q_3^2 - 1) \]

We split the Hamiltonian as \( H^1(p, q) = \frac{1}{2} (p_1^2 + p_2^2 + p_3^2) \) and \( H^2(p, q) = q_3 \), and we solve (1.45) with initial values on the manifold

\[ \mathcal{M} = \{(p, q) \mid q_1^2 + q_2^2 + q_3^2 - 1 = 0, p_1q_1 + p_2q_2 + p_3q_3 = 0\} \]

The kinetic energy \( H^1(p, q) \) leads to the system

\[ \dot{q} = p, \quad \dot{p} = -q \lambda, \quad q^T p = 0, \]

which gives \( \lambda = p_0^T p_0 \), so that the flow \( \varphi^1 \) is just a planar rotation around the origin. The potential energy \( H^2(p, q) \) leads to

\[ \dot{q} = 0, \quad \dot{p} = -(0, 0, 1)^T - q \lambda, \quad q^T p = 0. \]

The flow \( \varphi^2 \) keeps \( q(t) \) constant and changes \( p(t) \) linearly with time. Splitting methods give simple, explicit and symplectic time integrators for this problem.

**VII.2 Poisson Systems**

This section is devoted to an interesting generalization of Hamiltonian systems, where \( J^{-1} \) in (VI.2.5) is replaced with a nonconstant matrix \( B(y) \). Such structures were introduced by Sophus Lie (1888) and are today called Poisson systems. They result, in particular, from Hamiltonian systems on manifolds written in non-canonical coordinates. In a first subsection, however, we discuss the Poisson structure of Hamiltonian systems in canonical form.

**VII.2.1 Canonical Poisson Structure**

\[ \ldots \] quelques remarques sur la plus profonde découverte de M. Poisson, mais qui, je crois, n’a pas été bien comprise ni par Lagrange, ni par les nombreux géomètres qui l’ont citée, ni par son auteur lui-même.  
(C.G.J. Jacobi 1840, p. 350)
The derivative of a function \( F(p, q) \) along the flow of a Hamiltonian system
\[
\frac{d}{dt} F(p(t), q(t)) = \sum_{i=1}^{d} \left( \frac{\partial F}{\partial p_i} \dot{p}_i + \frac{\partial F}{\partial q_i} \dot{q}_i \right) = \sum_{i=1}^{d} \left( \frac{\partial F}{\partial q_i} \frac{\partial H}{\partial p_i} - \frac{\partial F}{\partial p_i} \frac{\partial H}{\partial q_i} \right).
\]
(2.2)

This remarkably symmetric structure motivates the following definition.

**Definition 2.1.** The (canonical) Poisson bracket of two smooth functions \( F(p, q) \) and \( G(p, q) \) is the function
\[
\{F, G\} = \sum_{i=1}^{d} \left( \frac{\partial F}{\partial q_i} \frac{\partial G}{\partial p_i} - \frac{\partial F}{\partial p_i} \frac{\partial G}{\partial q_i} \right),
\]
(2.3)
or in vector notation \( \{F, G\}(y) = \nabla F(y)^T J^{-1} \nabla G(y) \), where \( y = (p, q) \) and \( J \) is the matrix of \( \text{VI.2.3} \).

This Poisson bracket is bilinear, skew-symmetric (\( \{F, G\} = -\{G, F\} \)), it satisfies the Jacobi identity (Jacobi 1862, Werke 5, p. 46)
\[
\{\{F, G\}, H\} + \{\{G, H\}, F\} + \{\{H, F\}, G\} = 0
\]
(2.4)
(notice the cyclic permutations among \( F, G, H \)), and Leibniz’ rule
\[
\{F \cdot G, H\} = F \cdot \{G, H\} + G \cdot \{F, H\}.
\]
(2.5)

These formulas are obtained in a straightforward manner from standard rules of calculus (see also Exercise 1).

With this notation, the Lie derivative (2.2) becomes
\[
\frac{d}{dt} F(y(t)) = \{F, H\}(y(t)).
\]
(2.6)

It follows that a function \( I(p, q) \) is a first integral of (2.1) if and only if
\[
\{I, H\} = 0.
\]

If we take \( F(y) = y_i \), the mapping that selects the \( i \)th component of \( y \), we see that the Hamiltonian system (2.1) or (VI.2.5), \( \dot{y} = J^{-1} \nabla H(y) \), can be written as
\[
\dot{y}_i = \{y_i, H\}, \quad i = 1, \ldots, 2d.
\]
(2.7)
Poisson’s Discovery. At the beginning of the 19th century, the hope of being able to integrate a given system of differential equations by analytic formulas faded more and more, and the energy of researchers went to the construction of, at least, first integrals. In this enthusiasm, Jacobi declared the subsequent result to be “Poisson’s deepest discovery” (see citation) and his own identity, developed for its proof, a “gravissimum Theorema”.

**Theorem 2.2 (Poisson 1809).** If \( I_1 \) and \( I_2 \) are first integrals, then their Poisson bracket \( \{ I_1, I_2 \} \) is again a first integral.

**Proof.** This follows at once from the Jacobi identity with \( F = I_1 \) and \( G = I_2 \). \( \square \)

VII.2.2 General Poisson Structures

...the general concept of a Poisson manifold should be credited to Sophus Lie in his treatise on transformation groups ...


\[
\{ F, G \}(y) = \sum_{i,j=1}^n \frac{\partial F(y)}{\partial y_i} b_{ij}(y) \frac{\partial G(y)}{\partial y_j} \quad (2.8)
\]

(or more compactly \( \{ F, G \}(y) = \nabla F(y)^T B(y) \nabla G(y) \)).

**Lemma 2.3.** The bracket defined in (2.8) is bilinear, skew-symmetric and satisfies Leibniz’ rule (2.5) as well as the Jacobi identity (2.4) if and only if

\[
b_{ij}(y) = -b_{ji}(y) \quad \text{for all } i, j \quad (2.9)
\]

and for all \( i, j, k \) (notice the cyclic permutations among \( i, j, k \))

\[
\sum_{i=1}^n \left( \frac{\partial b_{ij}(y)}{\partial y_i} b_{ik}(y) + \frac{\partial b_{jk}(y)}{\partial y_j} b_{ij}(y) + \frac{\partial b_{ki}(y)}{\partial y_k} b_{ij}(y) \right) = 0. \quad (2.10)
\]

---

1 Siméon Denis Poisson, born: 21 June 1781 in Pithiviers (France), died: 25 April 1840 in Sceaux (near Paris).
Proof. The main observation is that condition (2.10) is the Jacobi identity for the
special choice of functions $F = y_i, G = y_j, H = y_k$ because of
\[ \{ y_i, y_j \} = b_{ij}(y). \] (2.11)
If equation (2.4) is developed for the bracket (2.8), one obtains terms containing
second order partial derivatives — these cancel due to the symmetry of the Jacobi
identity — and terms containing first order partial derivatives; for the latter we may
assume $F, G, H$ to be linear combinations of $y_i, y_j, y_k$, so we are back to (2.10).
The details of this proof are left as an exercise (see Exercise 1). \qed

**Definition 2.4.** If the matrix $B(y)$ satisfies the properties of Lemma 2.3, formula
(2.8) is said to represent a (general) Poisson bracket. The corresponding differential
system
\[ \dot{y} = B(y) \nabla H(y), \] (2.12)
is a Poisson system. We continue to call $H$ a Hamiltonian.

The system (2.12) can again be written in the bracket formulation (2.7). The
formula (2.6) for the Lie derivative remains also valid, as is seen immediately from
the chain rule and the definition of the Poisson bracket. Choosing $F = H$, this
shows in particular that the Hamiltonian $H$ is a first integral for general Poisson
systems.

**Definition 2.5.** A function $C(y)$ is called a Casimir function of the Poisson system
(2.12), if
\[ \nabla C(y)^T B(y) = 0 \quad \text{for all } y. \]

A Casimir function is a first integral of every Poisson system with structure
matrix $B(y)$, whatever the Hamiltonian $H(y)$ is.

**Example 2.6.** The Lotka–Volterra equations of Sect. I.1.1 can be written as
\[ \begin{pmatrix} \dot{u} \\ \dot{v} \end{pmatrix} = \begin{pmatrix} 0 & uv \\ -uv & 0 \end{pmatrix} \nabla H(u, v), \] (2.13)
where $H(u, v) = u - \ln u + v - 2 \ln v$ is the invariant (I.1.4). This is of the form
(2.12) with a matrix that is skew-symmetric and satisfies the identity (2.10).

Higher dimensional Lotka–Volterra systems can also have a Poisson structure
(see, e.g., Perelomov (1995) and Suris (1999)). For example, the system
\[ \dot{y}_1 = y_1(y_2 + y_3), \quad \dot{y}_2 = y_2(y_1 - y_3 + 1), \quad \dot{y}_3 = y_3(y_1 + y_2 + 1) \]
can be written as
\[ \begin{pmatrix} \dot{y}_1 \\ \dot{y}_2 \\ \dot{y}_3 \end{pmatrix} = \begin{pmatrix} 0 & y_1y_2 & y_1y_3 \\ -y_1y_2 & 0 & -y_2y_3 \\ -y_1y_3 & y_2y_3 & 0 \end{pmatrix} \nabla H(y) \] (2.14)
with \( H(y) = -y_1 + y_2 + y_3 + \ln y_2 - \ln y_3 \). Again one can check by direct computation that (2.10) is satisfied.

In contrast to the structure matrix \( J^{-1} \) of Hamiltonian systems in canonical form, the matrix \( B(y) \) of (2.12) need not be invertible. All odd-dimensional skew-symmetric matrices are singular, and so is the matrix \( B(y) \) of (2.14). In this case, the vector \( v(y) = (-1/y_1, -1/y_2, 1/y_3)^T \) satisfies \( v(y)^T B(y) = 0 \). Since \( v(y) = \nabla C(y) \) with \( C(y) = -\ln y_1 - \ln y_2 + \ln y_3 \), the function \( C(y) \) is a Casimir function.

### VII.2.3 Hamiltonian Systems on Symplectic Submanifolds

An important motivation for studying Poisson systems is given by Hamiltonian problems expressed in non-canonical coordinates.

**Example 2.7 (Constrained Mechanical Systems).** Consider the system (1.9) written as the differential equation

\[
\dot{x} = J^{-1} \left( \nabla H(x) + \sum_{i=1}^{m} \lambda_i(x) \nabla g_i(x) \right)
\]

(2.15)

on the manifold \( \mathcal{M} = \{ x ; c(x) = 0 \} \) with \( c(x) = \left( g(q), G(q)H_p(p, q) \right)^T \) and \( x = (p, q)^T \) (see (1.14)). As in the proof of Theorem 1.2, \( \lambda_i(x) \) and \( g_i(x) \) are the components of \( \lambda(x) \) and \( g(x) \), and \( \lambda(x) \) is the function obtained from (1.12). We use \( y \in \mathbb{R}^{2(d-m)} \) as local coordinates of the manifold \( \mathcal{M} \) via the transformation \( x = \chi(y) \).

In these coordinates, the differential equation (2.15) becomes, with \( X(y) = \chi'(y) \),

\[
X(y) \dot{y} = J^{-1} \left( \nabla H(\chi(y)) + \sum_{i=1}^{m} \lambda_i(\chi(y)) \nabla g_i(\chi(y)) \right).
\]

We multiply this equation from the left with \( X(y)^T J \) and note that the columns of \( X(y) \), which are tangent vectors, are orthogonal to the gradients \( \nabla g_i \) of the constraints. This yields

\[
X(y)^T J X(y) \dot{y} = X(y)^T \nabla H(\chi(y)).
\]

By assumption (1.13) the matrix \( X(y)^T J X(y) \) is invertible. This is seen as follows: \( X(y)^T J X(y) v = 0 \) implies \( J X(y) v = c'(x)^T w \) for some \( w (x = \chi(y)) \). By \( c(\chi(y)) = 0 \) and \( c'(x) X(y) = 0 \) we get \( c'(x) J^{-1} c'(x)^T w = 0 \). It then follows from the structure of \( c'(x) \) and from (1.13) that \( w = 0 \) and hence also \( v = 0 \).

With \( B(y) = \left( X(y)^T J X(y) \right)^{-1} \) and \( K(y) = H(\chi(y)) \), the above equation for \( \dot{y} \) thus becomes the Poisson system \( \dot{y} = B(y) \nabla K(y) \). The matrix \( B(y) \) is skew-symmetric and satisfies (2.10), see Theorem 2.8 below or Exercise 11.
More generally, consider a symplectic submanifold $\mathcal{M}$ of $\mathbb{R}^{2d}$, that is, a manifold for which the symplectic two-form\(^2\)

$$\omega_x(\xi_1, \xi_2) = (J\xi_1, \xi_2) \quad \text{for} \quad \xi_1, \xi_2 \in T_x\mathcal{M}$$

(2.16)

(with $(\cdot, \cdot)$ denoting the Euclidean inner product on $\mathbb{R}^{2d}$) is non-degenerate for every $x \in \mathcal{M}$; for $\xi_1$ in the tangent space $T_x\mathcal{M}$,

$$\omega_x(\xi_1, \xi_2) = 0 \quad \text{for all} \quad \xi_2 \in T_x\mathcal{M} \quad \text{implies} \quad \xi_1 = 0.$$  

In local coordinates $x = \chi(y)$, this condition is equivalent to the invertibility of the matrix $X(y)^T J X(y)$ with $X(y) = \chi'(y)$, since every tangent vector at $x = \chi(y)$ is of the form $\xi = X(y)\eta$ and $X(y)$ has linearly independent columns. A manifold defined by constraints, $\mathcal{M} = \{ x \in \mathbb{R}^{2d} | \phi(x) = 0 \}$, is symplectic if the matrix $c'(x)J^{-1}c(x)^T$ is invertible for every $x \in \mathcal{M}$ (see the argument at the end of the previous example). This condition can be restated as saying that the matrix $(\{c_i, c_j\}(x))$ of canonical Poisson brackets of the constraint functions is invertible.

We consider the reduction of the Hamiltonian system to the symplectic submanifold $\mathcal{M}$, which determines solution curves $t \mapsto x(t) \in \mathcal{M}$ by the equations

$$(J \dot{x} - \nabla H(x), \xi) = 0 \quad \text{for all} \quad \xi \in T_x\mathcal{M}.$$  

(2.17)

With the interpretation $(\nabla H(x), \xi) = H'(x)\xi = \frac{d}{dt}|_{t=0} H(\gamma(t))$ as a directional derivative along a path $\gamma(t) \in \mathcal{M}$ with $\gamma(0) = x$ and $\dot{\gamma}(0) = \xi$, it is sufficient that the Hamiltonian $H$ is defined and differentiable on the manifold $\mathcal{M}$. Equation (2.17) can also be expressed as

$$\omega_x(\dot{x}, \xi) = H'(x)\xi \quad \text{for all} \quad \xi \in T_x\mathcal{M},$$

(2.18)

a formulation that is susceptible to further generalization; cf. Marsden & Ratiu (1999), Chap. 5.4, and Exercise 2. Choosing $\xi = \dot{x}$ we obtain $0 = H'(x)\dot{x} = \frac{d}{dt} H(x(t))$, and hence the Hamiltonian is conserved along solutions.

Note that for $\mathcal{M}$ of Example 2.7, the formulation (2.17) is equivalent to the equations of motion (2.15) of the constrained mechanical system. It corresponds to d’Alembert’s principle of virtual variations in constrained mechanics; see Arnold (1989), p. 92. In quantum mechanics the Hamiltonian reduction (2.17) to a manifold (in that case, a submanifold of the Hilbert space $L^2(\mathbb{R}^N, \mathbb{R}^2)$ instead of $\mathbb{R}^{2d}$) is known as the Dirac–Frenkel time-dependent variational principle and is the basic tool for deriving reduced models of the many-body Schrödinger equation; see Sect. VII.6 for an example. From a numerical analysis viewpoint, (2.17) can also be viewed as a Galerkin method on the solution-dependent tangent space $T_x\mathcal{M}$.

In terms of the symplectic projection $P(x) : \mathbb{R}^{2d} \to T_x\mathcal{M}$ for $x \in \mathcal{M}$, defined by determining $P(x)v \in T_x\mathcal{M}$ for $v \in \mathbb{R}^{2d}$ from the condition

$$(JP(x)v, \xi) = (Jv, \xi) \quad \text{for all} \quad \xi \in T_x\mathcal{M},$$

(2.19)

\(^2\) Notice that this two-form is the negative of that introduced in Sect. VI.2. This slight inconsistency makes the subsequent formulas nicer.
formula (2.17) can be reformulated as the differential equation on $\mathcal{M}$,
\[ \dot{x} = P(x)J^{-1}\nabla H(x). \]  
(2.20)

In coordinates $x = \chi(y)$, and again with $X(y) = \chi'(y)$, formula (2.17) becomes
\[ X(y)^T \left( JX(y)\dot{y} - \nabla H(\chi(y)) \right) = 0, \]
and with
\[ B(y) = (X(y)^T JX(y))^{-1} \quad \text{and} \quad K(y) = H(\chi(y)), \]  
(2.21)
we obtain the differential equation
\[ \dot{y} = B(y)\nabla K(y). \]  
(2.22)

**Theorem 2.8.** For a Hamiltonian system (2.17) on a symplectic submanifold $\mathcal{M}$, the equivalent differential equation in local coordinates, (2.22) with (2.21), is a Poisson system.

**Proof.** In coordinates, the symplectic projection is given by
\[ P(x) = X(y)B(y)X(y)^T J \quad \text{for} \quad x = \chi(y) \in \mathcal{M}, \]

since for every tangent vector $\xi = X(y)\eta$ we have by (2.21),
\[ (JXBX^T Jv, X\eta) = (X^T JXBX^T Jv, \eta) = (X^T Jv, \eta) = (Jv, X\eta). \]

From the decomposition $\mathbb{R}^{2d} = P(x)\mathbb{R}^{2d} \oplus (I - P(x))\mathbb{R}^{2d}$ we obtain, by the implicit function theorem, a corresponding splitting in a neighbourhood of the manifold $\mathcal{M}$ in $\mathbb{R}^{2d}$,
\[ v = x + w \quad \text{with} \quad x \in \mathcal{M}, \ P(x)w = 0. \]

This permits us to extend smooth functions $F(y)$ to a neighbourhood of $\mathcal{M}$ by setting
\[ \hat{F}(v) = F(y) \quad \text{for} \quad v = x + w \quad \text{with} \quad x = \chi(y), \ P(x)w = 0. \]

We then have for the derivative $\hat{F}'(x) = \hat{F}'(x)P(x)$ for $x \in \mathcal{M}$ and hence for its transpose, the gradient, $\nabla \hat{F}(x) = P(x)^T \nabla \hat{F}(x)$. Moreover, by the chain rule we have $\nabla F(y) = X(y)^T \nabla \hat{F}(x)$ for $x = \chi(y)$. For the canonical bracket this gives, at $x = \chi(y)$,
\[ \{\hat{F}, \hat{G}\}_{\text{can}}(x) = \nabla \hat{F}(x)^T P(x)J^{-1}P(x)^T \nabla \hat{G}(x) \]
\[ = \nabla F(y)^T B(y)\nabla G(y) = \{F, G\}(y), \]
and hence the required properties of the bracket defined by $B(y)$ follow from the corresponding properties of the canonical bracket. \[ \square \]
VII.3 The Darboux–Lie Theorem

Theorem 2.8 also shows that a Hamiltonian system without constraints becomes a Poisson system in non-canonical coordinates. Interestingly, a converse also holds: every Poisson system can locally be written in canonical Hamiltonian form after a suitable change of coordinates. This result is a special case of the Darboux–Lie Theorem. Its proof was the result of several important papers: Jacobi’s theory of simultaneous linear partial differential equations (Jacobi 1862), the works by Clebsch (1866) and Darboux (1882) on Pfaffian systems, and, finally, the paper of Lie (1888). We shall now retrace this development. Our first tool is a result on the commutativity of Poisson flows.

VII.3.1 Commutativity of Poisson Flows and Lie Brackets

The elegant formula (2.6) for the Lie derivative is valid for general Poisson systems with the vector field \( f(y) = B(y) \nabla H(y) \) of (2.12). Acting on a function \( F : \mathbb{R}^n \to \mathbb{R} \), the Lie operator (III.5.2) becomes

\[
DF = \nabla F^T f = \nabla f^T B(y) \nabla H = \{F, H\}
\]

and is again the Poisson bracket. This observation is the key for the following lemma, which shows an interesting connection between the Lie bracket and the Poisson bracket.

**Lemma 3.1.** Let two smooth Hamiltonians \( H^{[1]}(y) \) and \( H^{[2]}(y) \) be given.

If \( D_1 \) is the Lie operator of \( B(y) \nabla H^{[1]} \)

and \( D_2 \) is the Lie operator of \( B(y) \nabla H^{[2]} \),

then \( [D_1, D_2] \) is the Lie operator of \( B(y) \nabla \{H^{[2]}, H^{[1]}\} \)

(notice, once again, that the indices 1 and 2 have been reversed).

**Proof.** After some clever permutations, the Jacobi identity (2.4) can be written as

\[
\{\{F, H^{[2]}\}, H^{[1]}\} - \{\{F, H^{[1]}\}, H^{[2]}\} = \{F, \{H^{[2]}, H^{[1]}\}\}.
\]

By (3.1) this is nothing other than \( D_1 D_2 F - D_2 D_1 F = [D_1, D_2] F \). \( \square \)

**Lemma 3.2.** Consider two smooth Hamiltonians \( H^{[1]}(y) \) and \( H^{[2]}(y) \) on an open connected set \( U \), with \( D_1 \) and \( D_2 \) the corresponding Lie operators and \( \varphi^{[1]}_s(y) \) and \( \varphi^{[2]}_t(y) \) the corresponding flows. Then, if the matrix \( B(y) \) is invertible, the following are equivalent in \( U \):

(i) \( \{H^{[1]}, H^{[2]}\} = Const \);

(ii) \( [D_1, D_2] = 0 \);

(iii) \( \varphi^{[2]}_t \circ \varphi^{[1]}_s = \varphi^{[1]}_s \circ \varphi^{[2]}_t \).

The conclusions “(i) \( \Rightarrow \) (ii) \( \Leftrightarrow \) (iii)” also hold for a non-invertible \( B(y) \).
Proof. This is obtained by combining Lemma III.5.4 and Lemma 3.1. We need the invertibility of $B(y)$ to conclude that $\{H^{[1]}, H^{[2]}\} = Const$ follows from $B(y)\nabla\{H^{[1]}, H^{[2]}\} = 0$. \hfill $\square$

VII.3.2 Simultaneous Linear Partial Differential Equations

If two functions $F(y)$ and $G(y)$ are given, formula (2.8) determines a function $h(y) = \{F, G\}(y)$ by differentiation. We now ask the inverse question: Given functions $G(y)$ and $h(y)$, can we find a function $F(y)$ such that $\{F, G\}(y) = h(y)$? This problem represents a first order linear partial differential equation for $F$. So we are led to the following problem, which we first discuss in two dimensions.

One Equation. Given functions $a(y_1, y_2)$, $b(y_1, y_2)$, $h(y_1, y_2)$, find all solutions $F(y_1, y_2)$ satisfying

$$a(y_1, y_2) \frac{\partial F}{\partial y_1} + b(y_1, y_2) \frac{\partial F}{\partial y_2} = h(y_1, y_2). \tag{3.4}$$

This equation is, for any point $(y_1, y_2)$, a linear relation between the partial derivatives of $F$, but does not determine them individually. There is one direction, however, where the derivative is uniquely determined, namely that of the vector $n = (a(y_1, y_2), b(y_1, y_2))$, since the left-hand side of equation (3.4) is the directional derivative $\frac{\partial F}{\partial n}$. The lines, which everywhere respect this direction, are called characteristic lines (see left picture of Fig. 3.1). If we parametrize them with a parameter $t$, we can compute $y_1(t), y_2(t)$ as well as $F(t) = F(y_1(t), y_2(t))$ as solutions of the following ordinary differential equations

$$\dot{y}_1 = a(y_1, y_2), \quad \dot{y}_2 = b(y_1, y_2), \quad \dot{F} = h(y_1, y_2). \tag{3.5}$$

The initial values $(y_1(0), y_2(0))$ can be chosen on an arbitrary curve $\gamma$ (which must be transversal to the characteristic lines) and the values $F|_{\gamma}$ can be arbitrarily prescribed. The solution $F(y_1, y_2)$ of (3.4) is then created by the curves (3.5) wherever the characteristic lines go (right picture of Fig. 3.1).

Fig. 3.1. Characteristic lines and solution of a first order linear partial differential equation.
For one equation in $n$ dimensions, the initial values $(y_1(0), \ldots, y_n(0))$ can be freely chosen on a manifold of dimension $n-1$ (e.g., the subspace orthogonal to the characteristic line passing through a given point), and $F$ can be arbitrarily prescribed on this manifold. This guarantees the existence of $n-1$ independent solutions in the neighbourhood of a given point. Here, independent means that the gradients of these functions are linearly independent.

Two Simultaneous Equations. Two simultaneous equations of dimension two are trivial. We therefore suppose $y = (y_1, y_2, y_3)$ and two equations of the form

\[
\begin{align*}
a_1^1(y) \frac{\partial F}{\partial y_1} + a_1^2(y) \frac{\partial F}{\partial y_2} + a_1^3(y) \frac{\partial F}{\partial y_3} &= h_1(y), \\
a_2^1(y) \frac{\partial F}{\partial y_1} + a_2^2(y) \frac{\partial F}{\partial y_2} + a_2^3(y) \frac{\partial F}{\partial y_3} &= h_2(y)
\end{align*}
\]

for an unknown function $F(y_1, y_2, y_3)$. This system can also be written as $D_1F = h_1, D_2F = h_2$, where $D_i$ denotes the Lie operator corresponding to the vector field $a_i^1(y)$. Here, we have two directional derivatives prescribed, namely $\frac{\partial F}{\partial n_1}$ and $\frac{\partial F}{\partial n_2}$ where $n_i = a_i^1(y)$ (see Fig. 3.2). Therefore, we will have to follow both directions and, instead of (3.5), we will have two sets of ordinary differential equations

\[
\begin{align*}
\dot{y}_1 &= a_1^1(y), & \dot{y}_2 &= a_2^1(y), & \dot{y}_3 &= a_3^1(y), & \dot{F} &= h_1(y), \\
\ddot{y}_1 &= a_1^2(y), & \ddot{y}_2 &= a_2^2(y), & \ddot{y}_3 &= a_3^2(y), & \dddot{F} &= h_2(y).
\end{align*}
\]

If we prescribe $F$ on a curve that is orthogonal to $n_1$ and $n_2$, and if we follow the solutions of (3.7), we obtain the function $F$ on two 2-dimensional surfaces $S_1$ and $S_2$ containing the prescribed curve. Continuing from $S_1$ along the second flow and from $S_2$ along the first flow, we may be led to the same point, but nothing guarantees that the obtained values for $F$ are identical. To get a well-defined $F$, additional assumptions on the differential operators and on the inhomogeneities have to be made.

The following theorem, which is due to Jacobi (1862), has been extended by Clebsch (1866), who created the theory of complete systems ("vollständige Sys-
These papers contained long analytic calculations with myriades of formula-
las. The wonderful geometric insight is mainly due to Sophus Lie.

**Theorem 3.3.** Let \( D_1, \ldots, D_m \) be \( m (m < n) \) linear differential operators in \( \mathbb{R}^n \)
corresponding to vector fields \( a^{[1]}(y), \ldots, a^{[m]}(y) \) and suppose that these vectors
are linearly independent for \( y = y_0 \). If

\[
[D_i, D_j] = 0 \quad \text{for all } i, j.
\]  

then the homogeneous system

\[ D_i F = 0 \quad \text{for } i = 1, \ldots, m \]

possesses (in a neighbourhood of \( y_0 \)) \( n - m \) solutions for which the gradients
\( \nabla F(y_0) \) are linearly independent.

Furthermore, the inhomogeneous system of partial differential equations

\[ D_i F = h_i \quad \text{for } i = 1, \ldots, m \]

possesses a particular solution in a neighbourhood of \( y_0 \), if and only if in addition
to (3.8) the functions \( h_1(y), \ldots, h_m(y) \) satisfy the integrability conditions

\[
D_i h_j = D_j h_i \quad \text{for all } i, j.
\]  

**Proof.** (a) Let \( V \) denote the space of vectors in \( \mathbb{R}^n \) that are orthogonal to \( a^{[1]}(y_0), \ldots, a^{[m]}(y_0) \), and consider the \( (n - m) \)-dimensional manifold \( M = y_0 + V \). We then extend an arbitrary smooth function \( F: M \rightarrow \mathbb{R} \) to a neighbourhood of \( y_0 \) by

\[
F(\varphi^{[m]}_{t_m} \circ \cdots \circ \varphi^{[1]}_{t_1}(y_0 + v)) = F(y_0 + v).
\]  

Notice that \( (t_1, \ldots, t_m, v) \mapsto y = \varphi^{[m]}_{t_m} \circ \cdots \circ \varphi^{[1]}_{t_1}(y_0 + v) \) defines a local diffeomorphism between neighbourhoods of \( 0 \) and \( y_0 \). Since the application of the operator \( D_m \) to (3.10) corresponds to a differentiation with respect to \( t_m \) and the expression
\( F(\varphi^{[m]}_{t_m} \circ \cdots \circ \varphi^{[1]}_{t_1}(y_0 + v)) \) is independent of \( t_m \) by (3.10), we get \( D_m F(y) = 0 \).

To prove \( D_i F(y) = 0 \) for \( i < m \), we first have to change the order of the flows \( \varphi^{[j]}_{t_j} \)
in (3.10), which is permitted by Lemma III.5.4 and assumption (3.8), so that \( \varphi^{[i]}_{t_i} \) is
in the left-most position.

(b) The necessity of (3.9) follows immediately from \( D_i h_j = D_i D_j F = D_j D_i F = D_j h_i \). For given \( h_i \) satisfying (3.9) we define \( F(y) \) in a neighbourhood of \( y_0 \) (i.e., for small \( t_1, \ldots, t_m \) and small \( v \)) by

\[
F(\varphi^{[m]}_{t_m} \circ \cdots \circ \varphi^{[1]}_{t_1}(y_0 + v)) = \int_0^{t_1} h_1(\varphi^{[1]}_{t_1}(y_0 + v)) \, dt \\
+ \cdots + \int_0^{t_m} h_m(\varphi^{[m]}_{t_m} \circ \cdots \circ \varphi^{[1]}_{t_1}(y_0 + v)) \, dt,
\]
and we prove that it is a solution of the system $D_i F = h_i$ for $i = 1, \ldots, m$. Since only the last integral depends on $t_m$, we immediately get by differentiation with respect to $t_m$ that $D_m F = h_m$. For the computation of $D_i F$ we differentiate with respect to $t_i$. The first $i - 1$ integrals are independent of $t_i$. The derivative of the $i$th integral gives $h_i \left( \varphi_{t_i}^{[i]} \circ \cdots \circ \varphi_{t_1}^{[1]}(y_0 + v) \right)$, and the derivative of the remaining integrals gives

$$
\int_0^{t_i} D_j h_j \left( \varphi_{t_i}^{[j]} \circ \cdots \circ \varphi_{t_1}^{[1]}(y_0 + v) \right) dt = \int_0^{t_i} D_j h_i \left( \varphi_{t_i}^{[j]} \circ \cdots \circ \varphi_{t_1}^{[1]}(y_0 + v) \right) dt
$$

for $j = i + 1, \ldots, m$. Summing up, this proves $D_i F = h_i$.

### VII.3.3 Coordinate Changes and the Darboux–Lie Theorem

The emphasis here is to simplify a given Poisson structure as much as possible by a coordinate transformation. We change from coordinates $y_1, \ldots, y_n$ to $\tilde{y}_1(y), \ldots, \tilde{y}_n(y)$ with continuously differentiable functions and an invertible Jacobian $A(y) = \partial \tilde{y}/\partial y$.

and we denote $\tilde{F}(\tilde{y}) := F(y)$ and $\tilde{G}(\tilde{y}) := G(y)$ (see Fig. 3.3). The Poisson structure as well as the Poisson flow on one space will become another Poisson structure and flow on the other space by simply applying the chain rule:

$$
\sum_{i,j} \frac{\partial F(y)}{\partial \tilde{y}_i} b_{ij}(y) \frac{\partial G(y)}{\partial \tilde{y}_j} = \sum_{i,j,k,l} \frac{\partial \tilde{F}(\tilde{y})}{\partial \tilde{y}_k} \frac{\partial \tilde{G}(\tilde{y})}{\partial \tilde{y}_l} b_{ij}(y(\tilde{y})) \frac{\partial \tilde{y}_k}{\partial \tilde{y}_j} \frac{\partial \tilde{y}_l}{\partial \tilde{y}_i}.
$$

This is another Poisson structure with

$$
\tilde{b}_{kl} = \{\tilde{y}_k, \tilde{y}_l\} \quad \text{or} \quad \tilde{B}(\tilde{y}) = A(y) B(y) A(y)^T.
$$

---

3 Jean Gaston Darboux, born: 14 August 1842 in Nîmes (France), died: 23 February 1917 in Paris.
The same structure matrix is obtained if the Poisson system (2.12) is written in these new coordinates (Exercise 5).

Since $A$ is invertible, the structure matrices $B$ and $\tilde{B}$ have the same rank. We now want to obtain the simplest possible form for $\tilde{e}_B$.

**Theorem 3.4 (Darboux 1882, Lie 1888).** Suppose that the matrix $B(y)$ defines a Poisson bracket and is of constant rank $n - q = 2m$ in a neighbourhood of $y_0 \in \mathbb{R}^n$. Then, there exist functions $P_1(y), \ldots, P_m(y)$, $Q_1(y), \ldots, Q_m(y)$, and $C_1(y), \ldots, C_q(y)$ satisfying

\[
\begin{align*}
\{P_i, P_j\} &= 0 & \{P_i, Q_j\} &= -\delta_{ij} & \{P_i, C_l\} &= 0 \\
\{Q_i, P_j\} &= \delta_{ij} & \{Q_i, Q_j\} &= 0 & \{Q_i, C_l\} &= 0 \\
\{C_k, P_j\} &= 0 & \{C_k, Q_j\} &= 0 & \{C_k, C_l\} &= 0
\end{align*}
\]  

(3.13)
on a neighbourhood of $y_0$. The gradients of $P_1, Q_1, C_k$ are linearly independent, so that $y \mapsto (P_1(y), Q_1(y), C_k(y))$ constitutes a local change of coordinates to canonical form.

The functions $C_1(y), \ldots, C_q(y)$ are called distinguished functions (ausgezeichnete Funktionen) by Lie.

**Proof.** We follow Lie’s original proof. Similar ideas, and the same notation, are also present in Darboux’s paper. The proof proceeds in several steps, satisfying the conditions of (3.13), from one line to the next, by solving systems of linear partial differential equations.

(a) If all $b_{ij}(y_0) = 0$, the constant rank assumption implies $b_{ij}(y) = 0$ in a neighbourhood of $y_0$. We thus have $m = 0$ and all coordinates $C_j(y) = y_i$ are Casimirs.

(b) If there exist $i, j$ with $b_{ij}(y_0) \neq 0$, we set $Q_1(y) = y_i$ and we determine $P_1(y)$ as the solution of the linear partial differential equation

\[
\{Q_1, P_1\} = 1.
\]  

(3.14)

Because of $b_{ij}(y_0) \neq 0$ the assumption of Theorem 3.3 is satisfied and this yields the existence of $P_1$. We next consider the homogeneous system

\[
\{Q_1, F\} = 0 \quad \text{and} \quad \{P_1, F\} = 0
\]  

(3.15)
of partial differential equations. By Lemma 3.2 and (3.14) the Lie operators corresponding to $Q_1$ and $P_1$ commute, so that by Theorem 3.3 the system (3.15) has $n - 2$ independent solutions $F_3, \ldots, F_n$. Their gradients together with those of $Q_1$ and $P_1$ form a basis of $\mathbb{R}^n$. We therefore can change coordinates from $y_1, \ldots, y_n$ to $Q_1, P_1, F_3, \ldots, F_n$ (mapping $y_0$ to $\tilde{y}_0$). In these coordinates the first two rows and the first two columns of the structure matrix $\tilde{B}(\tilde{y})$ have the required form.

(c) If $b_{ij}(\tilde{y}_0) = 0$ for all $i, j \geq 3$, we have $m = 1$ (similar to step (a)) and the coordinates $F_3, \ldots, F_n$ are Casimirs.
(d) If there exist \( i \geq 3 \) and \( j \geq 3 \) with \( b_{ij}(y_0) \neq 0 \), we set \( Q_2 = F_1 \) and we determine \( P_2 \) from the inhomogeneous system

\[
\{Q_1, P_2\} = 0, \quad \{P_1, P_2\} = 0, \quad \{Q_2, P_2\} = 1.
\]

The inhomogeneities satisfy (3.9), and the Lie operators corresponding to \( Q_1, P_1, Q_2 \) commute (by Lemma 3.2). Theorem 3.3 proves the existence of such a \( P_2 \). We then consider the homogeneous system

\[
\{Q_1, F\} = 0, \quad \{P_1, F\} = 0, \quad \{Q_2, F\} = 0, \quad \{P_2, F\} = 0
\]

and apply once more Theorem 3.3. We get \( n - 4 \) independent solutions, which we denote again \( F_5, \ldots, F_n \). As in part (b) of the proof we get new coordinates \( Q_1, P_1, Q_2, P_2, F_5, \ldots, F_n \), for which the first four rows and columns of the structure matrix are canonical.

(e) The proof now continues by repeating steps (c) and (d) until the structure matrix has the desired form.

Corollary 3.5 (Casimir Functions). In the situation of Theorem 3.4 the functions \( C_1(y), \ldots, C_q(y) \) satisfy

\[
\{C_i, H\} = 0 \quad \text{for all smooth } H. \quad (3.16)
\]

Proof. Theorem 3.4 states that \( \nabla C_i(y)^T B(y) \nabla H(y) = 0 \), when \( H(y) \) is one of the functions \( P_j(y), Q_j(y) \) or \( C_j(y) \). However, the gradients of these functions form a basis of \( \mathbb{R}^n \). Consequently, \( \nabla C_i(y)^T B(y) = 0 \) and (3.16) is satisfied for all differentiable functions \( H(y) \).

□

This property implies that all Casimir functions are first integrals of (2.12) whatever \( H(y) \) is. Consequently, (2.12) is (close to \( y_0 \)) a differential equation on the manifold

\[
\mathcal{M} = \{ y \in U \mid C_i(y) = \text{Const}_i, \ i = 1, \ldots, m \}. \quad (3.17)
\]

Corollary 3.6 (Transformation to Canonical Form). Denote the transformation of Theorem 3.4 by \( z = \vartheta(y) = (P_i(y), Q_i(y), C_k(y)) \). With this change of coordinates, the Poisson system \( \dot{y} = B(y) \nabla H(y) \) becomes

\[
\dot{z} = B_0 \nabla K(z) \quad \text{with} \quad B_0 = \begin{pmatrix} J^{-1} & 0 \\ 0 & 0 \end{pmatrix}, \quad (3.18)
\]

where \( K(z) = H(y) \). Writing \( z = (p, q, c) \), this system becomes

\[
\dot{p} = -K_q(p, q, c), \quad \dot{q} = K_p(p, q, c), \quad \dot{c} = 0.
\]

Proof. The transformed differential equation is

\[
\dot{z} = \vartheta'(y) B(y) \vartheta'(y)^T \nabla K(z) \quad \text{with} \quad y = \vartheta^{-1}(z),
\]

and Theorem 3.4 states that \( \vartheta'(y) B(y) \vartheta'(y)^T = B_0 \).

□
VII.4 Poisson Integrators

Before discussing geometric numerical integrators, we show that many important properties of Hamiltonian systems in canonical form remain valid for systems

$$\dot{y} = B(y)\nabla H(y), \quad (4.1)$$

where $B(y)$ represents a Poisson bracket.

VII.4.1 Poisson Maps and Symplectic Maps

We have already seen that the Hamiltonian $H(y)$ is a first integral of (4.1). We shall show here that the flow of (4.1) satisfies a property closely related to symplecticity.

**Definition 4.1.** A transformation $\varphi : U \to \mathbb{R}^n$ (where $U$ is an open set in $\mathbb{R}^n$) is called a Poisson map with respect to the bracket (2.8), if its Jacobian matrix satisfies

$$\varphi'(y)B(y)\varphi'(y)^T = B(\varphi(y)). \quad (4.2)$$

An equivalent condition is that for all smooth real-valued functions $F, G$ defined on $\varphi(U)$,

$$\{F \circ \varphi, G \circ \varphi\}(y) = \{F, G\}(\varphi(y)), \quad (4.3)$$

as is seen by the chain rule and choosing $F, G$ as the coordinate functions. It is clear from this condition that the composition of Poisson maps is again a Poisson map. A comparison with (3.12) shows that Poisson maps leave the structure matrix invariant.

For the canonical symplectic structure, where $B(y) = J^{-1}$, condition (4.2) is equivalent to the symplecticity of the transformation $\varphi(y)$. This can be seen by taking the inverse of both sides of (4.2), and by multiplying the resulting equation with $\varphi'(y)$ from the right and with $\varphi'(y)^T$ from the left. Also in the situation of a Hamiltonian system (2.17) on a symplectic submanifold $M$, where $B(y)$ is the structure matrix of the differential equation in coordinates $y$ as in Theorem 2.8, condition (4.2) is equivalent to symplecticity in the sense of preserving the symplectic two-form (2.16) on the tangent space, as in (1.16):

**Definition 4.2.** A map $\psi : M \to M$ on a symplectic manifold $M$ is called symplectic if for every $x \in M$,

$$\omega_{\psi(x)}(\psi'(x)\xi_1, \psi'(x)\xi_2) = \omega_x(\xi_1, \xi_2) \quad \text{for all} \quad \xi_1, \xi_2 \in T_xM. \quad (4.4)$$

A near-identity map $\psi : M \to M$ is symplectic if and only if the conjugate map $\varphi$ in local coordinates $x = \chi(y)$, with $\varphi(y)$ given by $\psi(x) = \chi(\varphi(y))$ for $x = \chi(y)$, is a Poisson map for the structure matrix of (2.21), $B(y) = (X(y)^TJX(y))^{-1}$ with $X(y) = \chi'(y)$. This holds because $\psi'(x)\xi = X(\varphi(y))\varphi'(y)\eta$ for $x = \chi(y)$ and $\xi = X(y)\eta$, and because (4.2) is equivalent to $\varphi'(y)^T X(\varphi(y))^T J X(\varphi(y))\varphi'(y) = X(y)^TJX(y)$.
Theorem 4.3. If \( B(y) \) is the structure matrix of a Poisson bracket, then the flow \( \varphi_t(y) \) of the differential equation (4.1) is a Poisson map.

Proof. (a) For \( B(y) = J^{-1} \) this is exactly the statement of Theorem VI.2.4 on the symplecticity of the flow of Hamiltonian systems. This result can be extended in a straightforward way to the matrix \( B_0 \) of (3.18).

(b) For the general case consider the change of coordinates \( z = \vartheta(y) \) which transforms (4.1) to canonical form (Theorem 3.4), i.e., \( \vartheta'(y)B(y)\vartheta'(y)^T = B_0 \) and \( \dot{z} = B_0 \nabla K(z) \) with \( K(z) = H(y) \) (Corollary 3.6). Denoting the flows of (4.1) and \( \dot{z} = B_0 \nabla K(z) \) by \( \varphi_t(y) \) and \( \psi_t(z) \), respectively, we have \( \psi_t(\vartheta(y)) = \vartheta(\varphi_t(y)) \) and by the chain rule \( \psi_t'(\vartheta(y))\vartheta'(y) = \vartheta'(\varphi_t(y))\varphi_t'(y) \). Inserting this relation into \( \psi_t(z)B_0\psi_t'(z)^T = B_0 \), which follows from (a), proves the statement.

A direct proof, avoiding the use of Theorem 3.4, is indicated in Exercise 6. \( \square \)

From Theorems 2.8 and 4.3 and the remark after Definition 4.2 we note the following.

Corollary 4.4. The flow of a Hamiltonian system (2.17) on a symplectic submanifold is symplectic.

The inverse of Theorem 4.3 is also true. It extends Theorem VI.2.6 from canonically symplectic transformations to Poisson maps.

Theorem 4.5. Let \( f(y) \) and \( B(y) \) be continuously differentiable on an open set \( U \subset \mathbb{R}^m \), and assume that \( B(y) \) represents a Poisson bracket (Definition 2.4). Then, \( \dot{y} = f(y) \) is locally of the form (4.1), if and only if

- its flow \( \varphi_t(y) \) respects the Casimirs of \( B(y) \), i.e., \( C_i(\varphi_t(y)) = \text{Const}, \) and
- its flow is a Poisson map for all \( y \in U \) and for all sufficiently small \( t \).

Proof. The necessity follows from Corollary 3.5 and from Theorem 4.3. For the proof of sufficiency we apply the change of coordinates \( (u, c) = \vartheta(y) \) of Theorem 3.4, which transforms \( B(y) \) into canonical form (3.18). We write the differential equation \( \dot{y} = f(y) \) in the new variables as

\[
\begin{align*}
\dot{u} &= g(u, c), \\
\dot{c} &= h(u, c).
\end{align*}
\]

(4.5)

Our first assumption expresses the fact that the Casimirs, which are the components of \( c \), are first integrals of this system. Consequently, we have \( h(u, c) \equiv 0 \). The second assumption implies that the flow of (4.5) is a Poisson map for \( B_0 \) of (3.18). Writing down explicitly the blocks of condition (4.2), we see that this is equivalent to the symplecticity of the mapping \( u_0 \mapsto u(t, u_0, c_0) \), with \( c_0 \) as a parameter. From Theorem VI.2.6 we thus obtain the existence of a function \( K(u, c) \) such that \( g(u, c) = J^{-1}\nabla_u K(u, c) \). Notice that for flows depending smoothly on a parameter, the Hamiltonian also depends smoothly on it. Consequently, the vector field (4.5) is of the form \( B_0 \nabla K(u, c) \). Transforming back to the original variables we obtain \( f(y) = B(y)\nabla H(y) \) with \( H(y) = K(\vartheta(y)) \) (see Corollary 3.6). \( \square \)
VII. Non-Canonical Hamiltonian Systems

VII.4.2 Poisson Integrators

The preceding theorem shows that “being a Poisson map and respecting the Casimirs” is characteristic for the flow of a Poisson system. This motivates the following definition.

Definition 4.6. A numerical method \( y_1 = \Phi_h(y_0) \) is a Poisson integrator for the structure matrix \( B(y) \), if the transformation \( y_0 \mapsto y_1 \) respects the Casimirs and if it is a Poisson map whenever the method is applied to (4.1).

Observe that for a Poisson integrator one has to specify the class of structure matrices \( B(y) \). A method will never be a Poisson integrator for all possible \( B(y) \).

Example 4.7. The symplectic Euler method reads

\[
\begin{align*}
    u_{n+1} &= u_n + hu_{n+1}v_nH_u(u_{n+1}, v_n), \\
    v_{n+1} &= v_n - hv_{n+1}v_nH_v(u_{n+1}, v_n)
\end{align*}
\]

for the Lotka–Volterra problem (2.13). It produces an excellent long-time behaviour (Fig. 4.1, left picture). We shall show that this is a Poisson integrator for all separable Hamiltonians \( H(u, v) = K(u) + L(v) \). For this we compute the Jacobian of the map \((u_n, v_n) \mapsto (u_{n+1}, v_{n+1})\),

\[
\begin{pmatrix}
    1 - hv_nH_v \\
    hv_n(H_u + u_{n+1}H_{uu})
\end{pmatrix}
\begin{pmatrix}
    \frac{\partial (u_{n+1}, v_{n+1})}{\partial (u_n, v_n)}
\end{pmatrix}
= \begin{pmatrix}
    1 & hu_{n+1}(H_v + v_nH_{vv}) \\
    0 & 1 - hu_{n+1}H_u
\end{pmatrix}
\]

(the argument of the partial derivatives of \( H \) is \((u_{n+1}, v_n)\) everywhere), and we check in a straightforward fashion the validity of (4.2). A different proof, using differential forms, is given in Sanz-Serna (1994) for a special choice of \( H(u, v) \). Similarly, the adjoint of the symplectic Euler method is a Poisson integrator, and so is their composition — the Störmer–Verlet scheme. Composition methods based on this scheme yield high order Poisson integrators, because the composition of Poisson maps is again a Poisson map.

The implicit midpoint rule, though symplectic when applied to canonical Hamiltonian systems, turns out not to be a Poisson map for the structure matrix \( B(u, v) \) of (2.13). Figure 4.1 (right picture) shows that the numerical solution does not remain near a closed curve.

It is a difficult task to construct Poisson integrators for general Poisson systems; cf. the overview by Karasözen (2004). First of all, for non-constant \( B(y) \) condition (4.2) is no longer a quadratic first integral of the problem augmented by its variational equation (see Sect. VI.4.1). Secondly, the Casimir functions can be arbitrary and we know that only linear and quadratic first integrals can be conserved automatically (Chap. IV). Therefore, Poisson integrators will have to exploit special structures of the particular problem.

Splitting Methods. Consider a (general) Poisson system \( \dot{y} = B(y)\nabla H(y) \) and suppose that the Hamiltonian permits a decomposition as \( H(y) = H^{[1]}(y) + \ldots + \)
Fig. 4.1. Numerical solutions of the Lotka–Volterra equations (2.13) (step size $h = 0.25$, which is very large compared to the period of the solution; 1000 steps; initial values $(4, 2)$ and $(6, 2)$ for all methods.)

$H^{[m]}(y)$, such that the individual systems $\dot{y} = B(y) \nabla H^{[i]}(y)$ can be solved exactly. The flow of these subsystems is a Poisson map and automatically respects the Casimirs, and so does their composition. McLachlan (1993), Reich (1993), and McLachlan & Quispel (2002) present several interesting examples.

Example 4.8. In the previous example of a Lotka–Volterra equation with separable Hamiltonian $H(u, v) = K(u) + L(v)$, the systems with Hamiltonian $K(u)$ and $L(v)$ can be solved explicitly. Since the flow of each of the subsystems is a Poisson map, so is their composition. Combining a half-step with $L$, a full step with $K$, and again a half-step with $L$, we thus obtain the following Verlet-like second-order Poisson integrator:

$$
\begin{align*}
    u_{n+1/2} &= \exp\left(\frac{h}{2} v_n \nabla L(v_n)\right) u_n \\
    v_{n+1} &= \exp\left(-hu_{n+1/2} \nabla K(u_{n+1/2})\right) v_n \\
    u_{n+1} &= \exp\left(\frac{h}{2} v_{n+1} \nabla L(v_{n+1})\right) u_{n+1/2}.
\end{align*}
$$

(4.6)

In the setting of Hamiltonian systems on a manifold, the splitting approach can be formulated in the following way.

Variational Splitting. Consider a Hamiltonian system (2.17) on a symplectic manifold $\mathcal{M}$, and use a splitting $H = H^{[1]} + H^{[2]}$ of the Hamiltonian in the following algorithm:

1. Let $x_n^+ \in \mathcal{M}$ be the solution at time $h/2$ of the equation for $x$,

$$
(J\dot{x} - \nabla H^{[1]}(x), \xi) = 0 \quad \text{for all } \xi \in T_x\mathcal{M}
$$

(4.7)

with initial value $x(0) = x_n$. 

with
2. Let \( x_n^{n+1} \) be the solution at time \( h \) of
\[
(\dot{J}\dot{x} - \nabla H^{(2)}(x), \xi) = 0 \quad \text{for all} \quad \xi \in T_xM
\] (4.8)
with initial value \( x(0) = x_n^+ \).

3. Take \( x_n^{n+1} \) as the solution at time \( h = 2 \) of (4.7) with initial value \( x(0) = x_n^{n+1} \).

Splitting algorithms for Hamiltonian systems on manifolds have been studied by Dullweber, Leimkuhler & McLachlan (1997) and Benettin, Cherubini & Fasso (2001) in the context of rigid body dynamics; see Sect. VII.5. Lubich (2004) and Faou & Lubich (2004) have studied the above splitting method for applications in quantum molecular dynamics; see Sect. VII.6 for an example.

By Theorem 2.8, the substeps 1.–3. written in coordinates \( x = (y) \) are Poisson systems \( \dot{y} = B(y)\nabla K^{[i]}(y) \) with \( K^{[i]}(y) = H^{[i]}(\chi(y)) \), but the algorithm itself is independent of the choice of coordinates. Since the substeps are exact ows of Hamiltonian systems on the manifold \( M \), their composition yields a symplectic map. In the coordinates \( y \) the substeps are the exact ows of Poisson systems, and hence their composition yields a Poisson map.

**Poisson Integrators and Symplectic Integrators.** Generally we note the following correspondence, which rephrases the remark on symplectic maps and Poisson maps after Definition 4.2. It applies in particular to the symplectic integrators for constrained mechanics of Sect. VII.1.

**Lemma 4.9.** An integrator \( x_1 = \psi_h(x_0) \) for a Hamiltonian system (2.17) on a manifold \( M \) is symplectic if and only if the integrator written in local coordinates, \( y_1 = \phi_h(y_0) \) corresponding to a coordinate map \( x = \chi(y) \), is a Poisson integrator for the structure matrix \( B(y) \) of (2.21).

**VII.4.3 Integrators Based on the Darboux–Lie Theorem.**

If we explicitly know a transformation \( z = \vartheta(y) \) that brings the system \( \dot{y} = B(y)\nabla H(y) \) to canonical form (as in Corollary 3.6), we can proceed as follows: compute \( z_n = \vartheta(y_n) \); apply a symplectic integrator to the transformed system \( \dot{z} = B_0\nabla K(z) \) (\( B_0 \) is the matrix (3.18) and \( K(z) = H(y) \)) which yields \( z_{n+1} = \psi_h(z_n) \); compute finally \( y_{n+1} \) from \( z_{n+1} = \vartheta(y_{n+1}) \). This yields a Poisson integrator by the following lemma.

**Lemma 4.10.** Let \( z = (u, c) = \vartheta(y) \) be the transformation of Theorem 3.4. Suppose that the integrator \( \psi_h(y) \) takes the form
\[
\psi_h(z) = \begin{pmatrix} \psi_h^1(u, c) \\ c \end{pmatrix}
\]
in the new variables \( z = (u, c) \). Then, \( \psi_h^1(u, c) \) is a Poisson integrator if and only if \( u \mapsto \psi_h^1(u, c) \) is a symplectic integrator for every \( c \).
Proof. The integrator $\Psi_h(y)$ is Poisson for the structure matrix $B(y)$ if and only if $\Psi_h(z)$ is Poisson for the matrix $B_0$ of (3.18); see Exercise 7. By assumption, $\Psi_h(z)$ preserves the Casimirs of $B_0$. The identity

$$\Psi_h'(z)B_0\Psi_h'(z)^T = \begin{pmatrix} AJ^{-1}A^T & 0 \\ 0 & 0 \end{pmatrix}$$

with $A = \partial\Psi_h'/\partial u$ proves the statement. \qed

Notice that the transformation $\vartheta$ has to be global in the sense that it has to be the same for all integration steps. Otherwise a degradation in performance, similar to that of the experiment in Example V.4.3, has to be expected.

Example 4.11. As a first illustration consider the Lotka–Volterra system (2.13). Applying the transformation $\vartheta(u,v) = (\ln u, \ln v) = (p, q)$, this system becomes canonically Hamiltonian with

$$K(p, q) = -H(u,v) = -H(e^p, e^q).$$

If we apply the symplectic Euler method to this Hamiltonian system, and if we transform back to the original variables, we obtain the method

$$u_{n+1} = u_n \exp(hv_n H_v(u_{n+1}, v_n)),$$
$$v_{n+1} = v_n \exp(-hu_{n+1} H_u(u_{n+1}, v_n)). \tag{4.9}$$

In contrast to the method of Example 4.7, (4.9) is also a Poisson integrator for (2.13) if $H(u,v)$ is not separable. If we compose a step with step size $h/2$ of the symplectic Euler method with its adjoint method, then we obtain again, in the case of a separable Hamiltonian, the method (4.6).

Example 4.12 (Ablowitz–Ladik Discrete Nonlinear Schrödinger Equation). An interesting space discretization of the nonlinear Schrödinger equation is the Ablowitz–Ladik model

$$i y_k + \frac{1}{\Delta x^2} (y_{k+1} - 2y_k + y_{k-1}) + |y_k|^2 (y_{k+1} + y_{k-1}) = 0,$$

which we consider under periodic boundary conditions $y_{k+N} = y_k$ ($\Delta x = 1/N$). It is completely integrable (Ablowitz–Ladik 1976) and, as we shall see below, it is a Poisson system with noncanonical Poisson bracket. Splitting the variables into real and imaginary parts, $y_k = u_k + iv_k$, we obtain

$$u_k = -\frac{1}{\Delta x^2} (v_{k+1} - 2v_k + v_{k-1}) - (u_k^2 + v_k^2) (v_{k+1} + v_{k-1}),$$
$$v_k = \frac{1}{\Delta x^2} (u_{k+1} - 2u_k + u_{k-1}) + (u_k^2 + v_k^2) (u_{k+1} + u_{k-1}).$$

With $u = (u_1, \ldots, u_N), v = (v_1, \ldots, v_N)$ this system can be written as
\[
\begin{pmatrix}
\dot{u} \\
\dot{v}
\end{pmatrix} =
\begin{pmatrix}
0 & -D(u, v) \\
D(u, v) & 0
\end{pmatrix}
\begin{pmatrix}
\nabla_u H(u, v) \\
\nabla_v H(u, v)
\end{pmatrix},
\tag{4.10}
\]
where \(D = \text{diag}(d_1, \ldots, d_N)\) is the diagonal matrix with entries
\[d_k(u, v) = 1 + \Delta x^2 (u_k^2 + v_k^2),\]
and the Hamiltonian is
\[H(u, v) = \frac{1}{\Delta x^2} \sum_{i=1}^N (u_i u_{i-1} + v_i v_{i-1}) - \frac{1}{\Delta x^4} \sum_{i=1}^N \ln(1 + \Delta x^2 (u_i^2 + v_i^2)).\]

We thus get a Poisson system (the conditions of Lemma 2.3 are directly verified). There are many possibilities to transform this system to canonical form. Tang, Pérez-García & Vázquez (1997) propose the transformation
\[p_k = \frac{1}{\Delta x \sqrt{1 + \Delta x^2 v_k^2}} \arctan\left(\frac{\Delta x}{\sqrt{1 + \Delta x^2 v_k^2}} \cdot u_k\right), \quad q_k = v_k,
\]
for which the inverse can be computed in a straightforward way. Here, we suggest the transformation
\[p_k = u_k \sigma(\Delta x^2 (u_k^2 + v_k^2)) \quad \text{with} \quad \sigma(x) = \frac{\ln(1 + x)}{x}, \quad q_k = v_k \sigma(\Delta x^2 (u_k^2 + v_k^2)) \tag{4.11}
\]
which treats the variables more symmetrically. Its inverse is
\[u_k = p_k \tau(\Delta x^2 (p_k^2 + q_k^2)) \quad \text{with} \quad \tau(x) = \frac{\exp x - 1}{x}, \quad v_k = q_k \tau(\Delta x^2 (p_k^2 + q_k^2)) \tag{4.11}
\]
Both transformations take the system (4.10) to canonical form. For the transformation (4.11) the Hamiltonian in the new variables is
\[H(p, q) = \frac{1}{\Delta x^2} \sum_{i=1}^N \tau(\Delta x^2 (p_i^2 + q_i^2)) \tau(\Delta x^2 (p_{i-1}^2 + q_{i-1}^2))(p_ip_{i-1} + q_iq_{i-1}) - \frac{1}{\Delta x^2} \sum_{i=1}^N (p_i^2 + q_i^2).\]

Applying standard symplectic schemes to this Hamiltonian yields Poisson integrators for (4.10).

**VII.5 Rigid Body Dynamics and Lie–Poisson Systems**

... these topics, which, after all, have occupied workers in geometric mechanics for many years. (R. McLachlan 2003)

An important Poisson system is given by Euler’s famous equations for the motion of a rigid body (see left picture of Fig. 5.1), for which we recall the history and derivation and present various structure-preserving integrators. Euler’s equations are a particular case of Lie–Poisson systems, which result from a reduction process of Hamiltonian systems on a Lie group.
VII.5.1 History of the Euler Equations

“A great challenge for Euler were his efforts to establish a mathematical analysis for the motion of a rigid body. Due to the fact that such a body can have an arbitrary shape and mass distribution (see left picture of Fig. 5.2), and that the rotation axis can arbitrarily move with time, the problem is difficult and Euler struggled for many years (all these articles are collected in *Opera Omnia*, Ser. II, Vols. 7 and 8). The breakthrough was enabled by the discovery that any body, as complicated as may be its configuration, reduces to an inertia ellipsoid with three principal axes and three numbers, the principal moments of inertia (Euler 1758a; see the middle picture of Fig. 5.2 and the citation).

The Inertia Ellipsoid. We choose a moving coordinate system connected to the body $B$ and we consider motions of the body where the origin is fixed. By another of Euler’s famous theorems, any such motion is infinitesimally a rotation around an axis. We represent the rotation axis of the body by the direction of a vector $\omega$ and the speed of rotation by the length $\omega$. Then the velocity of a mass point $x$ of $B$ is given by the exterior product

$$v = \omega \times x = \begin{pmatrix} \omega_2 x_3 - \omega_3 x_2 \\ \omega_3 x_1 - \omega_1 x_3 \\ \omega_1 x_2 - \omega_2 x_1 \end{pmatrix} = \begin{pmatrix} 0 & -\omega_3 & \omega_2 \\ \omega_3 & 0 & -\omega_1 \\ -\omega_2 & \omega_1 & 0 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}$$

(orthogonal to $\omega$, orthogonal to $x$, and of length $|\omega| \cdot |x| \cdot \sin \gamma$; see the left picture of Fig. 5.2). The kinetic energy is obtained by integrating the energy of the mass...
points $dm$ over the body

$$T = \frac{1}{2} \int_B \| \omega \times x \|^2 \, dm$$

$$= \frac{1}{2} \int_B \left( (\omega_2 x_3 - \omega_3 x_2)^2 + (\omega_3 x_1 - \omega_1 x_3)^2 + (\omega_1 x_2 - \omega_2 x_1)^2 \right) \, dm .$$

If this is multiplied out, one obtains

$$T = \frac{1}{2} \omega^T \Theta \omega \text{, where } \Theta_{ii} = \int_B (x_i^2 + x_i^2) \, dm, \quad \Theta_{ik} = -\int_B x_i x_k \, dm, \quad (i \neq k, \ell).$$

(5.3)

Euler (1758a) showed, by endless trigonometric transformations, that there exist principal axes of the body in which this expression takes the form

$$T = \frac{1}{2} \left( I_1 \omega_1^2 + I_2 \omega_2^2 + I_3 \omega_3^2 \right) .$$

(5.4)

This was historically the first transformation of such a $3 \times 3$ quadratic form to diagonal form. Later, Lagrange (1788) discovered that these axes were the eigenvectors of the matrix $\Theta$ and the moments of inertia $I_k$ the corresponding eigenvalues (without calling them so, see the right picture of Fig. 5.1).

The Angular Momentum. The first law of Newton’s *Principia* states that the momentum $v \cdot m$ of a mass point remains constant in the absence of exterior forces. The corresponding quantity for rotational motion is the angular momentum, i.e., the exterior product $x \times v$ times the mass. Integrating over the body we obtain, with (5.1),

$$y = \int_B (x \times v) \, dm = \int_B \left( x \times (\omega \times x) \right) \, dm .$$

If this is multiplied out, the matrix $\Theta$ appears again and one obtains the surprising result (due to Poinsot 1834)

**Fig. 5.2.** A rigid body rotating around a variable axis (left); the corresponding inertia ellipsoid (middle); the corresponding angular momentum (right).
\[ y = \Theta \omega, \quad \text{or, in the principal axes coordinates,} \quad y_k = I_k \omega_k. \tag{5.6} \]

Such a relation is familiar from the theory of conjugate diameters (Apollonius, Book II, Prop. VI): the angular momentum is a vector orthogonal to the plane of vectors conjugate to \( \omega \) (see the right picture of Fig. 5.2).

**The Euler Equations.** Euler’s paper (1758a), on his discovery of the principal axes, is immediately followed by Euler (1758b), where he derives his equations for the motion of a rigid body by long, doubtful and often criticized calculations, repeated in a little less doubtful manner in Euler’s monumental treatise (1765). Beauty and elegance, not only of the result, but also of the proof, is due to Poinsot (1834) and Hayward (1856). It is masterly described by Klein & Sommerfeld (1897), and in Chapter 6 of Arnold (1989).

From now on we choose the coordinate system, moving with the body, such that the inertia tensor remains diagonal. We also watch the motion of the body from a coordinate system stationary in the space. The transformation of a vector \( x \in \mathbb{R}^3 \) in the body frame \( 4 \), to the corresponding \( \tilde{x} \in \mathbb{R}^3 \) in the stationary frame, is denoted by

\[ \tilde{x} = Q(t)x. \tag{5.7} \]

The matrix \( Q(t) \) is orthogonal and describes the motion of the body: for \( x = e_i \) we see that the columns of \( Q(t) \) are the coordinates of the body’s principal axes in the stationary frame.

The analogous statement to Newton’s first law for rotational motion is: *in the absence of exterior angular forces, the angular momentum \( \dot{y} \), seen from the fixed coordinate system, is a constant vector* \(^5\). This same vector \( y \), seen from the moving frame, which at any instance rotates with the body around the vector \( \omega \), rotates in the *opposite* direction. Therefore we have from (5.1), by changing the signs of \( \omega \), the derivatives

\[ \begin{pmatrix} \dot{y}_1 \\ \dot{y}_2 \\ \dot{y}_3 \end{pmatrix} = \begin{pmatrix} 0 & \omega_3 & -\omega_2 \\ -\omega_3 & 0 & \omega_1 \\ \omega_2 & -\omega_1 & 0 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix}. \tag{5.8} \]

If we insert \( \omega_k = y_k/I_k \) from (5.6), we obtain

\[ \begin{pmatrix} \dot{y}_1 \\ \dot{y}_2 \\ \dot{y}_3 \end{pmatrix} = \begin{pmatrix} 0 & y_3/I_3 & -y_2/I_2 \\ -y_3/I_3 & 0 & y_1/I_1 \\ y_2/I_2 & -y_1/I_1 & 0 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix} = \begin{pmatrix} (I_3^{-1} - I_2^{-1}) y_3 y_2 \\ (I_1^{-1} - I_3^{-1}) y_1 y_3 \\ (I_2^{-1} - I_1^{-1}) y_2 y_1 \end{pmatrix} \tag{5.9} \]

or, by rearranging the products the other way round,

\[ \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix} = \begin{pmatrix} 0 & -y_3 & y_2 \\ y_3 & 0 & -y_1 \\ -y_2 & y_1 & 0 \end{pmatrix} \begin{pmatrix} y_1/I_1 \\ y_2/I_2 \\ y_3/I_3 \end{pmatrix}, \tag{5.10} \]

\(^4\) Long-standing tradition, from Klein to Arnold, uses capitals for denoting the coordinates in this moving frame; but this would lead to confusion with our subsequent matrix notation.

\(^5\) For a proof of this statement by d’Alembert’s Principle, see Sommerfeld (1942), §II.13.
written in two different ways as a Poisson system, whose right hand vectors are
the gradients of \( C(y) = \frac{1}{2} \sum_{k=1}^{3} y_k^2 \) and \( H(y) = \frac{1}{2} \sum_{k=1}^{3} I_k^{-1} y_k^2 \), respectively. These are the two quadratic invariants of Chap. IV. The first represents the length of the constant angular momentum \( \vec{y} \) in the orthogonal body frame, and the second represents the energy (5.4).

**Computation of the Position Matrix \( Q(t) \).** Once we have solved the Euler equations for \( y(t) \), we obtain the rotation vector \( \omega(t) \) by (5.6). It remains to find the matrix \( Q(t) \) which gives the position of our rotating body. We know that the columns of the matrix \( Q \), seen in the stationary frame, correspond to the unit vectors \( e_i \) in the body frame. These rotate, by (5.1), with the velocity

\[
\left( \omega \times e_1, \omega \times e_2, \omega \times e_3 \right) = \begin{pmatrix}
0 & -\omega_3 & \omega_2 \\
\omega_3 & 0 & -\omega_1 \\
-\omega_2 & \omega_1 & 0
\end{pmatrix} =: W. \tag{5.11}
\]

We thus obtain \( \dot{Q} \), the rotational velocity expressed in the stationary frame, by the back transformation (5.7):

\[
\dot{Q} = QW \quad \text{or} \quad Q^T \dot{Q} = W. \tag{5.12}
\]

This is a differential system for \( Q \) which, because \( W \) is skew-symmetric, preserves the orthogonality of \( Q \). The problem is solved — in theory.

**VII.5.2 Hamiltonian Formulation of Rigid Body Motion**

In order to open the door for efficient numerical algorithms, we treat the rigid body as a constrained Hamiltonian system.

**Position Variables.** The position of the rigid body at time \( t \) is determined, in view of (5.7), by a three-dimensional orthogonal matrix \( Q(t) \). The constraints to be respected are thus \( Q^T Q - I = 0 \).

**Kinetic Energy.** As in (5.12), we associate with \( Q \) and \( \dot{Q} \) the skew-symmetric matrix \( W = Q^T \dot{Q} \) whose entries \( \omega_k \), arranged as in (5.11), determine the kinetic energy by (5.4):

\[
T = \frac{1}{2} \left( I_1 \omega_1^2 + I_2 \omega_2^2 + I_3 \omega_3^2 \right).
\]

For any diagonal matrix \( D = \text{diag}(d_1, d_2, d_3) \) we observe

\[
\text{trace } (WDW^T) = (d_2 + d_3)\omega_1^2 + (d_3 + d_1)\omega_2^2 + (d_1 + d_2)\omega_3^2.
\]

Therefore, with

\[
I_1 = d_2 + d_3, \quad I_2 = d_3 + d_1, \quad I_3 = d_1 + d_2 \quad \text{or} \quad d_k = \int_B x_k^2 \, dm \tag{5.13}
\]
(note that \( d_k > 0 \) for all bodies that have interior points), we obtain the kinetic energy as

\[
T = \frac{1}{2} \text{trace} (WDW^T).
\]

Inserting \( W = Q^T \dot{Q} \), we have

\[
T = \frac{1}{2} \text{trace} (Q^T \dot{Q} D \dot{Q}^T Q) = \frac{1}{2} \text{trace} (\dot{Q} D \dot{Q}^T),
\]

since \( Q \) is an orthogonal matrix.

**Conjugate Variables.** We now have an expression for the kinetic energy in terms of derivatives of position coordinates and are able to introduce the conjugate momenta

\[
P = \frac{\partial T}{\partial \dot{Q}} = \dot{Q} D.
\]

If we suppose to have, in addition to \( T \), a potential \( U(Q) \), we get the Hamiltonian

\[
H(P, Q) = \frac{1}{2} \text{trace} (PD^{-1}P^T) + U(Q).
\]

**Lagrange Multipliers.** The constraints are given by the orthogonality of \( Q \), i.e., the equation \( g(Q) = Q^T Q - I = 0 \). Since this matrix is always symmetric, this consists of \( \frac{1}{2} n(n + 1) = 6 \) independent algebraic conditions, calling for six Lagrange multipliers. If the expression \( G(Q)^T \lambda \) in (1.9) is actually computed, it turns out that this term becomes the product \( QA \), where the six Lagrange multipliers are arranged in a symmetric matrix \( A \); see also formula (IV.9.6). Thus, the constrained Hamiltonian system (1.9) reads in our case, with \( \nabla U = (\partial U/\partial Q_{ij}) \),

\[
\dot{Q} = PD^{-1},
\]

\[
\dot{P} = -\nabla U(Q) - QA \quad (A \text{ symmetric})
\]

\[
0 = Q^T Q - I.
\]

**Reduction to the Euler Equations.** The key idea is to introduce the matrix

\[
Y = Q^T P = Q^T \dot{Q} D = WD = \begin{pmatrix}
0 & -d_1 \omega_3 & d_2 \omega_2 \\
d_1 \omega_3 & 0 & -d_3 \omega_1 \\
-d_2 \omega_2 & d_3 \omega_1 & 0
\end{pmatrix},
\]

where the \( \omega_k \) can be further expressed in terms of the angular momenta \( y_k = I_k \omega_k \). Using the notation \( \text{skew} (A) = \frac{1}{2}(A - A^T) \), we see, with (5.13), that

\[
Y - Y^T = 2 \text{skew} (Y) = \begin{pmatrix}
0 & -y_3 & y_2 \\
y_3 & 0 & -y_1 \\
-y_2 & y_1 & 0
\end{pmatrix}
\]

contains just the angular momenta. Moreover, \( DY \) is skew-symmetric. By (5.18) the derivative of \( Y \) is seen to be
\[ \dot{Y} = \dot{Q}^T P + Q^T \dot{P} = D^{-1} P^T P - Q^T \nabla U(Q) - \Lambda = D^{-1} Y^T Y - Q^T \nabla U(Q) - \Lambda. \]

Taking the skew-symmetric part of this equation, the symmetric matrix \( \Lambda \) drops out and we obtain
\[
\text{skew}(\dot{Y}) = \text{skew}(D^{-1} Y^T Y) - \text{skew}(Q^T \nabla U(Q)). \tag{5.21}
\]

These are, for \( U = 0 \), precisely the above Euler equations, obtained a second time.

### VII.5.3 Rigid Body Integrators

For a numerical simulation of rigid body motions, one can either solve the constrained Hamiltonian system (5.18), or one can solve the differential equation (5.21) for the angular momentum \( Y(t) \) in tandem with the equation (5.12) for \( Q(t) \).

We consider the following approaches: (I) an efficient application of the \textsc{RATTLE} algorithm (1.26), and (II) various splitting methods.

#### (I) \textsc{RATTLE}

We apply the symplectic \textsc{RATTLE} algorithm (1.26) to the system (5.18), and rewrite the formulas in terms of the variables \( Y \) and \( Q \). This approach has been proposed and developed independently by McLachlan & Scovel (1995) and Reich (1994).

An application of the \textsc{RATTLE} algorithm (1.26) to the system (5.18) yields
\[
\begin{align*}
P_{1/2} &= P_0 - \frac{h}{2} \nabla U(Q_0) - \frac{h}{2} Q_0 A_0, \\
Q_1 &= Q_0 + h P_{1/2} D^{-1}, \quad Q_1^T Q_1 = I, \\
P_1 &= P_{1/2} - \frac{h}{2} \nabla U(Q_1) - \frac{h}{2} Q_1 A_1, \quad Q_1^T P_1 D^{-1} + D^{-1} P_1^T Q_1 = 0,
\end{align*}
\]

where both \( A_0 \) and \( A_1 \) are symmetric matrices. We let \( Y_0 = Q_0^T P_0, Y_1 = Q_1^T P_1, \) and \( Z = Q_0^T P_{1/2} D^{-1} \). We multiply the first relation of (5.22) by \( Q_0^T \), the last relation by \( Q_1^T \), and we eliminate the symmetric matrices \( A_0 \) and \( A_1 \) by taking the skew-symmetric parts of the resulting equations. The orthogonality of \( Q_0^T Q_1 = I + hZ \) implies \( hZ^T Z = -(Z + Z^T) \), which can then be used to simplify the last relation. Altogether this results in the following algorithm.

**Algorithm 5.1.** Let \( Q_0 \) be orthogonal and \( D Y_0 \) be skew-symmetric. One step \((Q_0, Y_0) \mapsto (Q_1, Y_1)\) of the method then reads as follows:

- find \( Z \) such that \( I + hZ \) is orthogonal and
  \[
  \text{skew}(ZD) = \text{skew}(Y_0) - \frac{h}{2} \text{skew}(Q_0^T \nabla U(Q_0)), \tag{5.23}
  \]
- compute \( Q_1 = Q_0(I + hZ) \),
- compute \( Y_1 \) such that \( D Y_1 \) is skew-symmetric and
  \[
  \text{skew}(Y_1) = \text{skew}(ZD) - \text{skew}((Z + Z^T)D) - \frac{h}{2} \text{skew}(Q_1^T \nabla U(Q_1)).
  \]
The second step is explicit, and the third step represents a linear equation for the elements of $Y_1$.

**Computation of the First Step.** We write for the known part of equation (5.23)

$$\text{skew}(Y_0) - \frac{\hbar}{2} \text{skew}(Q_0^T \nabla U(Q_0)) = \begin{pmatrix} 0 & -\alpha_3 & \alpha_2 \\ -\alpha_3 & 0 & -\alpha_1 \\ \alpha_2 & \alpha_1 & 0 \end{pmatrix} = A \quad (5.24)$$

and have to solve

$$\frac{1}{2} (ZD - DZ^T) = A, \quad (I + hZ^T)(I + hZ) = I, \quad \frac{1}{2} (ZD + DZ^T) = S$$

(the trick was to add the last equation with $S$ an unknown symmetric matrix). Elimination gives $Z = (A + S)D^{-1}$ and $Z^T = D^{-1}(S - A)$. Both inserted into the second equation lead to a Riccati equation for $S$. There exist efficient algorithms for such problems; see the reference in Sect. IV.5.3 and a detailed explanation in McLachlan & Zanna (2005).

**Remark 5.2 (Moser–Veselov Algorithm).** An independent access to the above formulas is given in a remarkable paper by Moser & Veselov (1991), by treating the rigid body through a discretized variational principle, similar to the ideas of Sect. VI.6.2. The equivalence is explained by McLachlan & Zanna (2005), following a suggestion of B. Leimkuhler and S. Reich.

**Quaternions (Euler Parameters).** An efficient implementation of the above algorithm requires suitable representations of orthogonal matrices, and the use of quaternions is a standard approach.

After having revolutionized Lagrangian mechanics (see Chapt. VI), Hamilton struggled for years to generalize complex analysis to three dimensions. He finally achieved his dream, however not in three dimensions, but in four, and founded in 1843 the theory of quaternions.

For an introduction to quaternions (whose coefficients are sometimes called Euler parameters) we refer to Sects. IV.2 and IV.3 of Klein (1908), and for their use in numerical simulations to Sects. 9.3 and 11.3 of Haug (1989). Quaternions can be written as $e = e_0 + ie_1 + je_2 + ke_3$, where multiplication is defined via the relations $i^2 = j^2 = k^2 = -1$, $ij = k$, $jk = i$, $ki = j$, and $ji = -k$, $kj = -i$, $ik = -j$. The product of two quaternions $e \cdot f$ (written in matrix notation) is

$$e \cdot f = \begin{pmatrix} e_0 & e_1 & e_2 & e_3 \\ e_1 & e_0 & -e_3 & e_2 \\ e_2 & e_3 & e_0 & -e_1 \\ e_3 & -e_2 & e_1 & e_0 \end{pmatrix} \begin{pmatrix} f_0 \\ f_1 \\ f_2 \\ f_3 \end{pmatrix} \quad (5.25)$$

We see (in grey) that in dimensions 1, 2, 3 appears a skew-symmetric matrix $E$ whose structure is familiar to us. This part of the matrix changes sign if the two factors are permuted.
An important discovery, for three dimensional applications of the quaternions, is the following: if a quaternion $p$ is a 3-vector (i.e., has $p_0 = 0$), then $p' = e \cdot p \overline{\tau}$ is a 3-vector, too, and the map $p \mapsto p'$ is described by the matrix

$$Q(e) = \|e\|^2 I + 2e_0 E + 2E^2, \quad E = \begin{pmatrix} 0 & -e_3 & e_2 \\ e_3 & 0 & -e_1 \\ -e_2 & e_1 & 0 \end{pmatrix}$$

(5.26)

where $\overline{\tau} = e_0 - ie_1 - je_2 - ke_3$ and $\|e\|^2 = e \cdot e = e_0^2 + e_1^2 + e_2^2 + e_3^2$.

**Lemma 5.3.** If $\|e\| = 1$, then the matrix $Q(e)$ is orthogonal. Every orthogonal matrix with dot $Q = 1$ can be written in this form. We have $Q(e)Q(f) = Q(ef)$, so that the multiplication of orthogonal matrices corresponds to the multiplication of quaternions.

Geometrically, the matrix $Q$ effects a rotation around the axis $e = (e_1, e_2, e_3)^T$ with rotation angle $\phi$ which satisfies $\tan(\phi/2) = \|e\|/e_0$.

**Proof.** The condition $Q^TQ = I$ can be verified directly using $E^T = -E$ and $E^3 = -(e_1^2 + e_2^2 + e_3^2)E$. The reciprocal statement is a famous theorem of Euler; it is based on the fact that $e$ is an eigenvector of $Q$, which in dimension $3 \times 3$ always exists. The formula for $Q(e)Q(f)$ follows from $e \cdot f = (e \cdot f) \cdot (e \cdot f)$.

The geometric property follows from the virtues of the exterior product, because by (5.1) the matrix $Q$ maps a vector $x$ to

$$x + 2e_0 e \times x + 2 \varepsilon (e \times e).$$

This consists in a rectangular movement in a plane orthogonal to $e$; first vertical to $x$ by an amount $2e_0 \|e\|$ (times the distance of $x$), then parallel to $x$ by an amount $2\|e\|^2$.

Applying Pythagoras’ Theorem as $(2e_0 \|e\|)^2 + (2\|e\|^2 - 1)^2 = 1$, it turns out that the map is norm preserving if $e_0^2 + \|e\|^2 = 1$. The angle $\phi/2$, whose tangens can be seen to be $\|e\|/e_0$, is an angle at the circumference of the circle for the rotation angle $\phi$ at the center.

For an efficient implementation of Algorithm 5.1 we represent the orthogonal matrices $Q_0$, $Q_1$, and $I + hZ$ by quaternions. This reduces the dimension of the systems, and step 2 becomes a simple multiplication of quaternions. For solving the nonlinear system of step 1, we let $I + hZ = Q(e)$. With the values of $\alpha_i$ from (5.24) and with skew $(hZD) = 2e_0 \mathrm{skew}(ED) + 2 \mathrm{skew}(E^2D)$, the equation (5.23) becomes

$$\begin{pmatrix} h\alpha_1 \\ h\alpha_2 \\ h\alpha_3 \end{pmatrix} = 2e_0 \begin{pmatrix} I_1e_1 \\ I_2e_2 \\ I_3e_3 \end{pmatrix} + 2 \begin{pmatrix} (I_1 - I_2)e_2e_3 \\ (I_2 - I_3)e_3e_1 \\ (I_3 - I_1)e_1e_2 \end{pmatrix},$$

(5.27)

which, together with $e_0^2 + e_1^2 + e_2^2 + e_3^2 = 1$, represent four quadratic equations for four unknowns. We solve them very quickly by a few fixed-point iterations: update...
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force free body

symmetric body

y_1

y_2

y_3

non-symmetric body

y_1

y_2

y_3

heavy body

y_1

y_2

y_3

Fig. 5.3. Numerical solutions of the rigid body equations; without/with gravitation, with/without symmetry. Initial values \( y_{10} = 0.2, y_{20} = 1.0, y_{30} = 0.4 \); initial position of \( Q_0 \) determined by the quaternion \( e_0 = 0.4, e_1 = 0.2, e_2 = 0.4, e_3 = 0.8 \); moments of inertia \( I_1 = 0.5, I_2 = 0.85 \) (0.5 in the symmetric case), \( I_3 = 1 \); step size \( h = 0.1 \), integration interval \( 0 \leq t \leq 30 \).

successively \( e_i \) from the \( i \)th equation of (5.27) and then \( e_0 \) from the normalization condition. A Fortran subroutine RATORI for this algorithm is available on the homepage <http://www.unige.ch/~hairer>.

Conservation of Casimir and Hamiltonian. It is interesting to note that, in the absence of a potential, the Algorithm 5.1 preserves exactly the Casimir \( y_1^2 + y_2^2 + y_3^2 \) and, more surprisingly, also the Hamiltonian \( \frac{1}{2}(y_1^2/I_1 + y_2^2/I_2 + y_3^2/I_3) \). This can be seen as follows: without any potential we have skew \((Y_0) = \) skew \((ZD)\) and skew \((Y_1) = -\) skew \((Z^TF)\), so that the vectors \((y_{10}, y_{20}, y_{30})^T\) and \((y_{11}, y_{21}, y_{31})^T\) are equal to \(u + v\) and \(u - v\), respectively, where \(u\) and \(v\) are the vectors of the right-hand side of (5.27). Since \(u\) and \(v\) are orthogonal, we have \(\|u + v\| = \|u - v\|\), which proves the conservation of the Casimir.

To prove the conservation of the Hamiltonian, we first multiply the relation (5.27) with \( G = \text{diag}(1/\sqrt{I_1}, 1/\sqrt{I_2}, 1/\sqrt{I_3})\), and then apply the same arguments. The vectors \(Gu\) and \(Gv\) are still orthogonal.

Example 5.4 (Force-Free and Heavy Top). We present in Fig. 5.3 the numerical solutions \(y_i\) obtained by the above algorithm. In the case of the heavy top, we assume the centre of gravity to be \((0, 0, 1)\) in the body frame, and assume that the third coordinate of the stationary frame is vertical. The potential energy due to gravity is
then given by \( U(Q) = q_{33} \) and, expressed by quaternions (5.26), it is \( U = e_3^3 - e_2^3 + e_1^3 \).

### (II) Splitting Methods

As before we consider the differential equation (5.21) for the angular momenta in the body \( y_1, y_2, y_3 \) together with the differential equation (5.12) for the rotation matrix \( Q \). An obvious splitting in the presence of a potential is

\[
\varphi_{h/2} U^T \circ \varphi_{h} U^T \varphi_{h/2},
\]

where \( \varphi_{h/2} U^T \) represents the exact flow of \( \dot{\omega} = 0, \quad \text{skew} (\dot{Y}) = -\text{skew} (Q^T \nabla U(Q)) \), and \( \varphi_{h} U^T \) is a suitable numerical approximation of the system corresponding to kinetic energy only, i.e., without any potential \( U(Q) \). The use of splitting techniques for rigid body dynamics was proposed by Touma & Wisdom (1994), McLachlan (1993), Reich (1994), and Dullweber, Leimkuhler & McLachlan (1997). Fasso (2003) presents a careful study and comparison of various ways of splitting the kinetic energy.

#### Computation of \( \varphi_{h} U^T \).

We do this by splitting once again, by letting several moments of inertia tending to infinity (and the corresponding \( \omega_i \) tending to zero). In order to avoid formal difficulties with infinite denominators, we write the system (5.10) together with (5.12) in the form

\[
\begin{pmatrix}
\dot{y}_1 \\
\dot{y}_2 \\
\dot{y}_3
\end{pmatrix} =
\begin{pmatrix}
0 & -y_3 & y_2 \\
y_3 & 0 & -y_1 \\
-y_2 & y_1 & 0
\end{pmatrix}
\begin{pmatrix}
T_{y_1} (y) \\
T_{y_2} (y) \\
T_{y_3} (y)
\end{pmatrix},
\]

(5.59)

where \( T(y) = \frac{1}{2} (y_1^2/I_1 + y_2^2/I_2 + y_3^2/I_3) \) is the kinetic energy, and \( T_{y_i} (y) \) denote partial derivatives.

#### Three Rotations Splitting. An obvious splitting of the kinetic energy is

\[
T(y) = R_1(y) + R_2(y) + R_3(y), \quad R_i(y) = y_i^2/(2I_i),
\]

(5.31)

which results in the numerical method

\[
\varphi_{h} U^T = \varphi_{h/2} \circ \varphi_{h/2} \circ \varphi_{h/2} \circ \varphi_{h/2} \circ \varphi_{h/2},
\]

where \( \varphi_{h/2} R_i \) is the exact flow of (5.29)-(5.30) with \( T(y) \) replaced by \( R_i(y) \). The flow \( \varphi_{1} R_1 \) is easily obtained: \( y_1 \) remains constant and the second and third equation in (5.29) boil down to the harmonic oscillator. We obtain
\[ y(t) = S(\alpha t)y(0), \quad Q(t) = Q(0)S(\alpha t)^T \]  \quad (5.32)

with \( \alpha = y_1(0)/I_1 \) and the rotation matrix

\[
S(\theta) = \begin{pmatrix}
1 & 0 & 0 \\
0 & \cos \theta & \sin \theta \\
0 & -\sin \theta & \cos \theta
\end{pmatrix}.
\]

Similar simple formulas are obtained for the exact flows corresponding to \( R_2 \) and \( R_3 \).

**Symmetric + Rotation Splitting.** It is often advantageous, in particular for a nearly symmetric body \((I_1 \approx I_2)\), to consider the splitting

\[
T(y) = R(y) + S(y), \quad R(y) = \left( \frac{1}{I_1} - \frac{1}{I_2} \right) \frac{y_1^2}{2}, \quad S(y) = \frac{1}{2} \left( \frac{y_1^2 + y_2^2}{I_2} + \frac{y_3^2}{I_3} \right)
\]

and the corresponding numerical integrator

\[
\Phi_h^T = \varphi_{h/2}^R \circ \varphi_h^S \circ \varphi_{h/2}^R.
\]

The exact flow \( \varphi_{\alpha}^R \) is the same as (5.32) with \( I_1^{-1} \) replaced by \( I_1^{-1} - I_2^{-1} \). The flow of the symmetric force-free top \( \varphi_{\alpha}^S \) possesses simple analytic formulas, too (see the first picture of Fig. 5.3): we observe a precession of \( y \) with constant speed around a cone and a rotation of the body around \( \omega \) with constant speed. Therefore

\[
y(t) = B(\beta t)y(0), \quad Q(t) = Q(0)A(t)B(\beta t)^T, \quad (5.33)
\]

where \( \beta = (I_1^{-1} - I_2^{-1})y_3(0) \), and

\[
A(t) = \exp \left( t \frac{I_2}{I_1} \begin{pmatrix}
0 & -y_3(0) & y_2(0) \\
y_3(0) & 0 & -y_1(0) \\
-y_2(0) & y_1(0) & 0
\end{pmatrix} \right), \quad B(\theta) = \begin{pmatrix}
\cos \theta & \sin \theta & 0 \\
-\sin \theta & \cos \theta & 0 \\
0 & 0 & 1
\end{pmatrix}.
\]

This can also be checked directly by differentiation.

Similar to the previous algorithm it is advantageous to use a representation of the appearing orthogonal matrices by quaternions. The correspondence between the orthogonal rotation matrices appearing in (5.32) and (5.33) and their quaternions is, in accordance with Lemma 5.3, the following:

\[
S(\theta)^T \iff \cos(\theta/2) + i \sin(\theta/2)
\]
\[
B(\theta)^T \iff \cos(\theta/2) + k \sin(\theta/2)
\]
\[
A(t) \iff \cos(\theta/2) + a^{-1} \sin(\theta/2) (iy_1(0) + jy_2(0) + ky_3(0)),
\]

where \( a = \sqrt{y_1(0)^2 + y_2(0)^2 + y_3(0)^2} \) and \( \vartheta = \alpha t/I_2 \). The matrix multiplications in the algorithm can therefore be done very efficiently. A Fortran subroutine QUATER for the ‘symmetric + rotation splitting’ algorithm is available on the homepage <http://www.unige.ch/~hairer/>.
VII.5.4 Lie–Poisson Systems

In Sect. VII.5.1 we have seen that the reduction of the equations of motion of the rigid body leads to the Poisson system (5.10) with a structure matrix whose entries are linear functions. Here we consider more general Poisson systems

\[ \dot{y} = B(y) \nabla H(y), \]

where the structure matrix \( B(y) \) depends linearly on \( y \), i.e.,

\[ b_{ij}(y) = \sum_{k=1}^{n} C_{jk}^{i} y_k \quad \text{for } i, j = 1, \ldots, n. \]

Such systems, called Lie–Poisson systems, are closely related to differential equations on the dual of Lie algebras; see Marsden & Ratiu (1999), Chaps. 13 and 14, for an in-depth discussion of this theory.

Recall that a Lie algebra is a vector space with a bracket which is anti-symmetric and satisfies the Jacobi identity (Sect. IV.6). Let \( E_1, \ldots, E_n \) be a basis of a vector space, and define a bracket by

\[ [E_i, E_j] = \sum_{k=1}^{n} C_{ij}^{k} E_k \]  

(5.36)

with \( C_{ij}^{k} \) from (5.35). If the structure matrix \( B(y) \) of (5.35) is skew-symmetric and satisfies (2.10), then this bracket makes the vector space a Lie algebra (the verification is left as an exercise). The coefficients \( C_{ij}^{k} \) are called structure constants of the Lie algebra. Conversely, if we start from a Lie algebra with bracket given by (5.36), then the matrix \( B(y) \) defined by (5.35) is the structure matrix of a Poisson bracket.

Let \( \mathfrak{g} \) be a Lie algebra with a basis \( E_1, \ldots, E_n \), and let \( \mathfrak{g}^* \) be the dual of the Lie algebra, i.e., the vector space of all linear forms \( Y : \mathfrak{g} \to \mathbb{R} \). The duality is written as \( \langle Y, X \rangle \) for \( Y \in \mathfrak{g}^* \) and \( X \in \mathfrak{g} \). We denote by \( F_1, \ldots, F_n \) the dual basis defined by

\[ \langle F_i, E_j \rangle = \delta_{ij}, \]

the Kronecker \( \delta \).

**Theorem 5.5.** Let \( \mathfrak{g} \) be a Lie algebra with basis \( E_1, \ldots, E_n \) satisfying (5.36). To \( y = (y_1, \ldots, y_n)^T \in \mathbb{R}^n \) we associate \( Y = \sum_{j=1}^{n} y_j F_j \in \mathfrak{g}^* \), and we consider a Hamiltonian\(^6\) \( H(y) = H(Y) \).

Then, the Poisson system \( \dot{y} = B(y) \nabla H(y) \) with \( B(y) \) given by (5.35) is equivalent to the following differential equation on the dual \( \mathfrak{g}^* \):

\[ \langle \dot{Y}, X \rangle = \langle Y, [H'(Y), X] \rangle \quad \text{for all } X \in \mathfrak{g}, \]

(5.37)

where \( H'(Y) = \sum_{j=1}^{n} \frac{\partial H(Y)}{\partial y_j} E_j \).

\(^6\) We use the same symbol \( H \) for the functions \( H : \mathbb{R}^n \to \mathbb{R} \) and \( H : \mathfrak{g}^* \to \mathbb{R} \).
Proof. Differentiating $H(y) = H(Y)$ with respect to $y_i$ gives

$$\frac{\partial H(y)}{\partial y_i} = \langle F_i, H'(Y) \rangle$$

and

$$H'(Y) = \sum_{j=1}^{n} \frac{\partial H(y)}{\partial y_j} E_j.$$

Here we have used the identification $(\mathfrak{g}^*)^* = \mathfrak{g}$, because $H'(Y)$ is actually an element of $(\mathfrak{g}^*)^*$. With this formula for $H'(Y)$ we are able to compute

$$\langle Y, [H'(Y), E_i] \rangle = \left\langle Y, \sum_{j=1}^{n} \frac{\partial H(y)}{\partial y_j} [E_j, E_i] \right\rangle = \sum_{j=1}^{n} \sum_{k=1}^{n} \frac{\partial H(y)}{\partial y_j} C_{ji}^k \langle Y, E_k \rangle,$$

where we have used (5.36). Since $\langle \dot{Y}, E_i \rangle = \dot{y}_i$ and $\langle Y, E_k \rangle = y_k$, this shows that the differential equation (5.37) is equivalent to

$$\dot{y}_i = \sum_{j=1}^{n} \left( \sum_{k=1}^{n} C_{ji}^k y_k \right) \frac{\partial H(y)}{\partial y_j},$$

which is nothing more than $\dot{y} = B(y) \nabla H(y)$ with $B(y)$ from (5.35).

We remark that (5.37) can be reformulated as

$$\dot{Y} = \text{ad}_{H'(Y)}^* Y,$$

where $\text{ad}_{A}^*$ is the adjoint of the operator $\text{ad}_{A}(X) = [A, X]$.

Equation (5.37) is similar in appearance to the Lie bracket equation $\dot{L} = [A(L), L] = \text{ad}_{A(L)} L$ of Sect.IV.3.2. When $\mathfrak{g}$ is the Lie algebra of a matrix Lie group $G$, then solutions of that equation are of the form $L(t) = \text{Ad}_{U(t)} L_0$ where

$$\text{Ad}_{U} X = UXU^{-1};$$

see the proof of Lemma IV.3.4. Similarly, for the solution of (5.37) we have the following.

**Theorem 5.6.** Consider a matrix Lie group $G$ with Lie algebra $\mathfrak{g}$. Then, the solution $Y(t) \in \mathfrak{g}^*$ of (5.37) with initial value $Y_0 \in \mathfrak{g}^*$ is given by

$$\langle Y(t), X \rangle = \langle Y_0, U(t)^{-1} X U(t) \rangle \quad \text{for all } X \in \mathfrak{g},$$

where $U(t) \in G$ satisfies

$$\dot{U} = -H'(Y(t))U, \quad U(0) = I.$$  (5.40)

Equation (5.39) can be written as

$$Y(t) = \text{Ad}_{U(t)^{-1}}^* Y_0,$$

where $\text{Ad}_{U(t)^{-1}}^*$ is the adjoint of $\text{Ad}_{U(t)^{-1}}$. The solution $Y(t)$ of (5.37) thus lies on the coadjoint orbit

$$Y(t) \in \{ \text{Ad}_{U(t)^{-1}}^* Y_0 ; U \in G \}.$$  (5.41)

In coordinates $Y = \sum_{j=1}^{n} y_j F_j$, we note $y_j = \langle Y_0, U(t)^{-1} E_j U(t) \rangle$. 

Proof. Differentiating the ansatz (5.39) for the solution we obtain
\[
\langle \dot{Y}, X \rangle = \langle Y_0, -U^{-1}\dot{U}U^{-1}XU + U^{-1}XU \rangle \\
= \langle Y_0, U^{-1}[X, \dot{U}U^{-1}]U \rangle = \langle Y, [X, \dot{U}U^{-1}] \rangle,
\]
where we have used (5.39) in the first and the last equation. This shows that (5.37) is satisfied with the choice \( \dot{U}U^{-1} = -H'(Y) \).

Example 5.7 (Rigid Body). The Lie group corresponding to the rigid body is \( \text{SO}(3) \) with the Lie algebra \( \mathfrak{so}(3) \) of skew-symmetric \( 3 \times 3 \) matrices, with the basis
\[
E_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}, \quad E_2 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix}, \quad E_3 = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.
\]
If we let \( x = (x_1, x_2, x_3)^T \) be the coordinates of \( X \in \mathfrak{so}(3) \), then we have \( Xv = x \times v \) for all \( v \in \mathbb{R}^3 \). Since for \( U \in \text{SO}(3) \),
\[
U^{-1}XUv = U^{-1}(x \times Uv) = U^{-1}x \times v,
\]
the vector \( U^{-1}x \) consists of the coordinates of \( U^{-1}XU \in \mathfrak{so}(3) \).

Let \( y = (y_1, y_2, y_3)^T \) be the coordinates of \( Y \in \mathfrak{so}(3)^* \) with respect to the dual basis of \( E_1, E_2, E_3 \). Since
\[
\langle Y, U^{-1}XU \rangle = \left\langle \sum_{j=1}^3 y_j F_j, \sum_{i=1}^3 (U^{-1}x)_i E_i \right\rangle = y^T U^{-1}x = (Uy)^T x,
\]
the coordinates of \( \text{Ad}_{U^{-1}} Y \) are given by the vector \( Uy \). Therefore, the coordinates of the coadjoint orbit of \( Y \) lie on a sphere of radius \( \|y\| \). The conservation of the coadjoint orbit thus reduces here to the preservation of the Casimir \( C(y) = y_1^2 + y_2^2 + y_3^2 \).

Lie–Poisson integrators seem to have first been considered by Ge & Marsden (1988), who extend the construction of symplectic methods by generating functions to Lie–Poisson systems. Channel & Scovel (1991) propose an implementation of these methods based on a coordinatization of the group by the exponential map.

McLachlan (1993) proposes integrators based on splitting the Hamiltonian and illustrates this approach for various examples of Lie-Poisson systems. When applicable, such splitting integrators yield Poisson integrators that preserve the coadjoint orbits, since they are composed of exact flows of Lie-Poisson systems.

Engø & Faltinsen (2001) propose to solve numerically the Lie–Poisson system (5.34) by applying Lie group integrators such as those of Sect. IV.8 to the differential equation (5.40) with (5.39). This approach keeps the solution on the coadjoint orbit by construction, but it does not, in general, give a Poisson integrator.
VII.5 Lie–Poisson Reduction

The reduction of the Hamiltonian equations of motion of the free rigid body to the Euler equations is an instance of a general reduction process from Hamiltonian systems with symmetry on a Lie group to Lie–Poisson systems, which we now describe; cf. Marsden & Ratiu (1999), Chap. 13, for a presentation in a more abstract framework and for an historical account.

Let us assume that the Lie group \( G \) is a subgroup of \( \text{GL}(n) \) given by
\[
G = \{ Q : g_i(Q) = 0, \ i = 1, \ldots, m \},
\]
and consider a Hamiltonian system on \( G \),
\[
\dot{P} = -\nabla_Q H(P,Q) - \sum_{i=1}^{m} \lambda_i \nabla_Q g_i(Q),\quad \dot{Q} = \nabla_P H(P,Q)
\]
\[
0 = g_i(Q), \quad i = 1, \ldots, m,
\]
where \( P, Q \) are square matrices, and \( \nabla_Q H = \frac{\partial H}{\partial Q_{ij}} \). This is of the form discussed in Sect. VII.1.2. In regions where the matrix
\[
\left( \frac{\partial^2 H(P,Q)}{\partial P^2} \left( \nabla_Q g_i(Q), \nabla_Q g_j(Q) \right) \right)_{i,j=1}^{m}
\]
is invertible, \( \lambda_i \) can be expressed in terms of \( P \) and \( Q \) (cf. formula (1.13)). Hence, a unique solution exists locally provided the initial values \( (P_0, Q_0) \) are consistent, i.e., \( g_i(Q_0) = 0 \) and
\[
g_i(Q_0) \left( \nabla_P H(P_0, Q_0) \right) = \text{trace} \left( \nabla_Q g_i(Q_0)^T \nabla_P H(P_0, Q_0) \right) = 0,
\]
or equivalently, \( Q_0 \in G \) and \( \nabla_P H(P_0, Q_0) \in T_{Q_0} G \).

We now assume that the Hamiltonian \( H \) is quadratic in \( P \). As we have seen in Sect. VII.1.2, the equations (5.43) can be viewed as a differential equation on the cotangent bundle \( T^* G = \{ (P, Q) : Q \in G, \ P \in T_Q^* G \} \), where the cotangent space \( T_Q^* G \) is identified with a subspace of matrices such that
\[
P \in T_Q^* G \quad \text{if and only if} \quad \nabla_P H(P, Q) \in T_Q G.
\]
With this identification, the duality between \( T_Q^* G \) and \( T_Q G \) is given by the matrix inner product
\[
(P, V) = \text{trace} \left( P^T V \right) \quad \text{for} \quad P \in T_Q^* G, \ V \in T_Q G.
\]
We call the Hamiltonian left-invariant, if
\[
H(U^T P, U^{-1} Q) = H(P, Q) \quad \text{for all} \ U \in G.
\]
In this case we have $H(P, Q) = H(Q^T P, I)$ and by differentiating we obtain
$$\nabla_P H(P, Q) = Q^T \nabla_P H(Q^T P, I).$$
By (5.45) and since $T_Q G = \{ Q X ; X \in \mathfrak{g} \}$ with the Lie algebra $\mathfrak{g} = T_I G$ (cf. Sect. IV.6), this relation implies
$$P \in T^*_Q G \quad \text{if and only if} \quad Q^T P \in T^*_Q G = \mathfrak{g}^*. \quad (5.47)$$
Now $H(P, Q)$ depends, for $(P, Q) \in T^* G$, only on the product $Y = Q^T P \in \mathfrak{g}^*$, and we write $\nabla^H(P, Q) = H(Y)$ with a function $H : \mathfrak{g}^* \to \mathbb{R}$.

Left-invariant Hamiltonian systems can be reduced to a Lie–Poisson system of half the dimension by a process that generalizes the derivation of the Euler equations for the rigid body.

**Theorem 5.8.** Consider a Hamiltonian system (5.43) on a matrix Lie group $G$ with a left-invariant quadratic Hamiltonian $H(P, Q) = H(Y)$ for $Y = Q^T P$. If $(P(t), Q(t)) \in T^* G$ is a solution of the system (5.43), then $Y(t) = Q(t)^T P(t) \in \mathfrak{g}^*$ solves the differential equation (5.37).

**Proof.** It is convenient for the proof (though not necessary, see the lines following (2.17)) to extend the Hamiltonian $H : \mathfrak{g}^* \to \mathbb{R}$ to a function of arbitrary matrices $Y$ by setting $H(Y) = H(IIY)$, where $I$ is the projection onto $\mathfrak{g}^*$ given by $(II Y, X) = (Y, X)$ for all $X \in \mathfrak{g}$, with the matrix inner product $(Y, X) = \text{trace}(Y^T X)$.

We first compute the derivatives of $H(P, Q) = H(Y) = H(IIY) = H(y)$ where $Q^T P = Y$ and, using the notation of Theorem 5.5, $IIY = \sum_{j=1}^d y_j E_j$. Since $y_j = (II Q^T P, E_j) = (Q^T P, E_j)$, it follows from $\nabla_A \text{trace}(A^T B) = B$ that
$$\nabla_P H(P, Q) = \sum_{j=1}^d \frac{\partial H(y)}{\partial y_j} \nabla_P y_j = \sum_{j=1}^d \frac{\partial H(y)}{\partial y_j} \text{trace}(P^T Q E_j) = QH'(Y),$$
where $H'(Y) = \sum_{j=1}^d \frac{\partial H(y)}{\partial y_j} E_j \in \mathfrak{g}$ as in Theorem 5.5. Using the identity $y_j = \text{trace}(P^T Q E_j) = \text{trace}(Q^T P E_j^T)$ we get in a similar way
$$\nabla_Q H(P, Q) = PH'(Y)^T. \quad (5.49)$$
Consequently, the differential equations (5.43) become
$$\dot{P} = -PH'(Q^T P)^T = \sum_{i=1}^m \lambda_i \nabla_Q g_i(Q), \quad \dot{Q} = QH'(Q^T P). \quad (5.50)$$
The product rule $\dot{Y} = \dot{Q}^T P + Q^T \dot{P}$ for $Y = Q^T P$ thus yields
$$\dot{Y} = H'(Y)^T Y - Y H'(Y)^T - \sum_{i=1}^m \lambda_i Q^T \nabla_Q g_i(Q). \quad (5.51)$$

\textsuperscript{7} We use again the same letter for different functions. Since they have either one or two arguments, no confusion should arise.
For $X \in \mathfrak{g}$, we now exploit the properties
\[
\langle Q^T \nabla_{Q g_i}(Q), X \rangle = \langle \nabla_{Q g_i}(Q), Q X \rangle = 0 \quad \text{(because $Q X \in T_Q G$)}
\]
\[
\langle [H'(Y)^T, Y], X \rangle = \text{trace} \left(\left(Y^T H'(Y) - H'(Y) Y^T\right) X\right)
\]
\[
= \text{trace} \left(Y^T \left(H'(Y)X - X H'(Y)\right)\right) = \langle Y, [H'(Y), X]\rangle.
\]
Since $Y(t) \in \mathfrak{g}^*$ for all $t$, this gives the equation (5.37).

**Reduced System and Reconstruction.** Combining Theorems 5.8 and 5.5, we have reduced the Hamiltonian system (5.43) to the Lie-Poisson system for $y(t) \in \mathbb{R}^d$,
\[
\dot{y} = B(y) \nabla H(y), \quad (5.52)
\]
of half the dimension. To recover the full solution $(P(t), Q(t)) \in T^* G$, we must solve this system along with
\[
\dot{Q} = Q H'(Y), \quad P = Q^{-T} Y \quad (5.53)
\]
where $Y = \sum_{j=1}^d y_j F_j \in \mathfrak{g}^*$.

**Poisson Structures.** The Poisson bracket on $\mathbb{R}^d$ defined by $B(y)$ is still closely related to the canonical Poisson bracket on $\mathbb{R}^{2n^2}$. Consider left-invariant real-valued functions $K, L$ on $T^* G$. These can be viewed as functions on $T^* G = \mathfrak{g}^* \subset \mathbb{R}^{n \times n}$,
\[
K(P, Q) = K(Y) \quad \text{for} \quad Y = Q^T P.
\]
(As we did previously in this section, we use the same symbol for these functions.) Via the projection $H : \mathbb{R}^{n \times n} \to \mathfrak{g}^*$ used in the above proof, we can extend $K(Y) = K(HY)$ to arbitrary $n \times n$ matrices $Y$, and via the above relation to a left-invariant function $K(P, Q)$ on $\mathbb{R}^{n \times n} \times \mathbb{R}^{n \times n}$, on which we have the canonical Poisson bracket
\[
\{K, L\}_{\text{can}} = \sum_{k, l=1}^n \left(\frac{\partial K}{\partial Q_{kl}} \frac{\partial L}{\partial P_{kl}} - \frac{\partial K}{\partial P_{kl}} \frac{\partial L}{\partial Q_{kl}}\right).
\]
On the other hand, we can view $K$ as a function on $\mathbb{R}^d$ by choosing coordinates on $\mathfrak{g}^*$,
\[
K(y) = K(Y) \quad \text{for} \quad Y = \sum_{j=1}^d y_j F_j \in \mathfrak{g}^*.
\]
On $\mathbb{R}^d$ we have the Poisson bracket defined by the structure matrix $B(y)$,
\[
\{K, L\} = \sum_{i, j=1}^d \frac{\partial K}{\partial y_i} b_{ij} \frac{\partial L}{\partial y_j}.
\]
Lemma 5.9. For left-invariant functions $K, L$ as described above, we have for $Q^T P = Y = \sum_{j=1}^{d} y_j F_j \in \mathfrak{g}^*$

$$\{K, L\}(y) = \langle Y, [L'(Y), K'(Y)] \rangle = \{K, L\}_{\text{can}}(P, Q)$$

where $K'(Y) = \sum_{i=1}^{d} \frac{\partial K}{\partial y_i}(y) E_i \in \mathfrak{g}$.

Proof. The first equality follows from the identity

$$b_{ij}(y) = \langle Y, [E_j, E_i] \rangle,$$

which is a direct consequence of the definition (5.35) with (5.36). For the second equality, the relations (5.48) and (5.49) for $K$ and $L$ yield

$$\{K, L\}_{\text{can}}(P, Q) = \text{trace} \left( K'(Y)^T L'(Y) - K'(Y) Y L'(Y)^T \right)$$

$$= \text{trace} \left( K'(Y)^T L'(Y) - L'(Y) Y^T K'(Y) \right)$$

$$= \text{trace} \left( Y^T [L'(Y), K'(Y)] \right) = \langle Y, [L'(Y), K'(Y)] \rangle,$$

which is the result.

Discrete Lie–Poisson Reduction. Consider a symplectic integrator

$$(P_1, Q_1) = \Phi_h(P_0, Q_0) \quad \text{on} \quad T^* G$$

for the left-invariant Hamiltonian system (5.43), and suppose that the method preserves the left-invariance: if $\Phi_h(P_0, Q_0) = (P_1, Q_1)$, then

$$\Phi_h(U^T P_0, U^{-1} Q_0) = (U^T P_1, U^{-1} Q_1) \quad \text{for all} \quad U \in G. \quad (5.54)$$

For example, this is satisfied by the RATTLE algorithm. The method then induces a one-step map

$$Y_1 = \psi_h(Y_0) \quad \text{on} \quad \mathfrak{g}^*$$

by setting $Y_1 = Q_1^T P_1$ for $(P_1, Q_1) = \Phi_h(P_0, Q_0)$ with $Q_0^T P_0 = Y_0$. This is a numerical integrator for (5.37), and in the coordinates $y = (y_j)$ with respect to the basis $(F_j)$ of $\mathfrak{g}^*$ this gives a map

$$y_1 = \psi_h(y_0) \quad \text{on} \quad \mathbb{R}^d,$$

which is a numerical integrator for the Poisson system (5.52).

Example 5.10. For the rigid body, applying the RATTLE algorithm to the constrained Hamiltonian system (5.18) yields the integrator for the Euler equations discussed in Sect. VII.5.3. By the following result this is a Poisson integrator.

Theorem 5.11. If $\Phi_h(P, Q)$ is a symplectic and left-invariant integrator for (5.43), then its reduction $\psi_h(y)$ is a Poisson map.
**Proof.** We write \( \psi_h \) as the composition

\[
\psi_h : \mathbb{R}^d \xrightarrow{\xi} T^*G \xrightarrow{\Phi_h} T^*G \xrightarrow{\eta} \mathbb{R}^d
\]

where \( \eta = (\eta_j) \) is the function with \( \eta_j(P, Q) = y_j \) for \( Q^T P = \sum_{j=1}^d y_j F_j \), and \( \xi \) is any right inverse of \( \eta \), i.e., \( \eta \circ \xi = \text{id} \). For arbitrary smooth real-valued functions \( K, L \) on \( \mathbb{R}^d \) we then have for \( (P, Q) = (\xi(y)) \), using Lemma 5.9 in the outer equalities and the symplecticity of \( \Phi_h \) in the middle equality,

\[
\{ K \circ \psi_h, L \circ \psi_h \}(y) = \{ K \circ \eta \circ \Phi_h, L \circ \eta \circ \Phi_h \}_\text{can}(P, Q) = \{ K \circ \eta, L \circ \eta \}_\text{can}(\Phi_h(P, Q)) = \{ K, L \}(\psi_h(y)).
\]

This equation states that \( \psi_h \) is a Poisson map. \( \square \)

A similar reduction in a discrete Lagrangian framework is studied by Marsden, Pekarsky & Shkoller (1999).

The reduced numerical maps \( \psi_h \) and \( \psi_h \) have further structure-preserving properties: they preserve the Casimirs and the co-adjoint orbits. This will be shown in Sect. IX.5.3 with the help of backward error analysis.

### VII.6 Reduced Models of Quantum Dynamics

To incorporate quantum effects in molecular dynamics simulations, computations are done with models that are intermediate between classical molecular dynamics based on Newton’s equations of motion and full quantum dynamics described by the \( N \)-particle Schrödinger equation. The direct computational treatment of the latter is not feasible because of its high dimensionality. These intermediate models are obtained by the Hamiltonian reduction (2.17) from an infinite-dimensional Hilbert space to an appropriately chosen manifold. In chemical physics, this reduction is known as the Dirac–Frenkel time-dependent variational principle. We illustrate this procedure for the case where the quantum-mechanical wave function is approximated by a complex Gaussian as proposed by Heller (1975). It turns out that the resulting ordinary differential equations have a Poisson structure, which was recently described by Faou & Lubich (2004). Following that paper, we derive a structure-preserving explicit integrator for Gaussian wavepackets, which tends to the Störmer–Verlet method in the classical limit.

#### VII.6.1 Hamiltonian Structure of the Schrödinger Equation

The introduction of wave mechanics stands ... as Schrödinger’s monument and a worth one.  
(From Schrödinger’s obituary in *The Times* 1961; quoted from http://www-groups.dcs.st-and.ac.uk/history/Mathematicians/Schrodinger.html)
The time-dependent $N$-body Schrödinger equation reads (see, e.g., Messiah (1999) and Thaller (2000))

$$i\hbar \frac{\partial \psi}{\partial t} = H\psi \quad (6.1)$$

for the wave function $\psi = \psi(x,t)$ depending on the spatial variables $x = (x_1, \ldots, x_N)$ with $x_k \in \mathbb{R}^d$ (e.g., with $d = 1$ or $3$ in the partition) and the time $t \in \mathbb{R}$. The squared absolute value $|\psi(x,t)|^2$ represents the joint probability density for $N$ particles to be at the positions $x_1, \ldots, x_N$ at time $t$. In (6.1), \(\hbar\) is a (small) positive number representing the scaled Planck constant and $i$ is the complex imaginary unit. The Hamiltonian operator $H$ is written

$$H = T + V$$

with the kinetic and potential energy operators

$$T = -\sum_{k=1}^{N} \frac{\hbar^2}{2m_k} \Delta x_k \quad \text{and} \quad V = V(x),$$

where $m_k > 0$ is a particle mass and $\Delta x_k$ the Laplacian in the variable $x_k \in \mathbb{R}^d$, and where the real-valued potential $V$ acts as a multiplication operator $(V\phi)(x) = V(x)\phi(x)$. Under appropriate conditions on $V$ (boundedness of $V$ is sufficient, but by no means necessary), the operator $H$ is then a self-adjoint operator on the complex Hilbert space $L^2(\mathbb{R}^{dN}, \mathbb{C})$ with domain $D(H) = D(T) = \{\phi \in L^2(\mathbb{R}^{dN}, \mathbb{C}); T\phi \in L^2(\mathbb{R}^{dN}, \mathbb{C})\}$; see Sect. V.5.3 of Kato (1980).

We separate the real and imaginary parts of $\psi = v + iw \in L^2(\mathbb{R}^{dN}, \mathbb{C})$, the complex Hilbert space of Lebesgue square-integrable functions. The functions $v$ and $w$ are thus functions in the real Hilbert space $L^2(\mathbb{R}^{dN}, \mathbb{R})$. We denote the complex inner product by $\langle \cdot, \cdot \rangle$ and the real inner product by $\langle \cdot, \cdot \rangle$. The $L^2$ norms will be simply denoted by $\| \cdot \|$.

As $H$ is a real operator, formula (6.1) can be written

$$\begin{align*}
\hbar \dot{v} &= Hw, \\
\hbar \dot{w} &= -Hv,
\end{align*} \quad (6.2)$$

or equivalently, with the canonical structure matrix

$$J = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$$

and the Hamiltonian function (we use the same symbol $H$ as for the operator)

$$H(v,w) = \frac{1}{2} \langle \psi, H\psi \rangle = \frac{1}{2} \langle v, Hv \rangle + \frac{1}{2} \langle w, Hw \rangle$$

for $\psi = v + iw$ in the domain of the operator $H$. This becomes the canonical Hamiltonian system

$$\begin{pmatrix} \dot{v} \\ \dot{w} \end{pmatrix} = \hbar^{-1} J^{-1} \nabla H(v,w).$$
VII.6 Reduced Models of Quantum Dynamics

Note that the real multiplication with \( J \) corresponds to the complex multiplication with the imaginary unit \( i \). The flow of this system preserves the canonical symplectic two-form
\[
\omega(\xi_1, \xi_2) = (J\xi_1, \xi_2), \quad \xi_1, \xi_2 \in L^2(\mathbb{R}^N, \mathbb{R})^2.
\] (6.3)

VII.6.2 The Dirac–Frenkel Variational Principle

For dealing with atoms involving many electrons the accurate quantum theory, involving a solution of the wave equation in many-dimensional space, is far too complicated to be practicable. One must therefore resort to approximate methods. (P.A.M. Dirac 1930)

Reduced models of the Schrödinger equation are obtained by restricting the equation to an approximation manifold \( M \) via (2.17), viz.,
\[
(\varepsilon J\dot{u} - \nabla H(u), \xi) = 0 \quad \text{for all} \quad \xi \in T_uM,
\] (6.4)
or equivalently in complex notation for \( u = (v, w)^T = v + iw \),
\[
\text{Re} \langle \varepsilon i\dot{u} - Hu, \xi \rangle = 0 \quad \text{for all} \quad \xi \in T_uM.
\] (6.5)

Taking the real part can be omitted if the tangent space \( T_uM \) is complex linear. Equation (6.5) (usually without the real part) is known as the Dirac–Frenkel time-dependent variational principle, after Dirac (1930) and Frenkel (1934); see also McLachlan (1964), Heller (1976), Beck, Jäckle, Worth & Meyer (2000), and references therein.

We choose a (local) coordinate map \( u = \chi(y) \) of \( M \) and denote its derivative
\[
X_{\mathbb{C}}(y) = V(y) + iW(y) = \chi'(y) \quad \text{or in the real setting as} \quad X = \begin{pmatrix} V \\ W \end{pmatrix}.
\]
Denoting by \( X^T \) the adjoint of \( X \) with respect to the real inner product \( \langle \cdot, \cdot \rangle \), we thus obtain
\[
e\langle X(y)^T JX(y) \dot{y} \rangle = X(y)^T \nabla_u H(\chi(y)).
\]

With \( X_{\mathbb{C}}^* \) denoting the adjoint of \( X_{\mathbb{C}} \) with respect to the complex inner product \( \langle \cdot, \cdot \rangle \), we note \( X_{\mathbb{C}}^* X_{\mathbb{C}} = (V^T V + W^T W) + i(V^T W - W^T V) = X^T X - iX^T JX \) and hence
\[
X^T JX = -\text{Im} \ X_{\mathbb{C}}^* X_{\mathbb{C}}.
\] (6.6)

Lemma 6.1. If \( T_uM \) is a complex linear space for every \( u \in M \), then \( M \) is a symplectic submanifold of \( L^2(\mathbb{R}^N, \mathbb{R})^2 \), that is, the symplectic two-form (6.3) is non-degenerate on \( T_uM \) for all \( u \in M \). Expressed in coordinates,
\[
X(y)^T JX(y) \quad \text{is invertible for all} \quad y.
\]

Proof. We fix \( u = \chi(y) \in M \) and omit the argument \( y \) in the following. Since \( T_uM = \text{Range}(X_{\mathbb{C}}) \) is complex linear by assumption, there exists a real linear mapping \( L : \mathbb{R}^m \to \mathbb{R}^m \) such that \( i X_{\mathbb{C}} \eta = X_{\mathbb{C}} L \eta \) for all \( \eta \in \mathbb{R}^m \). This implies
\[
JX = XL \quad \text{and} \quad L^2 = -\text{Id}
\]
and hence \( X^T JX = X^T XL \), which is invertible. \( \square \)
Approximation properties of the Dirac–Frenkel variational principle can be obtained from the interpretation as the orthogonal projection \( \hat{\mathbf{u}} = P_\perp(\mathbf{u}) \frac{1}{\hbar} \hat{H} \mathbf{u} \), which corresponds to taking the imaginary part in (6.5), as opposed to the symplectic projection in (6.4) which corresponds to the real part. See Lubich (2005) for a near-optimality result for approximation on the manifold.

### VII.6.3 Gaussian Wavepacket Dynamics

We develop a new approach to semiclassical dynamics which exploits the fact that extended wavefunctions for heavy particles (or particles in harmonic potentials) may be decomposed into time-dependent wave packets, which spread minimally and which execute classical or nearly classical trajectories. A Gaussian form for the wave packets is assumed and equations of motion are derived for the parameters characterizing the Gaussian. (E.J. Heller 1975)

The variational Gaussian wavepacket dynamics of Heller (1976) is obtained by choosing the manifold \( \mathcal{M} \) in (6.5) as consisting of complex Gaussians. For ease of presentation we restrict our attention in the following to the one-particle case \( N = 1 \) (the extension to \( N > 1 \) is straightforward; cf. Heller (1976) and Faou & Lubich (2004)). Here we have

\[
\mathcal{M} = \left\{ \mathbf{u} = \chi(y) \in L^2(\mathbb{R}^d, \mathbb{C}) : y = (p, q, \alpha, \beta, \gamma, \delta) \in \mathbb{R}^{2d+4} \text{ with } \beta > 0 \right\}
\]

(6.7)

with

\[
\left( \chi(y) \right)(x) = \exp\left( \frac{i}{\hbar} \left( (\alpha + i\beta) |x-q|^2 + p \cdot (x-q) + \gamma + i\delta \right) \right),
\]

(6.8)

where \(|| \cdot ||\) and \( \cdot \) stand for the Euclidean norm and inner product on \( \mathbb{R}^d \). The parameters \( q \) and \( p \) represent the average position and momentum, respectively: for \( u = \chi(y) \) with \( y = (p, q, \alpha, \beta, \gamma, \delta) \) and \( ||u|| = 1 \), a direct calculation shows that

\[
q = \langle u, xu \rangle = \int_{\mathbb{R}^d} x |u(x)|^2 \, dx, \quad p = \langle u, -i \hbar \nabla u \rangle.
\]

The parameter \( \beta > 0 \) determines the width of the wavepacket. The tangent space \( T_u \mathcal{M} \subset L^2(\mathbb{R}^d, \mathbb{C}) \) at a given point \( u = \chi(y) \in \mathcal{M} \) is \((2d+4)\)-dimensional and is made of the elements of \( L^2(\mathbb{R}^d, \mathbb{C}) \) written as

\[
\frac{i}{\hbar} \left( (A + iB) |x-q|^2 + (P - 2(\alpha + i\beta)Q) \cdot (x-q) - p \cdot Q + C + iD \right) u
\]

(6.9)

with arbitrary \((P, Q, A, B, C, D)^T \in \mathbb{R}^{2d+4} \). We note that \( T_u \mathcal{M} \) is complex linear, and \( u \in T_u \mathcal{M} \). By choosing \( \xi = iu \) in (6.5), this yields \( (d/dt)||u||^2 = 2 \text{ Re } \langle \dot{u}, u \rangle = 0 \) and hence the preservation of the squared \( L^2 \) norm of \( u = \chi(y) \), which is given by
\[ I(y) = ||u||^2 = \int_{\mathbb{R}^d} |u(x)|^2 \, dx \]  
\[ = \int_{\mathbb{R}^d} \exp \left( -\frac{\omega}{\varepsilon} \beta|x-q|^2 + \delta \right) \, dx = \exp \left( -\frac{2\delta}{\varepsilon} \right) \left( \frac{\pi \varepsilon}{2\beta} \right)^{d/2}. \]

The physically reasonable situation is \( ||u||^2 = 1 \), which corresponds to the interpretation of \( |u(x)|^2 \) as a probability density.

With these preparations we have the following result of Faou & Lubich (2004).

**Theorem 6.2.** The Hamiltonian reduction of the Schrödinger equation to the Gaussian wavepacket manifold \( \mathcal{M} \) of (6.7)-(6.8) yields the Poisson system

\[ \dot{y} = B(y) \nabla K(y) \]  
(6.11)

where, for \( y = (p, q, \alpha, \beta, \gamma, \delta) \in \mathbb{R}^{2d+4} \) with \( \beta > 0 \), and with \( 1_d \) denoting the \( d \)-dimensional identity,

\[ B(y) = \frac{1}{I(y)} \begin{pmatrix}
0 & -1_d & 0 & 0 & -p & 0 \\
1_d & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & \frac{4\beta^2}{\varepsilon d} & 0 & -\beta \\
0 & 0 & -\frac{4\beta^2}{\varepsilon d} & 0 & \beta & 0 \\
p^T & 0 & 0 & -\beta & 0 & \frac{d+2}{4} \varepsilon \\
0 & 0 & \beta & 0 & -\frac{d+2}{4} \varepsilon & 0
\end{pmatrix} \]  
(6.12)

defines a Poisson structure, and for \( u = \chi(y) \),

\[ K(y) = \langle u, Hu \rangle = K_T(y) + K_V(y) \]  
(6.13)

is the total energy, with kinetic and potential parts

\[ K_T(y) = I(y) \left( \frac{|p|^2}{2m} + \frac{\varepsilon d}{2m} \frac{\alpha^2 + \beta^2}{\beta} \right) = \langle u, Tu \rangle \]

and

\[ K_V(y) = \int_{\mathbb{R}^d} V(x) \exp \left( -\frac{2}{\varepsilon} \beta|x-q|^2 + \delta \right) \, dx = \langle u, Vu \rangle. \]

Both \( K(y) \) and \( I(y) \) are first integrals of the system.

**Proof.** As in (2.22), the differential equation for \( y \) is \( \varepsilon X(y)^T J X(y) \dot{y} = \frac{1}{2} \nabla K(y) \). We note (6.6) and

\[ X_c(y) = \frac{i}{\varepsilon} \left( x - q, -2a(x - q) - p, |x-q|^2, i|x-q|^2, 1, i \right) u \]

where \( a = \alpha + i\beta \) and \( u = \chi(y) \) in the complex setting. Using the calculus of Gaussian integrals, we compute
$\varepsilon X^T(y)JX(y) = \frac{1}{2} I(y) \begin{pmatrix} 0 & 1_d & 0 & 0 & 0 & 0 \\ -1_d & 0 & 0 & \frac{dp}{2\varepsilon} & 0 & \frac{2p}{\varepsilon} \\ 0 & 0 & 0 & -\frac{c(d+2)}{8\varepsilon^2} & 0 & 0 \\ 0 & \frac{dp}{2\varepsilon} & \frac{c(d+2)}{8\varepsilon^2} & 0 & \frac{d}{2\varepsilon} & 0 \\ 0 & 0 & 0 & -\frac{d}{2\varepsilon} & 0 & -\frac{2}{\varepsilon} \\ 0 & \frac{2p}{\varepsilon} & \frac{d}{2\varepsilon} & 0 & \frac{2}{\varepsilon} & 0 \end{pmatrix}$,

and inversion yields the differential equation with $B(y) = (2\varepsilon X^T(y)JX(y))^{-1}$ as stated. The system is a Poisson system by Theorem 2.8. $\Box$

Assuming $I(y) = \|u\|^2 = 1$, we observe that the differential equations for the average position and momentum, $q$ and $p$, read

$$\dot{q} = \frac{p}{m}, \quad \dot{p} = -\langle u, \nabla V u \rangle$$

for $u = \chi(y)$ and $y = (p, q, \alpha, \beta, \gamma, \delta)$. We then note $\langle u, \nabla V u \rangle \to \nabla V(q)$ as $\varepsilon \to 0$. The differential equations for $q$ and $p$ thus tend to Newtonian equations of motion in the classical limit $\varepsilon \to 0$:

$$\dot{q} = \frac{p}{m}, \quad \dot{p} = -\nabla V(q).$$

It will be useful to consider also scaled variables

$$\tilde{y} = (p, q, \alpha, \beta, \gamma, \delta) \in \mathbb{R}^{2d+4} \quad \text{with} \quad \tilde{\beta} = \frac{\beta}{\varepsilon}, \quad \tilde{\delta} = \frac{\delta}{\varepsilon}. \quad (6.16)$$

Here we have

$$\tilde{y} = \tilde{B}(\tilde{y}) \nabla \tilde{K}(\tilde{y}) \quad (6.17)$$

where the structure matrix $\tilde{B}(\tilde{y})$ is independent of $\varepsilon$, and where $\tilde{K}(\tilde{y})$ depends regularly on $\varepsilon \geq 0$.

VII.6.4 A Splitting Integrator for Gaussian Wavepackets

With the natural splitting $H = T + V$ into kinetic and potential energy, we now consider the variational splitting integrator (4.7) – (4.8), which here becomes the following.

1. We define $u^+_n$ in $\mathcal{M}$ as the solution at time $h/2$ of the equation for $u$,

$$\langle i\varepsilon \dot{u} - Vu, \xi \rangle = 0 \quad \text{for all} \quad \xi \in T_u \mathcal{M} \quad (6.18)$$

with initial value $u(0) = u_n \in \mathcal{M}$.

2. We define $u^-_{n+1}$ as the solution at time $h$ of

$$\langle i\varepsilon \dot{u} - Tu, \xi \rangle = 0 \quad \text{for all} \quad \xi \in T_u \mathcal{M} \quad (6.19)$$

with initial value $u(0) = u^+_n$.

3. Then $u_{n+1}$ is the solution at time $h/2$ of (6.18) with initial value $u(0) = u^-_{n+1}$.
By Theorem 6.2, the substeps in the definition of this splitting method written in the coordinates \( y = (p, q, \alpha, \beta, \gamma, \delta) \) are the exact flows \( \varphi_{h/2}^V \) and \( \varphi_h^T \) of the Poisson systems

\[
\dot{y} = B(y) \nabla K_V (y) \quad \text{and} \quad \dot{y} = B(y) \nabla K_T (y).
\]

Note that both equations preserve the \( L^2 \) norm of \( u = \chi(y) \), which we assume to be 1 in the following.

Most remarkably, these equations can be solved explicitly. Let us consider first the equations (6.19). They are written, for \( a = \alpha + i \beta \) and \( c = \gamma + i \delta \), as

\[
\begin{align*}
\dot{q} &= \frac{p}{m}, & \dot{a} &= -2a^2/m, \\
\dot{p} &= 0, & \dot{c} &= \frac{1}{2}|p|^2 + i \varepsilon da / m,
\end{align*}
\]

with initial values \( y_0 = (p_0, q_0, a_0, c_0) \) corresponding to \( u_0 = \chi(y_0) \). They have the solution

\[
q(t) = q_0 + \frac{t}{m} p_0, \quad p(t) = p_0, \quad a(t) = \frac{a_0}{1 + 2a_0 t / m},
\]

and

\[
c(t) = c_0 + \frac{1}{2m} \frac{|p_0|^2}{2} + \frac{i \varepsilon d}{2} \log \left( 1 + \frac{2a_0 t}{m} \right).
\]

Let us now consider the equations (6.18). Taking into account the fact that the potential \( V \) is real, these equations are written

\[
\begin{align*}
\dot{p} &= -\langle u, \nabla V u \rangle, & \dot{q} &= 0, \\
\dot{a} &= -\frac{i}{2\varepsilon} \langle u, \Delta V u \rangle, & \dot{\beta} &= 0, \\
\dot{c} &= -\langle u, V u \rangle + \frac{\varepsilon}{2\delta} \langle u, \Delta V u \rangle, & \dot{\delta} &= 0,
\end{align*}
\]

with the \( L^2 \) inner products

\[
\langle u, W u \rangle = \int_{\mathbb{R}^d} W(x) \exp \left( -\frac{2}{\varepsilon} (\beta |x - q|^2 + \delta) \right) dx
\]

for \( W = V, \nabla V, \Delta V \). As the \( L^2 \) inner products in the equations for \( p, a, \gamma \) depend only on \( q, \beta, \delta \) which are constant along this trajectory, these equations can be solved trivially, requiring only the computation of the inner products at the initial value. We thus see that the splitting scheme \( \Phi_h = \varphi_{h/2}^V \circ \varphi_h^T \circ \varphi_{h/2}^V \) can be computed explicitly. This gives the following algorithm (Faou & Lubich 2004).

**Algorithm 6.3 (Gaussian Wavepacket Integrator).** A step from time \( t_n \) to \( t_{n+1} \), starting from the Gaussian wavepacket \( u_n = \chi(p_n, q_n, \alpha_n, \beta_n, \gamma_n, \delta_n) \), proceeds as follows:

1. With \( \langle W \rangle_n = \langle u_n, W u_n \rangle \) given by (6.22) for \( W = V, \nabla V, \Delta V \), compute
\[ p_{n+1/2} = p_n - \frac{h}{2} (\nabla V)_n \]
\[ \alpha_n^+ = \alpha_n + \frac{h}{4d} (\Delta V)_n \]
\[ \gamma_n^+ = \gamma_n + \frac{h \varepsilon}{16\beta_n} (\Delta V)_n. \] (6.23)

2. From the values \( p_{n+1/2}, \alpha_n^+, \) \( \alpha_n^- = \alpha_n + i\beta_n \) and \( c_n^+ = \gamma_n^+ + i\delta_n \), compute \( q_{n+1} \).

\[ \alpha_{n+1}^- = \alpha_{n+1}^- + i\beta_{n+1}, \text{ and } c_{n+1}^- = \gamma_{n+1}^- + i\delta_{n+1} \text{ via } \]
\[ q_{n+1} = q_n + \frac{h}{m} p_{n+1/2} \]
\[ a_{n+1}^- = a_n^+ \left( 1 + \frac{2h}{m} a_n^+ \right) \] (6.24)
\[ c_{n+1}^- = c_n^+ + i\varepsilon \frac{d}{2} \log \left( 1 + \frac{2h}{m} a_n^+ \right). \]

3. Compute \( p_{n+1}, \alpha_{n+1}, \gamma_{n+1} \) from

\[ p_{n+1} = p_{n+1/2} - \frac{h}{2} (\nabla V)_{n+1} \]
\[ \alpha_{n+1} = \alpha_{n+1}^- - \frac{h}{4d} (\Delta V)_{n+1} \] (6.25)
\[ \gamma_{n+1} = \gamma_{n+1}^+ + \frac{h \varepsilon}{16\beta_{n+1}} (\Delta V)_{n+1}. \]

Let us collect properties of this algorithm.

**Theorem 6.4.** The splitting scheme of Algorithm 6.3 is an explicit, symmetric, second-order numerical method for Gaussian wavepacket dynamics (6.11)–(6.13). It is a Poisson integrator for the structure matrix (6.12), and it preserves the unit \( L^2 \) norm of the wavepackets: \( \| u_n \| = 1 \) for all \( n \).

In the limit \( \varepsilon \to 0 \), the position and momentum approximations \( q_n, p_n \) of this method tend to those obtained by applying the Störmer–Verlet method to the associated classical mechanical system (6.15).

The statement for \( \varepsilon \to 0 \) follows directly from the equations for \( p_{n+1/2}, q_{n+1}, p_{n+1} \) and from noting \( (\nabla V)_n \to \nabla V(q_n) \).

In view of the small parameter \( \varepsilon \), the discussion of the order of the method requires more care. Here it is useful to consider the integrator in the scaled variables \( \tilde{y} = (p, q, \alpha, \beta \varepsilon, \gamma, \delta \varepsilon) \) of (6.16). Since the differential equation (6.17) contains \( \varepsilon \) only as a regular perturbation parameter, after \( n \) steps of the splitting integrator we have the \( \varepsilon \)-uniform error bound \( \tilde{y}_n - \tilde{y}(t_n) = O(h^2) \),

where the constants symbolized by the \( O \)-notation are independent of \( \varepsilon \) and of \( n \) and \( h \) with \( nh \leq \text{Const} \). For the approximation of the absolute values of the Gaussian wavepackets this yields
\[ \|u_n| - |u(t_n)|^2 = O(h^2), \]  
but the approximation of the phases is only such that
\[ \|u_n - u(t_n)\| = O(h^2/\varepsilon). \]

We refer to Faou & Lubich (2004) for the formulation of the corresponding algorithm for \( N > 1 \) particles, for further properties such as the exact conservation of linear and angular momentum and the long-time near-conservation of the total energy \( \langle u_n, Hu_n \rangle \), and for numerical experiments.

**VII.7 Exercises**

1. Prove that the Poisson bracket (2.8) satisfies the Jacobi identity (2.4) for all functions \( F, G, H \), if and only if it satisfies (2.4) for the coordinate functions \( y_i, y_j, y_k \).

**Hint** (F. Engel, in Lie’s *Gesammelte Abh*. vol. 5, p. 753). If the Jacobi identity is written as in (3.3), we see that there are no second partial derivatives of \( F \) (the left hand side is a Lie bracket, the right-hand side has no second derivatives of \( F \) anyway). Other permutations show the same result for \( G \) and \( H \).

2. For \( x \) in an open subset of \( \mathbb{R}^m \), let \( A(x) = (a_{ij}(x)) \) be an invertible skew-symmetric \( m \times m \)-matrix, with
\[ \frac{\partial a_{ij}}{\partial x_k} + \frac{\partial a_{ki}}{\partial x_j} + \frac{\partial a_{jk}}{\partial x_i} = 0 \]  
for all \( i, j, k \).  

(a) Show that \( B(x) = A(x)^{-1} \) satisfies (2.10) and hence defines a Poisson bracket.

(b) Generalize Theorem 2.8 to Hamiltonian equations (2.18) with the two-form \( \omega_x(\xi_1, \xi_2) = \xi_1^T A(x) \xi_2 \).

**Remark.** Condition (7.1) says that \( \omega \) is a closed differential form.

3. Solve the following first order partial differential equation:
\[ \begin{align*}
3 \frac{\partial F}{\partial y_1} + 2 \frac{\partial F}{\partial y_2} - 5 \frac{\partial F}{\partial y_3} &= 0.
\end{align*} \]

**Result.** \( f(2y_1 - 3y_2, 5y_2 + 2y_3) \).

4. Find two solutions of the homogeneous system
\[ \begin{align*}
3 \frac{\partial F}{\partial y_1} + \frac{\partial F}{\partial y_2} - 2 \frac{\partial F}{\partial y_3} - 5 \frac{\partial F}{\partial y_4} &= 0, \\
2 \frac{\partial F}{\partial y_1} - \frac{\partial F}{\partial y_2} - 3 \frac{\partial F}{\partial y_4} &= 0,
\end{align*} \]
such that their gradients are linearly independent.

5. Consider a Poisson system \( \dot{y} = B(y) \nabla H(y) \) and a change of coordinates \( z = \phi(y) \). Prove that in the new coordinates the system is of the form \( \dot{z} = \tilde{B}(z) \nabla K(z) \), where \( \tilde{B}(z) = \phi'(y) B(y) \phi'(y)^T \) (cf. formula (3.12)) and \( K(z) = H(y) \).
6. Give an elementary proof of Theorem 4.3. 
   Hint. Define $\delta(t) := \varphi'(y)B(y)\varphi'_r(y)^T - B(\varphi_r(y))$. Using the variational equation for (4.1) prove that $\delta(t)$ is the solution of a homogeneous linear differential equation. Therefore, $\delta(0) = 0$ implies $\delta(t) = 0$ for all $t$.

7. Let $z = \vartheta(y)$ be a transformation taking the Poisson system $\dot{y} = B(y)\nabla H(y)$ to $\dot{z} = \tilde{B}(z)\nabla K(z)$. Prove that $\Phi_h(y)$ is a Poisson integrator for $B(y)$ if and only if $\Phi_h(z) = \vartheta \circ \Phi_h \circ \vartheta^{-1}(z)$ is a Poisson integrator for $\tilde{B}(z)$.

8. Let $B$ be a skew-symmetric but otherwise arbitrary constant matrix, and consider the Poisson system $\dot{y} = B\nabla H(y)$. Prove that every symplectic Runge–Kutta method is a Poisson integrator for such a system. 
   Hint. Transform $B$ to block-diagonal form.

9. (M.J. Gander 1994). Consider the Lotka–Volterra equation (2.13) with separable Hamiltonian $H(u, v) = K(u) + L(v)$. Prove that

$$u_{n+1} = u_n + h u_n v_n H_v(u_n, v_n), \quad v_{n+1} = v_n - h u_{n+1} v_{n} H_u(u_{n+1}, v_n)$$

is a Poisson integrator for this system.

10. Find a change of coordinates that transforms the Lotka–Volterra system (2.14) into a Hamiltonian system (in canonical form). Following the approach of Example 4.11 construct Poisson integrators for this system.

11. Prove that the matrix $B(y)$ of Example 2.7 defines a Poisson bracket, by showing that the bracket is given as Dirac’s bracket (Dirac 1950)

$$\{F, G\} = \{\tilde{F}, \tilde{G}\} - \sum_{i,j} \{\tilde{F}, c_i\} \gamma_{ij} \{c_j, \tilde{G}\}. \quad (7.2)$$

Here $F$ and $G$ are functions of $y$, $\tilde{F}$ and $\tilde{G}$ are smooth functions of $x$ satisfying $\tilde{F}(\chi(y)) = F(y)$ and $\tilde{G}(\chi(y)) = G(y)$, $c_i(x)$ are the constraint functions defining the manifold $\mathcal{M}$, and $\gamma_{ij}$ are the entries of the inverse of the matrix $([c_i, c_j])$. The Poisson bracket to the left in (7.2) corresponds to $B(y)$ and those to the right are the canonical brackets evaluated at $x = \chi(y)$. Replacing $\tilde{F}(x)$ by $\tilde{F}(x) + \sum_{k} \mu_k(x)c_k(x)$ with $\mu_k(x)$ such that $\{\tilde{F}, c_k\} = 0$ on $\mathcal{M}$ eliminates the sum in (7.2) and proves the Jacobi identity for $B(y)$. 