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Time Integration and Discrete Hamiltonian Systems[1]

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This paper is dedicated to the memory of Juan C. Simo

Summary. This paper develops a formalism for the design of conserving time-integration schemes for Hamiltonian systems with symmetry. The main result is that, through the introduction of a discrete directional derivative, implicit second-order conserving schemes can be constructed for general systems which preserve the Hamiltonian along with a certain class of other first integrals arising from affine symmetries. Discrete Hamiltonian systems are introduced as formal abstractions of conserving schemes and are analyzed within the context of discrete dynamical systems; in particular, various symmetry and stability properties are investigated.

1. Background and Motivation

First integrals or conservation laws for Hamiltonian systems with symmetry are typically lost under numerical integration in time. In some cases, failure to maintain certain conservation laws can lead to physically impossible solutions [3], and in other cases to numerical instability [7], [21]–[24]. For Hamiltonian systems with symmetry it is thus generally desirable that numerical time-integration schemes preserve physically meaningful integrals from the underlying system. These types of integrators are usually referred to as *conserving integrators* and are the subject of this investigation.

This paper develops a formalism for the design of conserving time-integration schemes for Hamiltonian systems with symmetry. The main result is that, through the introduction of a discrete directional derivative, implicit second-order conserving schemes can be constructed for general systems which preserve the Hamiltonian along with quadratic integrals arising from affine symmetries. Discrete Hamiltonian systems are introduced as formal abstractions of conserving schemes and are analyzed within the context of discrete dynamical systems; in particular, various symmetry and stability properties are

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investigated. It is shown that the proposed class of schemes inherit equilibria and relative equilibria from the underlying system along with various notions of stability.

Only finite-dimensional Hamiltonian systems defined in open sets of Euclidean space are considered in this paper. However, the framework presented herein easily extends to infinite-dimensional systems on linear manifolds [6], [8], and can be extended to canonical systems with holonomic constraints [5]. For other treatments of conserving schemes, particularly within the context of specific applications, see [2]–[4], [9]–[15], [17], [19]–[24].

2. Preliminaries

In this section we recall some standard terminology and concepts to be used in the developments that follow. We refer to Abraham & Marsden [1], Olver [18] or Marsden & Ratiu [16] for further details not explained here.

2.1. Hamiltonian Differential Equations and First Integrals

Let (P, Ω) denote a symplectic space with P open in m-dimensional Euclidean space $\mathbb{R}^m$ with points denoted by $z = (z^1, \ldots, z^m)$, and symplectic structure $P \ni z \to \Omega_z \in \mathbb{R}^{m\times m}$, where each Ω_z is viewed as a bilinear form in $T_z P \cong \mathbb{R}^m$. For any $z \in P$ we recall that Ω_z is skew-symmetric in the sense that $\Omega_z(v, w) = -\Omega_z(w, v)$ for all $v, w \in \mathbb{R}^m$.

To any smooth function $H\colon P \to \mathbb{R}$ we associate a *Hamiltonian vector field* $X_H\colon P \to \mathbb{R}^m$ defined by

$$\Omega_z^\flat(X_H(z)) = DH(z), \tag{2.1}$$

where $DH(z) \in T_z^* P \cong \mathbb{R}^m$ denotes the derivative of H at z. If we denote the components of $\Omega_z \in \mathbb{R}^{m\times m}$ by $(\Omega_z)_{ij}$ $(i, j = 1, \ldots, m)$, then $\Omega_z^\flat\colon \mathbb{R}^m \to \mathbb{R}^m$ is defined in components by $(\Omega_z^\flat(v))_k = (\Omega_z)_{jk} v^j$ where summation on repeated indices is implied. Nondegeneracy conditions on the symplectic structure require that m be even, say $m = 2n$, and for each $z \in P$ we define $\Omega_z^\sharp\colon \mathbb{R}^m \to \mathbb{R}^m$ to be the inverse of $\Omega_z^\flat$.

Given a Hamiltonian system (P, Ω, H) we will be concerned with the associated *Hamiltonian differential equations*

$$\dot{z} = X_H(z) \tag{2.2}$$

where the Hamiltonian vector field X_H is assumed to be smooth. For any $z \in P$ we note that (2.2) generates a local evolution semigroup $F\colon B \times [0, T] \to P$, where B is a neighborhood of z and $T > 0$. For any $z_0 \in B$ the curve $\varphi(t) = F(z_0, t) = F_t(z_0)$ is a solution to (2.2), defined for all $t \in [0, T]$, with initial condition $\varphi(0) = z_0$.

By a (time-independent) *first integral* for the system (P, Ω, H), we mean a smooth function $f\colon P \to \mathbb{R}$ which is constant along any solution $\psi\colon [0, T] \to P$ of (2.2), i.e.,

$$f(\psi(t)) = f(\psi(0)), \qquad \forall t \in [0, T]. \tag{2.3}$$

Using straightforward arguments it can be shown that f is an integral if and only if the following *orthogonality condition* is satisfied:

$$Df(z) \cdot X_H(z) = 0, \qquad \forall z \in P. \tag{2.4}$$

Note that the skewness of Ω_z implies that the Hamiltonian $H\colon P \to \mathbb{R}$ is a first integral for (P, Ω, H).

2.2. Symplectic Actions of Lie Groups and Momentum Maps

Let G be a Lie group with tangent space at the identity denoted by T_eG, and let $\Phi\colon G \times P \to P$ denote a regular symplectic action of G on P. (See, e.g., Olver [18, p. 22] for the definition of a regular action.) Given $\xi \in T_eG$ the *infinitesimal generator* of the G-action corresponding to ξ is a vector field $\xi_P\colon P \to \mathbb{R}^m$ defined by the relation

$$\xi_P(z) = \left.\frac{d}{ds}\right|_{s=0} \Phi(\exp(s\xi), z), \tag{2.5}$$

where $\exp\colon T_eG \to G$ is the exponential map. For any $z \in P$ we denote by $G \cdot z$ the orbit of z under the action of G, and we denote by $\mathrm{Ad}^*\colon G \times T_e^*G \to T_e^*G$ the *coadjoint action* of G on T_e^*G.

By a *momentum map* for the action of G on P we mean a mapping of the form $J\colon P \to T_e^*G$ satisfying

$$DJ_\xi(z) = \Omega_z^\flat(\xi_P(z)) \quad \forall \xi \in T_eG, \tag{2.6}$$

where $J_\xi\colon P \to \mathbb{R}$ is defined by the relation $J_\xi(z) = J(z) \cdot \xi$. We say that J is Ad^*-*equivariant* if

$$J(\Phi(g, z)) = \mathrm{Ad}^*(g^{-1}, J(z)) \tag{2.7}$$

for all $g \in G$ and $z \in P$.

Given $\mu \in T_e^*G$ we denote by $G_\mu \subset G$ the *isotropy group* for μ under the coadjoint action, and we call the quotient space $P_\mu = J^{-1}(\mu)/G_\mu$, induced by the action of G_μ on $J^{-1}(\mu)$, the *reduced phase space* for the momentum value μ. Note that P_μ has the structure of a smooth manifold provided that μ is a regular value for J and G_μ acts regularly on $J^{-1}(\mu)$. In what follows we will assume that the symplectic structure Ω on P induces a well-defined symplectic structure Ω_μ in P_μ, and we will use π_μ to denote the natural projection from $J^{-1}(\mu)$ onto P_μ.

2.3. Symmetry, Conservation Laws and Relative Equilibria

Let (P, Ω) be a symplectic space as described above and let Φ denote the symplectic action of a Lie group G on P. Given a *G-invariant* function $H\colon P \to \mathbb{R}$, i.e.,

$$H(\Phi(g, z)) = H(z), \qquad \forall g \in G,\ z \in P, \tag{2.8}$$

we call the system (P, Ω, G, H) a Hamiltonian system with *symmetry*. This system has the property that if $\varphi\colon [0, T] \to P$ is a maximal trajectory for the Hamiltonian vector field X_H, then so is $\Phi_g \circ \varphi$ for any $g \in G$. Here we employ the notation $\Phi_g = \Phi(g, \cdot)\colon P \to P$.

Suppose the action of G possesses a momentum map $J\colon P \to T_e^*G$. Then J is conserved along trajectories of X_H in the sense that, for any $\xi \in T_eG$, the function $J_\xi = J \cdot \xi\colon P \to \mathbb{R}$ is an integral for (2.2). To see this result use (2.1) and (2.6) to write

$$DJ_\xi(z) \cdot X_H(z) = -DH(z) \cdot \xi_P(z). \tag{2.9}$$

The result then follows from the G-invariance of H, which implies $DH(z) \cdot \xi_P(z) = 0$ for any $\xi \in T_eG$ and $z \in P$.

For any regular value μ of J we recall that the G-invariance of H implies the existence of a well-defined function H_μ on the reduced phase space P_μ, which we call the *reduced Hamiltonian* associated with H and μ. Thus, given a Hamiltonian system with symmetry as discussed above, and a regular value μ for J, we have a well-defined reduced Hamiltonian system $(P_\mu, \Omega_\mu, H_\mu)$.

Finally, we recall the notion of a relative equilibria for a Hamiltonian system with symmetry. In particular, a point $z_e \in P$ is a *relative equilibrium* if the maximal trajectory of X_H with initial condition z_e, denoted by $\varphi(t)$, satisfies

$$\varphi(t) = \Phi(\exp(t\xi), z_e) \tag{2.10}$$

for some $\xi \in T_eG$. It is well known that, for any regular value μ of J, a point $z_e \in J^{-1}(\mu) \subset P$ is a relative equilibrium if $\pi_\mu(z_e) \in P_\mu$ is a critical point of the reduced Hamiltonian H_μ.

3. Conserving Time Integration

In this section we present a framework for the design and analysis of numerical schemes for (2.2). Our attention will be focused on schemes which inherit underlying integrals. Rather than view an algorithm as a discrete system which approximates a continuous one, we take the point of view that an algorithm defines a discrete system worthy of study in its own right. Hence, we introduce the notion of a discrete Hamiltonian system as a formal abstraction of a conserving scheme.

3.1. A Point of Departure

Given a Hamiltonian system (P, Ω, H) possessing an integral $f\colon P \to \mathbb{R}$, our goal is to construct a numerical approximation scheme for (2.2) which inherits f as an integral.

As a point of departure, we consider approximating solutions to (2.2) by numerical schemes of the form

$$z_{n+1} - z_n = h\mathsf{X}_H(z_n, z_{n+1}), \tag{3.1}$$

where $h > 0$ is a parameter interpreted as the time step and $\mathsf{X}_H\colon P \times P \to \mathbb{R}^m$ is a given smooth map which is viewed as a two-point approximation to the exact vector field X_H, e.g., $\mathsf{X}_H(z_n, z_{n+1}) \approx X_H(z_{n+\frac{1}{2}})$ where $z_{n+\frac{1}{2}} = \frac{1}{2}(z_n + z_{n+1})$.

For any $z \in P$ we assume the numerical scheme generates a local evolution semigroup in the sense that there exists a neighborhood B of z, real numbers $h_c, T > 0$, and a mapping $\mathsf{F}\colon B \times [0, h_c] \to P$ such that, for any $z_0 \in B$ and $h \in [0, h_c]$, the sequence (z_n) generated by $\mathsf{F}^n(z_0, h) = \mathsf{F}_h^n(z_0)$ satisfies (3.1) for all $nh \in [0, T]$. Note that a function $f\colon P \to \mathbb{R}$ is an integral for (3.1) if for any $z_0 \in P$ we have $f(z_n) = f(z_0)$ for all $nh \in [0, T]$.

The following observations illustrate how (3.1) may be constructed so that it inherits an arbitrary integral from the underlying system. To begin, let f be an integral for (2.2) and assume that, for any $x, y \in P$, there exists a vector $\mathsf{D}f(x, y) \in \mathbb{R}^m$ with the property that $\mathsf{D}f(x, y) \approx Df(\frac{x+y}{2})$ and

$$\mathsf{D}f(x, y) \cdot (y - x) = f(y) - f(x). \tag{3.2}$$

Along any solution sequence of (3.1) we could thus write

$$\begin{aligned} f(z_{n+1}) - f(z_n) &= \mathsf{D}f(z_n, z_{n+1}) \cdot (z_{n+1} - z_n) \\ &= h\mathsf{D}f(z_n, z_{n+1}) \cdot \mathsf{X}_H(z_n, z_{n+1}). \end{aligned} \tag{3.3}$$

Now note that if the approximate vector field X_H satisfied the discrete orthogonality condition

$$\mathsf{D}f(x, y) \cdot \mathsf{X}_H(x, y) = 0, \qquad \forall x, y \in P, \tag{3.4}$$

then f would be an integral for (3.1).

The preceding arguments suggest that a formalism for constructing conserving schemes can be based on both a discrete derivative operator "D" which allows one to write (3.2) and the discrete orthogonality condition (3.4).

In principle, by projecting $\mathsf{X}_H(x, y)$ onto the orthogonal complement of the linear space span$\{\mathsf{D}f(x, y)\}$, we could arrange for (3.1) to inherit an arbitrary integral from the underlying system (2.2). For multiple integrals such a projection would likely be inefficient and thus we are interested in simpler ways to satisfy the discrete orthogonality condition. As we will see below, a simplification can be achieved when the integrals of interest are the Hamiltonian and quadratic momentum maps associated with affine symmetries. The preceding ideas are formalized in the next few subsections.

3.2. Definitions

Consider a symplectic space (P, Ω) where the phase space P is an open subset of $\mathbb{R}^m$ and Ω denotes a symplectic structure on P. Motivated by the preceding developments we make the following definition.

Definition 3.1. A *discrete derivative* for a smooth function $f\colon P \to \mathbb{R}$ is a mapping $\mathsf{D}f\colon P \times P \to \mathbb{R}^m$ with the following properties:

(1) Directionality. $\mathsf{D}f(x, y) \cdot v_{xy} = f(y) - f(x)$ for any $x, y \in P$ where $v_{xy} = y - x$.
(2) Consistency. $\mathsf{D}f(x, y) = Df(\frac{x+y}{2}) + O(\|y - x\|)$ for all $x, y \in P$ with $\|y - x\|$ sufficiently small. (Here $\|\cdot\|$ denotes the standard Euclidean norm in $\mathbb{R}^m$.)

For any smooth function $H\colon P \to \mathbb{R}$ we call the system $(P, \Omega, \mathsf{D}, H)$ a *discrete Hamiltonian system*. We associate with this system a difference equation of the form

$$z_{n+1} - z_n = h\mathsf{X}_H(z_n, z_{n+1}), \tag{3.5}$$

where $h \in \mathbb{R}_+$ is a parameter and X_H is a *discrete Hamiltonian vector field* defined by the relation

$$\mathsf{X}_H(x, y) = \Omega^\sharp_{(x+y)/2}(\mathsf{D}H(x, y)) \tag{3.6}$$

for all $x, y \in P$. Any sequence $(z_n)_{n=0}^N$ in P satisfying (3.5), if it exists, will be called a *trajectory* or *solution sequence* for the discrete system.

We now give some constructive examples of discrete derivatives for functions defined on general inner-product spaces.

3.3. Discrete Derivative: Examples

We begin by considering the general case of functions defined on m-dimensional Euclidean space $\mathbb{R}^m$.

Proposition 3.1. *Let $f\colon \mathbb{R}^m \to \mathbb{R}$ be a smooth function and for any two points $x, y \in \mathbb{R}^m$ let $z = (x+y)/2$ and $v = y - x$. Then a discrete derivative for f is defined by the relation*

$$\mathsf{D}f(x,y) = Df(z) + \frac{f(y) - f(x) - Df(z)\cdot v}{\|v\|^2}\, v, \tag{3.7}$$

where $\|\cdot\|$ denotes the standard Euclidean norm in $\mathbb{R}^m$.

Proof. The result follows by direct verification of the directionality and consistency properties.

(1) To verify the directionality condition we apply $\mathsf{D}f(x,y)$ to v and get

$$\begin{aligned} \mathsf{D}f(x,y)\cdot v &= Df(z)\cdot v + \frac{f(y) - f(x) - Df(z)\cdot v}{\|v\|^2}\, v\cdot v \\ &= f(y) - f(x). \end{aligned} \tag{3.8}$$

(2) To verify the consistency condition we examine what happens to (3.7) as v approaches zero. As a first step, given $v = y - x$, we use Taylor's Theorem to write

$$\begin{aligned} f(y) &= f(z) + \tfrac{1}{2}Df(z)\cdot v + \tfrac{1}{4}D^2 f(z)\cdot(v,v) + \tfrac{1}{8}D^3 f(z)\cdot(v,v,v) \\ &\quad + \tfrac{1}{16}D^4 f(z)\cdot(v,v,v,v) + O(\|v\|^5), \end{aligned} \tag{3.9}$$

$$\begin{aligned} f(x) &= f(z) - \tfrac{1}{2}Df(z)\cdot v + \tfrac{1}{4}D^2 f(z)\cdot(v,v) - \tfrac{1}{8}D^3 f(z)\cdot(v,v,v) \\ &\quad + \tfrac{1}{16}D^4 f(z)\cdot(v,v,v,v) + O(\|v\|^5), \end{aligned} \tag{3.10}$$

which implies

$$f(y) - f(x) - Df(z)\cdot v = \tfrac{1}{4}D^3 f(z)\cdot(v,v,v) + O(\|v\|^5). \tag{3.11}$$

Let $v = y - x = \alpha w$ where $\alpha > 0$ and $w \in \mathbb{R}^m$ is a unit vector. Then the last expression can be written as

$$f(y) - f(x) - Df(z)\cdot v = \tfrac{1}{4}\alpha^3 D^3 f(z)\cdot(w,w,w) + O(\alpha^5). \tag{3.12}$$

Using the above result in (3.7) gives the relation

$$\mathsf{D}f(x,y) = Df(z) + \left(\tfrac{1}{4}\alpha^2 D^3 f(z)\cdot(w,w,w) + O(\alpha^4)\right) w, \tag{3.13}$$

which shows that $\mathsf{D}f(x,y)$ is well defined as $\alpha = \|y - x\| \to 0$. In particular, the expression for $\mathsf{D}f(x,y)$ given in (3.7) satisfies the consistency requirement. $\square$

Here we note that, for any $x, y \in \mathbb{R}^m$, the construction above yields a discrete derivative which, in the classical sense, is a second-order approximation to the exact derivative at the midpoint $z = \frac{1}{2}(x + y)$. For reference, we now list some (second-order) discrete derivatives for more general situations:

(1) General case. Let $(U, \langle\cdot, \cdot\rangle_U)$ be an inner-product space. Then, for any smooth function $f\colon U \to \mathbb{R}$, a second-order discrete derivative is given by

$$\mathsf{D}f(x, y) = Df(z) + \frac{f(y) - f(x) - \langle Df(z), v_{xy}\rangle_U}{\langle v_{xy}, v_{xy}\rangle_U} v_{xy}, \tag{3.14}$$

where $v_{xy} = y - x$.

(2) Partitioned case. Let $(U, \langle\cdot, \cdot\rangle_U)$ be an inner-product space where $U = U_1 \times \cdots \times U_k$ for some $k \geq 1$, and suppose each U_i $(i = 1, \ldots, k)$ is endowed with an inner-product $\langle\cdot, \cdot\rangle_{U_i}$. Here we would like a discrete derivative which respects the product structure of U. To this end, for any smooth function $f\colon U \to \mathbb{R}$ a second-order discrete derivative is defined by the relation

$$\tilde{\mathsf{D}}f(x, y) \cdot u = \sum_{i=1}^{k} \tfrac{1}{2} \left(\mathsf{D}f^i_{xy}(x_i, y_i) + \mathsf{D}f^i_{yx}(x_i, y_i)\right) \cdot u_i \tag{3.15}$$

for all $u = (u_1, \ldots, u_k) \in U$, where $x = (x_1, \ldots, x_k) \in U$, $y = (y_1, \ldots, y_k) \in U$, and $f^i_{xy}, f^i_{yx}\colon U_i \to \mathbb{R}$ are defined by the relations

$$f^i_{xy}(w) = f(x_1, x_2, \ldots, x_{i-1}, w, y_{i+1}, \ldots, y_k), \tag{3.16}$$

$$f^i_{yx}(w) = f(y_1, y_2, \ldots, y_{i-1}, w, x_{i+1}, \ldots, x_k). \tag{3.17}$$

3.4. *The Algorithmic Viewpoint*

The interpretation of the above developments within an algorithmic framework should be clear; in particular, we may view the Hamiltonian difference equation (3.5), together with (3.14) or (3.15), as defining an algorithm for the approximation of (2.2). Moreover, the approximation is formally second-order since $\mathsf{X}_H(z_n, z_{n+1})$ is a second-order approximation to $X_H(z_{n+\frac{1}{2}})$, where $z_{n+\frac{1}{2}} = \frac{1}{2}(z_n + z_{n+1})$.

To develop the theory for discrete Hamiltonian systems we assume that the algorithm defined by (3.5) generates an evolution semigroup so that, for any $z_0 \in P$, n sufficiently small, we may speak of unique solution sequences $(z_n)_{n=0}^N$. With this in mind, we may then view a discrete trajectory as being generated by a mapping F_h, defined at least locally, such that $z_n = \mathsf{F}_h^n(z_0)$. In particular, F_h^n has the semigroup properties $\mathsf{F}_h^{n+m} = \mathsf{F}_h^n \circ \mathsf{F}_h^m$ and $\mathsf{F}_h^0 = id$. Also, we note that for all fixed n the mapping F_h^n is continuous in h in the sense that $z_n = \mathsf{F}_h^n(z_0)$ and any $z_i = \mathsf{F}_h^i(z_0)$ for $i = 0, \ldots, n-1$ can be forced to remain in a neighborhood of z_0 for h sufficiently small.

3.5. *Discrete Brackets and First Integrals*

We next introduce the concept of a discrete bracket which we will use to define integrals for discrete Hamiltonian systems.

Let (P, Ω, D) be a symplectic space with a discrete derivative and, for any smooth function $H\colon P \to \mathbb{R}$, let X_H denote the associated discrete Hamiltonian vector field. For any $z_0 \in P$ let $(z_n)_{n=0}^N$ be the trajectory generated by X_H for some $h > 0$. We say that a smooth function $f\colon P \to \mathbb{R}$ is an *integral* for the discrete system $(P, \Omega, \mathsf{D}, H)$ if it is constant along trajectories. That is, f is an integral for X_H if, for any trajectory $(z_n)_{n=0}^N$, we have $f(z_n) = f(z_0)$ for all $n = 0, \ldots, N$.

The condition that f be an integral for X_H may be expressed locally by the condition $\{f, H\} = 0$ where the *discrete bracket* $\{f, H\}\colon P \times P \to \mathbb{R}$ is defined as

$$\{f, H\}(x, y) = \mathsf{D}f(x, y) \cdot \mathsf{X}_H(x, y) = -\{H, f\}(x, y). \tag{3.18}$$

This is the essence of the following proposition.

Proposition 3.2. *A smooth function $f\colon P \to \mathbb{R}$ is an integral for a discrete Hamiltonian system $(P, \Omega, \mathsf{D}, H)$ if the discrete bracket of f and H vanishes, i.e.,*

$$\{f, H\}(x, y) = 0, \qquad \forall x, y \in P. \tag{3.19}$$

Proof. For any $z_0 \in P$ let $(z_n)_{n=0}^N$ denote the trajectory generated by X_H for some $h > 0$. By the definitions of the discrete bracket, discrete Hamiltonian vector field and discrete derivative we have

$$\begin{aligned} \{f, H\}(z_n, z_{n+1}) &= \mathsf{D}f(z_n, z_{n+1}) \cdot \mathsf{X}_H(z_n, z_{n+1}) \\ &= \mathsf{D}f(z_n, z_{n+1}) \cdot (z_{n+1} - z_n)/h \\ &= (f(z_{n+1}) - f(z_n))/h. \end{aligned} \tag{3.20}$$

The result follows. □

Proposition 3.3 follows from the skew-symmetry property of the discrete bracket.

Proposition 3.3. *The Hamiltonian $H\colon P \to \mathbb{R}$ is an integral for the discrete Hamiltonian system $(P, \Omega, \mathsf{D}, H)$.*

Remark 3.1. The discrete brackets defined above are motivated by the discrete orthogonality condition (3.4). As defined, these brackets do not satisfy the Jacobi identity and hence are not Poisson brackets. The difficulty lies in the fact that the discrete brackets are defined for functions on P, while the discrete bracket of two functions is a function on $P \times P$. □

3.6. Symmetry and Conservation Laws

In this section we define a discrete derivative for G-invariant functions and use it to introduce the concept of a discrete Hamiltonian system with symmetry. In what follows we let P be an open set in m-dimensional Euclidean space $\mathbb{R}^m$ and we denote by Φ the symplectic action of a group G on P.

Definition 3.2. A *G-equivariant discrete derivative* for a smooth G-invariant function $f\colon P \to \mathbb{R}$ is a mapping $\mathsf{D}^G f\colon P \times P \to \mathbb{R}^m$ satisfying the requirements for a discrete derivative together with the following properties:

(1) Equivariance. $\mathsf{D}^G f(\Phi_g(x), \Phi_g(y)) = \left[D\Phi_g(\frac{x+y}{2})\right]^{-\mathrm{T}} \cdot \mathsf{D}^G f(x, y)$ for all $g \in G$ and $x, y \in P$. (For any $z \in P$ note that $D\Phi_g(z) \in \mathbb{R}^{m\times m}$.)
(2) Orthogonality Condition. $\mathsf{D}^G f(x, y) \cdot \xi_P(\frac{x+y}{2}) = 0$ for all $\xi \in T_e G$ and $x, y \in P$.

For any smooth G-invariant function H we call the system $(P, \Omega, G, \mathsf{D}^G, H)$ a discrete Hamiltonian system with *symmetry*. As before, we associate with this system a difference equation of the form

$$z_{n+1} - z_n = h\mathsf{X}_H(z_n, z_{n+1}), \tag{3.21}$$

where $h \in \mathbb{R}_+$ is a parameter and X_H is a discrete Hamiltonian vector field defined by the relation

$$\mathsf{X}_H(x, y) = \Omega^{\sharp}_{(x+y)/2}(\mathsf{D}^G H(x, y)) \tag{3.22}$$

for all $x, y \in P$.

Remark 3.2. The equivariance and orthogonality conditions stated above are motivated by properties of the derivatives of G-invariant functions. □

Before giving some constructive examples of G-equivariant discrete derivatives, we first summarize some properties of discrete Hamiltonian systems with symmetry.

Proposition 3.4. *Let $(P, \Omega, G, \mathsf{D}^G, H)$ be a discrete Hamiltonian system with symmetry and let Φ denote an affine symplectic action of G on P. Then solution sequences satisfying (3.21) are invariant under G. That is, if $(z_n)_{n=0}^N$ is a solution sequence, then so is $(\Phi_g(z_n))_{n=0}^N$ for any $g \in G$.*

Proof. For arbitrary $z_0 \in P$ let $(z_n)_{n=0}^N$ be the trajectory for X_H defined by (3.21) for some $h > 0$. For any $g \in G$ consider the transformed sequence $(\Phi_g(z_n))_{n=0}^N$. Since by assumption Φ_g is affine, we may write

$$\begin{aligned} \Phi_g(z_{n+1}) - \Phi_g(z_n) &= D\Phi_g(z_{n+\frac{1}{2}}) \cdot (z_{n+1} - z_n) \\ &= hD\Phi_g(z_{n+\frac{1}{2}}) \cdot \mathsf{X}_H(z_n, z_{n+1}). \end{aligned} \tag{3.23}$$

The above statement implies that the transformed sequence $(\Phi_g(z_n))_{n=0}^N$ is a trajectory of H if and only if the discrete vector field X_H satisfies the equivariance relation

$$\mathsf{X}_H(\Phi_g(z_n), \Phi_g(z_{n+1})) = D\Phi_g(z_{n+\frac{1}{2}}) \cdot \mathsf{X}_H(z_n, z_{n+1}). \tag{3.24}$$

The result follows from the fact that (3.24) is equivalent to the equivariance condition on $\mathsf{D}^G H$. □

Recall that, under certain circumstances, the action of a group G on a phase space P possesses a momentum map $J\colon P \to T_e^*G$. Furthermore, if a momentum map exists, it is conserved by the system (P, Ω, G, H) in the sense that the function $J_\xi = J \cdot \xi$ is an integral for any $\xi \in T_eG$. We now state a similar result for the discrete case.

Proposition 3.5. *Let $(P, \Omega, G, \mathsf{D}^G, H)$ be a discrete Hamiltonian system with symmetry and denote by Φ a symplectic action of G on P. Suppose this action possesses a momentum map $J\colon P \to T_e^*G$. If J is at most quadratic in $z \in P$, then J is conserved by the discrete system in the sense that the function $J_\xi = J \cdot \xi$ is an integral for any $\xi \in T_eG$.*

Proof. To begin, note that if the map $J\colon P \to T_e^*G$ is at most quadratic, then for any $x, y \in P$ we have

$$J_\xi(y) - J_\xi(x) = DJ_\xi\left(\tfrac{x+y}{2}\right) \cdot (y - x). \tag{3.25}$$

Now let $(z_n)_{n=0}^N$ be any trajectory generated by the discrete system (3.21). For any $\xi \in T_eG$ we use (3.25), (3.21) and (2.6) to write

$$\begin{aligned} J_\xi(z_{n+1}) - J_\xi(z_n) &= DJ_\xi(z_{n+\frac{1}{2}}) \cdot (z_{n+1} - z_n) \\ &= hDJ_\xi(z_{n+\frac{1}{2}}) \cdot \mathsf{X}_H(z_n, z_{n+1}) \\ &= h\Omega^\flat_{z_{n+\frac{1}{2}}}(\xi_P(z_{n+\frac{1}{2}})) \cdot \mathsf{X}_H(z_n, z_{n+1}) \\ &= -h\Omega^\flat_{z_{n+\frac{1}{2}}}(\mathsf{X}_H(z_n, z_{n+1})) \cdot \xi_P(z_{n+\frac{1}{2}}) \\ &= -h\mathsf{D}^G H(z_n, z_{n+1}) \cdot \xi_P(z_{n+\frac{1}{2}}), \end{aligned} \tag{3.26}$$

which vanishes in view of the orthogonality condition on $\mathsf{D}^G H$. □

We next give some constructive examples of G-equivariant discrete derivatives.

3.7. Discrete Derivative: G-Equivariant Case

Let (P, Ω, G) be a phase space with symmetry where P is an open set in m-dimensional Euclidean space $\mathbb{R}^m$, and denote by Φ a regular affine symplectic action of G on P. Assume the action of G has orbits of dimension s, so that the quotient or orbit space P/G can be identified locally with $\mathbb{R}^{m-s}$. In particular, let $\pi_i\colon P \to \mathbb{R}$ $(i = 1, \ldots, m - s)$ be invariants of G (assumed to be globally defined, for simplicity) so that $P/G \cong \pi(P) \subset \mathbb{R}^{m-s}$ where $\pi\colon P \to \mathbb{R}^{m-s}$ is defined by $\pi = (\pi_1, \ldots, \pi_{m-s})$. With this setup a G-equivariant discrete derivative is contained in the following proposition.

Proposition 3.6. *Let $f\colon P \to \mathbb{R}$ be a smooth G-invariant function and denote by $\tilde{f}\colon \pi(P) \subset \mathbb{R}^{m-s} \to \mathbb{R}$ the associated reduced function, defined by the expression $\tilde{f}(\pi(z)) = f(z)$ for all $z \in P$. Consider any two points $x, y \in P$ and let $z = (x + y)/2$*

and $v = y - x$. If the invariants $\pi_i \colon P \to \mathbb{R}$ are at most quadratic, then a G-equivariant discrete derivative for f is defined by the relation

$$
\begin{aligned}
\mathsf{D}^G f(x, y) &= \mathsf{D}\tilde{f}(\pi(x), \pi(y)) \circ D\pi(z) \\
&= [D\pi(z)]^{\mathrm{T}} \cdot \mathsf{D}\tilde{f}(\pi(x), \pi(y)),
\end{aligned} \tag{3.27}
$$

where on the right-hand side D represents a discrete derivative for functions on $\mathbb{R}^{m-s}$. (For any $z \in P$ note that $D\pi(z) \in \mathbb{R}^{(m-s)\times m}$.)

Proof. The result follows by direct verification of the defining conditions.

(1) To verify the directionality condition we apply $\mathsf{D}^G f(x, y)$ to v and obtain

$$
\mathsf{D}^G f(x, y) \cdot v = \mathsf{D}\tilde{f}(\pi(x), \pi(y)) \cdot (D\pi(z) \cdot v). \tag{3.28}
$$

Since by assumption π is at most quadratic we have that $D\pi(z) \cdot v = \pi(y) - \pi(x)$. Hence

$$
\begin{aligned}
\mathsf{D}^G f(x, y) \cdot v &= \mathsf{D}\tilde{f}(\pi(x), \pi(y)) \cdot (\pi(y) - \pi(x)) \\
&= \tilde{f}(\pi(y)) - \tilde{f}(\pi(x)) \\
&= f(y) - f(x).
\end{aligned} \tag{3.29}
$$

(2) Consistency follows from the consistency of the discrete derivative for functions defined on $\mathbb{R}^{m-s}$.

(3) To verify the equivariance condition we note that, since π is invariant, i.e., $\pi(\Phi_g(z)) = \pi(z)$ for all $z \in P$ and $g \in G$, we have

$$
D\pi(\Phi_g(z)) = D\pi(z) \circ \left[D\Phi_g(z)\right]^{-1}. \tag{3.30}
$$

Since $\Phi_g \colon P \to P$ is affine we have $\frac{1}{2}(\Phi_g(x) + \Phi_g(y)) = \Phi_g(z)$, and thus

$$
\begin{aligned}
\mathsf{D}^G f(\Phi_g(x), \Phi_g(y)) &= \mathsf{D}\tilde{f}(\pi(\Phi_g(x)), \pi(\Phi_g(y))) \circ D\pi(\Phi_g(z)) \\
&= \mathsf{D}\tilde{f}(\pi(x), \pi(y)) \circ D\pi(\Phi_g(z)) \\
&= \mathsf{D}\tilde{f}(\pi(x), \pi(y)) \circ D\pi(z) \circ \left[D\Phi_g(z)\right]^{-1} \\
&= \left[D\Phi_g(z)\right]^{-\mathrm{T}} \cdot \left(\mathsf{D}\tilde{f}(\pi(x), \pi(y)) \circ D\pi(z)\right) \\
&= \left[D\Phi_g(z)\right]^{-\mathrm{T}} \cdot \mathsf{D}^G f(x, y).
\end{aligned} \tag{3.31}
$$

(4) To verify the orthogonality condition we again exploit the invariance of the mapping $\pi \colon P \to \mathbb{R}^{m-s}$. In particular, we have $D\pi(z) \cdot \xi_P(z) = 0$ for all $\xi \in T_eG$. So

$$
\mathsf{D}^G f(x, y) \cdot \xi_P(z) = \mathsf{D}\tilde{f}(\pi(x), \pi(y)) \cdot (D\pi(z) \cdot \xi_P(z)) = 0, \tag{3.32}
$$

for all $\xi \in T_eG$. □

We next give an example to clarify the above ideas.

Example 3.1. Let P be an open set in $\mathbb{R}^3 \times \mathbb{R}^3$ of the form

$$P = \{(q, p) \in \mathbb{R}^3 \times \mathbb{R}^3 \mid q \times p \neq 0\}, \tag{3.33}$$

and let Ω denote the canonical symplectic structure on P. Let $H\colon P \to \mathbb{R}$ be a smooth function of the form

$$H(q, p) = V(q) + K(p), \tag{3.34}$$

where $V(q) = \hat{V}(\|q\|)$ for some function $\hat{V}\colon \mathbb{R}_+ \to \mathbb{R}$ and $K(p) = \hat{K}(\|p\|) = \|p\|^2/2m$ for some $m > 0$.

Clearly, the above Hamiltonian system (P, Ω, H) has symmetry under the regular affine action of $G = SO(3)$ on P defined as $\Phi(\Lambda, (q, p)) = (\Lambda q, \Lambda p)$, i.e., the Hamiltonian is invariant under this action. Moreover, this action is symplectic with momentum map $J\colon P \to T_e^*G \cong \mathbb{R}^3$ given by $J(q, p) = q \times p$, which is called the angular momentum for the system.

To construct an associated discrete system with symmetry we need to construct a G-equivariant discrete derivative for G-invariant functions on P. To do this, we need to find a set of independent invariants of G which are at most quadratic. In particular, since P is of dimension $k = 6$ and the action of G has orbits of dimension $s = 3$, we need to find $k - s = 3$ independent invariants of G. By inspection, we have that

$$\left.\begin{aligned} \pi_1(q, p) &= \|q\|^2 = q \cdot q \\ \pi_2(q, p) &= q \cdot p \\ \pi_3(q, p) &= \|p\|^2 = p \cdot p \end{aligned}\right\} \tag{3.35}$$

are a set of independent invariants which are quadratic. Hence we have $P/G \cong \pi(P) \subset \mathbb{R}^3$ where

$$\pi(P) = \{(x_1, x_2, x_3) \in \mathbb{R}^3 \mid x_1 > 0,\ x_3 > 0,\ |x_2| < x_1 x_3\}, \tag{3.36}$$

and the associated reduced function $\tilde{H}\colon \pi(P) \subset \mathbb{R}^3 \to \mathbb{R}$ for H is

$$\begin{aligned} \tilde{H}(\pi_1, \pi_2, \pi_3) &= \hat{V}(\sqrt{\pi_1}) + \hat{K}(\sqrt{\pi_3}) \\ &= \tilde{V}(\pi_1) + \tilde{K}(\pi_3), \end{aligned} \tag{3.37}$$

where $\tilde{V}(\pi_1) = \hat{V}(\sqrt{\pi_1})$ and $\tilde{K}(\pi_3) = \hat{K}(\sqrt{\pi_3}) = \pi_3/2m$.

Now, for any $x, y \in P$ let $z = (x + y)/2$. Then, using a partitioned discrete derivative for $\tilde{H}$, a G-equivariant discrete derivative for H is

$$\mathsf{D}^G H(x, y) = \mathsf{D}\tilde{V}(\pi_1(x), \pi_1(y)) \circ D\pi_1(z) + \mathsf{D}\tilde{K}(\pi_3(x), \pi_3(y)) \circ D\pi_3(z). \tag{3.38}$$

Since $\tilde{V}\colon \mathbb{R}_+ \to \mathbb{R}$ we have

$$\begin{aligned} \mathsf{D}\tilde{V}(\tau, t) &= \tilde{V}'(\tfrac{\tau+t}{2}) + \frac{\tilde{V}(t) - \tilde{V}(\tau) - \tilde{V}'(\frac{\tau+t}{2})(t - \tau)}{|t - \tau|^2}(t - \tau) \\ &= \frac{\tilde{V}(t) - \tilde{V}(\tau)}{t - \tau}. \end{aligned} \tag{3.39}$$

Similarly,

$$\mathsf{D}\tilde{K}(\tau, t) = \frac{\tilde{K}(t) - \tilde{K}(\tau)}{t - \tau} = \frac{1}{2m}. \tag{3.40}$$

So

$$\mathsf{D}^G H(x, y) = \frac{\tilde{V}(\pi_1(y)) - \tilde{V}(\pi_1(x))}{\pi_1(y) - \pi_1(x)} D\pi_1(z) + \frac{1}{2m} D\pi_3(z). \tag{3.41}$$

If we let $x = (q_n, p_n)$ and $y = (q_{n+1}, p_{n+1})$ then $z = (q_{n+\frac{1}{2}}, p_{n+\frac{1}{2}})$, and we get

$$\begin{aligned}
&\mathsf{D}^G H((q_n, p_n), (q_{n+1}, p_{n+1})) \\
&\quad = \frac{\tilde{V}(\|q_{n+1}\|^2) - \tilde{V}(\|q_n\|^2)}{\|q_{n+1}\|^2 - \|q_n\|^2} (2q_{n+\frac{1}{2}}, 0) + \frac{1}{2m} (0, 2p_{n+\frac{1}{2}}) \\
&\quad = \left(\frac{\hat{V}(\|q_{n+1}\|) - \hat{V}(\|q_n\|)}{\|q_{n+1}\| - \|q_n\|} \frac{q_{n+\frac{1}{2}}}{\frac{1}{2}(\|q_{n+1}\| + \|q_n\|)}, m^{-1} p_{n+\frac{1}{2}} \right).
\end{aligned} \tag{3.42}$$

With the canonical symplectic structure, we obtain the difference equations for our discrete system with symmetry as

$$\left.\begin{aligned}
q_{n+1} - q_n &= hm^{-1} p_{n+\frac{1}{2}} \\
p_{n+1} - p_n &= -h \frac{\hat{V}(\|q_{n+1}\|) - \hat{V}(\|q_n\|)}{\|q_{n+1}\| - \|q_n\|} \frac{q_{n+\frac{1}{2}}}{\frac{1}{2}(\|q_{n+1}\| + \|q_n\|)}
\end{aligned}\right\}, \tag{3.43}$$

where $h > 0$ is a parameter. □

Remarks 3.3.

(1) Within an algorithmic framework the above system is a second-order, implicit, one-step approximation to the underlying Hamiltonian differential equation which preserves the Hamiltonian and the angular momentum. This scheme is studied in detail in [7]. For an n-body generalization of the above scheme, together with a numerical assessment of performance, see [24].

(2) Generally speaking, the idea of replacing the derivative of a potential with a finite-difference quotient in order to achieve energy and momentum conservation goes back to the work of Greenspan [9] and LaBudde & Greenspan [12]–[14]. □

3.8. Reduced Trajectories

Given a discrete system with symmetry possessing a momentum map J, we can introduce the notion of reduced trajectories as is done for the underlying system. The existence of these reduced trajectories will be crucial when we consider questions of stability in later sections.

Let $(P, \Omega, G, \mathsf{D}^G, H)$ be a discrete Hamiltonian system with symmetry and let Φ denote a regular affine symplectic action of G on P. Assume this action possesses an Ad^*-equivariant momentum map $J\colon P \to T_e^*G$ which is an integral for the discrete system, and let $\mu \in T_e^*G$ be a regular value for J so that the preimage $J^{-1}(\mu)$ is a smooth manifold in P. Since J is an integral for the system, any trajectory which starts in $J^{-1}(\mu)$ remains there. Hence, given any $z_0 \in J^{-1}(\mu)$, there is a well-defined trajectory $(z_n)_{n=0}^N$ in $J^{-1}(\mu)$, which implies the existence of a well-defined discrete system on $J^{-1}(\mu)$.

As before, let G_μ denote the isotropy subgroup of μ under the coadjoint action of G on T_e^*G, i.e., $G_\mu = \{g \in G \mid \mathrm{Ad}^*_{g^{-1}}(\mu) = \mu\}$. Then $J^{-1}(\mu)$ is invariant under the action of G_μ. Since G_μ is a subgroup of G, we have, by Proposition 3.4, that any trajectory maps to a trajectory under the action of G_μ. In particular, the action of G_μ maps trajectories in $J^{-1}(\mu)$ to trajectories in $J^{-1}(\mu)$. Hence, the restriction of the discrete system to $J^{-1}(\mu)$ is a well-defined system with symmetry.

Since by assumption the action of G_μ is regular, there is a well-defined reduced phase space $P_\mu = J^{-1}(\mu)/G_\mu$ and a natural projection $\pi_\mu\colon J^{-1}(\mu) \to P_\mu$. If $(z_n)_{n=0}^N$ is a trajectory for the original system lying in $J^{-1}(\mu)$, then $(\pi_\mu(z_n))_{n=0}^N$ is a well-defined trajectory in the reduced space. In particular, trajectories in $J^{-1}(\mu)$ and P_μ differ by some sequence of transformations under the action. More importantly, since the reduced Hamiltonian $H_\mu\colon P_\mu \to \mathbb{R}$ depends only on the original Hamiltonian H and the momentum value μ, it follows that H_μ is an integral for the reduced trajectory, i.e., $H_\mu(\pi_\mu(z_n)) = H_\mu(\pi_\mu(z_0))$ for all $n = 0, \dots, N$.

3.9. *Fixed Points*

Consider a discrete Hamiltonian system $(P, \Omega, \mathsf{D}, H)$ where P is open in m-dimensional Euclidean space $\mathbb{R}^m$. An *equilibrium point* or *equilibria* of the system is a point $z_0 \in P$ for which the constant sequence $(z_0)_{n=0}^\infty$ satisfies the associated Hamiltonian difference equation (3.5). In terms of the discrete vector field, it follows by induction that z_0 is an equilibrium point if and only if $\mathsf{X}_H(z_0, z_0) = 0$.

We can characterize equilibria of general discrete Hamiltonian systems with the following proposition.

Proposition 3.7. *Let $(P, \Omega, \mathsf{D}, H)$ be a discrete Hamiltonian system. Then a point $z_0 \in P$ is an equilibrium point if and only if z_0 is a critical point of the Hamiltonian H, i.e., $D_{z_0}H = 0$.*

Proof. A point z_0 is an equilibria if and only if $\mathsf{X}_H(z_0, z_0) = 0$. Since $\mathsf{X}_H(z_0, z_0) = \Omega^\sharp_{z_0}(\mathsf{D}_{(z_0,z_0)}H)$, and Ω_{z_0} is nondegenerate, z_0 is an equilibria if and only if $\mathsf{D}_{(z_0,z_0)}H = 0$. The result follows from the fact that $\mathsf{D}_{(z_0,z_0)}H = D_{z_0}H$. □

Comparing the discrete system with the underlying system (P, Ω, H) we see that both possess equilibrium points which are critical points of the Hamiltonian function H. In particular, the trajectory $(z_0)_{n=0}^\infty$ is a discrete analog of the equilibrium solution $\varphi(t) = z_0$ for all $t \in \mathbb{R}$ of the underlying system.

We next consider discrete Hamiltonian systems with symmetry and determine whether they inherit discrete analogs of relative equilibria.

3.10. Relative Equilibria

Let $(P, \Omega, G, \mathsf{D}^G, H)$ be a discrete Hamiltonian system with symmetry and denote by Φ a regular affine symplectic action of G on P. Suppose the action has a momentum map $J\colon P \to T_e^*G$ which is conserved along trajectories of this system. We say a point $z_e \in P$ is a *relative equilibria* of the discrete system with symmetry if, for given $h > 0$, the local trajectory $(z_n)_{n=0}^N$ through z_e is of the form

$$z_n = \Phi(g^n, z_e), \tag{3.44}$$

for some $g \in G$ where g^n denotes n products of g. Note that this definition is just a discrete analog of the definition for the underlying system, and is motivated from that definition by considering $z(t_n)$ where $t_n = hn$. Regarding relative equilibria for discrete systems with symmetry, we have the following proposition.

Proposition 3.8. *Let $(P, \Omega, G, \mathsf{D}^G, H)$ be a discrete Hamiltonian system with symmetry and denote by Φ a regular affine symplectic action of G on P. Assume this action possesses an* Ad**-equivariant momentum map $J\colon P \to T_e^*G$ which is an integral for the discrete system. Then, for any regular momentum value μ, a point $z_e \in J^{-1}(\mu) \subset P$ is a relative equilibria if and only if, for given $h > 0$, the local trajectory at z_e projects to a constant trajectory (i.e., fixed point) in the reduced space P_μ.*

Proof. Consider a point $z_e \in J^{-1}(\mu)$ and recall that there exists a neighborhood B of z_e in P, real numbers $h_c, T > 0$, and an evolution semigroup $\mathsf{F}\colon B \times [0, h_c] \to P$ such that, for any $0 < h < h_c$, the local trajectory at z_e is given by $z_n = \mathsf{F}_h^n(z_e)$ for $n = 0, \dots, N$ where $N \geq 1$ is such that $Nh \leq T$. Furthermore, we have $z_n \in J^{-1}(\mu)$ for all $n = 0, \dots, N$.

Now, if z_e is a relative equilibria, then $z_n = \Phi(a^n, z_e)$ for all $n = 0, \dots, N$ for some $a \in G_\mu$. Hence, for each n it follows that $z_n \in G_\mu \cdot z_e$, i.e., z_n is in the orbit of z_e under the action of G_μ. By definition of the projection $\pi_\mu\colon J^{-1}(\mu) \to P_\mu$, we then have $\pi_\mu(z_n) = \pi_\mu(z_e)$ for all $n = 0, \dots, N$, and the reduced sequence $(\pi_\mu(z_n))_{n=0}^N$ in P_μ is a constant sequence.

Conversely, assume the local trajectory $(z_n)_{n=0}^N$ in $J^{-1}(\mu)$ projects to a constant sequence $(\pi_\mu(z_n))_{n=0}^N$ in P_μ, i.e., $\pi_\mu(z_n) = \pi_\mu(z_e)$ for all $n = 0, \dots, N$. By definition of π_μ, we must have $z_n \in G_\mu \cdot z_e$ for each n. That is, there exists a sequence $(g_n)_{n=0}^N$ in G_μ such that $z_n = \Phi(g_n, z_e)$. Since $z_n = \mathsf{F}_h^n(z_e)$ for $n = 0, \dots, N$ and the mappings F_h^n have the semigroup properties $\mathsf{F}_h^0 = id$ and $\mathsf{F}_h^{n+m} = \mathsf{F}_h^n \circ \mathsf{F}_h^m$, we can use properties of the action Φ to deduce that the sequence $(g_n)_{n=0}^N$ must have the properties $g_0 = e$ and $g_{n+m} = g_n g_m$. Let $g_1 = a \in G_\mu$, and for induction assume $g_n = a^n$. Then, since $g_{n+1} = g_n g_1$, it follows that $g_{n+1} = a^{n+1}$. Hence, the sequence $(g_n)_{n=0}^N$ is defined by $g_n = a^n$ for some $a \in G_\mu$. It then follows that z_e is a relative equilibria. □

As with equilibrium points, we would like to be able to characterize relative equilibria of discrete systems in terms of properties of the underlying system. To this end we have the following proposition.

Proposition 3.9. *Let (P, Ω, G, H) be a Hamiltonian system with symmetry with an* Ad^**-equivariant momentum map J. Assume this system possesses a relative equilibria z_e with a regular momentum value μ. If $\pi_\mu(z_e) \in P_\mu$ is a nondegenerate minima or maxima of the reduced Hamiltonian H_μ, and the parameter $h > 0$ is sufficiently small, then z_e is a relative equilibria for an associated discrete system with symmetry $(P, \Omega, G, \mathsf{D}^G, H)$ provided that the action of G on P is affine and J is an integral for this system.*

Proof. The result follows from Proposition 3.8, together with the observations that there is a well-defined discrete system in P_μ and H_μ is an integral for this system. □

The following proposition follows from the definitions of relative equilibria for both the underlying system and an associated discrete system.

Proposition 3.10. *If z_e is a relative equilibria for both the underlying system and an associated discrete system, then there is a sequence $(g_n)_{n=0}^N$ in G_μ such that the sampled trajectory $\varphi(hn)$ of the underlying system through z_e, and the local trajectory $(z_n)_{n=0}^N$ of the discrete system through z_e, differ by group transformations of the form*

$$\varphi(hn) = \Phi(g_n, z_n), \tag{3.45}$$

for all $n = 0, \dots, N$.

3.11. Notions of Stability

In analogy with the underlying Hamiltonian system we now introduce the notions of general dynamic stability and stability of equilibria and relative equilibria of an associated discrete system.

3.11.1. General Dynamic Stability. Consider a discrete Hamiltonian system $(P, \Omega, \mathsf{D}, H)$ with P open in $\mathbb{R}^m$ and consider the associated Hamiltonian difference equation (3.5). If the system has symmetry under the affine action of a group G, we suppose this action possesses a momentum map $J\colon P \to T_e^*G$ which is conserved along trajectories.

For any $z_0 \in P$ let (z_n) denote the maximal trajectory through z_0 for given $h > 0$. We say that the trajectory (z_n) is *dynamically stable* if it is defined for all $n \geq 0$ and if there is a constant $K > 0$, depending on h and z_0, such that $\|z_n\| \leq K$ for all $n \geq 0$. More generally, we say that the system is dynamically stable on a subset B of P if, for each $z_0 \in B$, there is a real number $h > 0$ such that the maximal trajectory through z_0 is dynamically stable.

An elementary criterion for dynamical stability is contained in the following proposition whose proof is straightforward.

Proposition 3.11. *Without loss of generality consider a discrete Hamiltonian system with symmetry $(P, \Omega, G, \mathsf{D}^G, H)$ possessing a momentum map J. Given $z_0 \in P$ such that $H(z_0) = c$ and $J(z_0) = \mu$, the trajectory through z_0 is dynamically stable if the subset $H^{-1}(c) \cap J^{-1}(\mu) \subset P$ is bounded, and the parameter $h > 0$ is sufficiently* *small. In particular, the system is dynamically stable on any bounded subset of the form* $H^{-1}(c) \cap J^{-1}(\mu)$.

3.11.2. Stability of Equilibria and Relative Equilibria. Our second notion of stability is that of stability of equilibria and relative equilibria, which is concerned with the behavior of solutions with nearby initial conditions. For concreteness consider a discrete Hamiltonian system $(P, \Omega, \mathsf{D}, H)$ where P is open in m-dimensional Euclidean space $\mathbb{R}^m$.

Suppose we are given an equilibrium point $z_0 \in P$. We say that z_0 is *stable* in the sense of Lyapunov if, for any neighborhood U of z_0, there is a neighborhood V of z_0 and a real number $h_{\max} > 0$ such that, for any $y \in V$ and $0 < h < h_{\max}$, the solution sequence (y_n) at y is defined and satisfies $y_n \in U$ for all $n \geq 0$. Roughly speaking, z_0 is stable if all solution sequences beginning in a neighborhood of z_0 remain in a neighborhood of z_0.

An elementary criterion for the Lyapunov stability of an equilibrium point of a discrete Hamiltonian system is contained in the following proposition whose proof is analogous to the time-continuous version [1].

Proposition 3.12. *Let* z_0 *be an equilibrium point of a discrete Hamiltonian system* $(P, \Omega, \mathsf{D}, H)$*. If the bilinear form* $D^2H(z_0)$ *is positive- or negative-definite, i.e.,* $D^2H(z_0)\cdot(v, v) > 0$ *or* $D^2H(z_0)\cdot(v, v) < 0$*, respectively, for all nonzero* $v \in T_{z_0}P \cong \mathbb{R}^m$*, then* z_0 *is stable in the sense of Lyapunov.*

The conditions of the above proposition are sufficient to guarantee Lyapunov stability of an equilibrium point for a general discrete Hamiltonian system. However, the proposition cannot be applied as is to systems with *symmetry*. The underlying reason is that the conditions of the above proposition imply the equilibrium point is isolated, which in general is not true for systems with symmetry. In particular, since equilibrium points z_0 correspond to critical points of the Hamiltonian, any point in the orbit $G \cdot z_0$ is also a critical point. In this case, the most we can hope for is stability of the set $G \cdot z_0$, i.e., stability up to the group action.

Similar difficulties are encountered when studying the stability of relative equilibria; in particular, for a relative equilibria with momentum value μ the most we can hope for is stability of the set $G_\mu \cdot z_e$. Since equilibrium points are special cases of relative equilibria—in particular, they are relative equilibria with $g = e$ (the group identity) in expression (3.44)—we can discuss their stability together as follows.

Let z_e be a relative equilibrium point with momentum value $J(z_e) = \mu$ and recall, from Proposition 3.8, that the trajectory in P through z_e projects to a fixed point in the reduced phase space P_μ. Also, for any trajectory in $J^{-1}(\mu) \subset P$, recall that the reduced Hamiltonian $H_\mu\colon P_\mu \to \mathbb{R}$ is an integral for the reduced trajectory. With this in mind, we can establish a criterion for the relative stability of a discrete relative equilibrium point z_e. In particular, we will say that z_e is *relatively stable* if the fixed point $\pi_\mu(z_e)$ in P_μ is stable in the sense of Lyapunov. As for the underlying time-continuous system [1], we have the following criterion for relative stability.

Proposition 3.13. *Let z_e be a relative equilibrium point with momentum μ of a discrete Hamiltonian system with symmetry $(P, \Omega, G, \mathsf{D}^G, H)$, and denote by π_μ the canonical projection from $J^{-1}(\mu)$ onto P_μ. If the bilinear form $D^2H_\mu(\pi_\mu(z_e))$ is positive- or negative-definite, i.e. $D^2H_\mu(\pi_\mu(z_e)) \cdot (v, v) > 0$ or $D^2H_\mu(\pi_\mu(z_e)) \cdot (v, v) < 0$, respectively, for all nonzero $v \in T_{\pi_\mu(z_e)}P_\mu$, then z_e is relatively stable.*

4. Concluding Remarks

Using the notion of a discrete Hamiltonian system, this paper has developed a framework for the design and analysis of conserving time-integration schemes for Hamiltonian systems with symmetry. Given a Hamiltonian system defined on an open set of Euclidean space, we have shown that a Hamiltonian-conserving scheme can always be constructed. Furthermore, if the system has symmetry under a group of affine transformations, we have shown how a conserving scheme that inherits this symmetry may be constructed. Regarding qualitative properties, it was shown that conserving schemes which fit within the proposed framework inherit invariant sets in phase space such as equilibria and relative equilibria, along with their stability properties.

The results summarized above were obtained for the case in which the underlying phase space was open in some Euclidean space and equipped with a symplectic structure. However, from the point of view of design, it is easy to see that the framework presented herein extends immediately to Euclidean phase spaces with more general Poisson structures. Moreover, the framework extends to infinite-dimensional systems. In this case, one introduces the idea of discrete functional derivatives, analogous to the discrete derivatives introduced in this paper, and then constructs a system of difference equations using the Poisson structure of the underlying problem (see [6] and [8] for details). For extensions of the ideas presented herein to constrained systems, see [5].

With regards to accuracy, we note that conserving schemes constructed using the discrete derivatives presented in this paper are formally second-order. However, one can employ time substepping procedures such as that proposed in [25] to increase the accuracy of a given conserving scheme.

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