

VARIATIONAL AND GEOMETRIC STRUCTURES OF DISCRETE DIRAC MECHANICS

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ABSTRACT. In this paper, we develop the theoretical foundations of discrete Dirac mechanics, that is, discrete mechanics of degenerate Lagrangian/Hamiltonian systems with constraints. We first construct discrete analogues of Tulczyjew's triple and induced Dirac structures by considering the geometry of symplectic maps and their associated generating functions. We demonstrate that this framework provides a means of deriving discrete Lagrange–Dirac and nonholonomic Hamiltonian systems. In particular, this yields nonholonomic Lagrangian and Hamiltonian integrators. We also introduce discrete Lagrange–d'Alembert–Pontryagin and Hamilton–d'Alembert variational principles, which provide an alternative derivation of the same set of integration algorithms. The paper provides a unified treatment of discrete Lagrangian and Hamiltonian mechanics in the more general setting of discrete Dirac mechanics, as well as a generalization of symplectic and Poisson integrators to the broader category of Dirac integrators.

Dedicated to the memory of Jerrold E. Marsden.

1. INTRODUCTION

Dirac structures, which can be viewed as simultaneous generalizations of symplectic and Poisson structures, were introduced in Courant [12, 13]. In the context of geometric mechanics [1, 3, 35], Dirac structures are of interest as they can directly incorporate Dirac constraints that arise in degenerate Lagrangian systems [16–18, 20–22, 28], interconnected systems [10, 45], and nonholonomic systems [6], and thereby provide a unified geometric framework for studying such problems.

From the Hamiltonian perspective, these systems are described by implicit Hamiltonian systems; see Bloch and Crouch [7] and van der Schaft [44] for applications of such a formulation to LC circuits and nonholonomic systems, and Dalsmo and van der Schaft [14] for a comprehensive review of Dirac structures in this setting. This approach is motivated by earlier work on almost-Poisson structures that describe nonholonomic systems using brackets that fail to satisfy the Jacobi identity [46]. These ideas are further extended to define port-Hamiltonian systems, which are intended to model interconnected systems (see van der Schaft [45] for a survey of such applications).

On the Lagrangian side, degenerate, interconnected, and nonholonomic systems can be described by Lagrange–Dirac (or implicit Lagrangian) systems introduced by Yoshimura and Marsden [50] in the context of Tulczyjew's triple [42, 43] and a certain class of representations of Dirac structures called induced Dirac structures [14]. The resulting Lagrange–Dirac equations generalize the Lagrange–d'Alembert equations for nonholonomic systems. The corresponding variational description of Lagrange–Dirac systems was developed in Yoshimura and Marsden [51], with the introduction of the Hamilton–Pontryagin principle on the Pontryagin bundle $TQ \oplus T^*Q$, which yields the generalized Legendre transformation, as well as Hamilton's principle for Lagrangian systems and Hamilton's phase space principle for Hamiltonian systems. Yoshimura and Marsden [51] also introduced the Lagrange–d'Alembert–Pontryagin principle, a generalization of the Hamilton–Pontryagin

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principle, which yields Lagrange–Dirac systems with nonholonomic constraints. It also generalizes the Lagrange–d’Alembert principle for nonholonomic systems (see, e.g., Bloch [6]).

In the context of geometric numerical integration [23, 30], which is concerned with the development of numerical methods that preserve geometric properties of the corresponding continuous flow, variational integrators that preserve the symplectic structure can be systematically derived from a discrete Hamilton’s principle [36], and can be extended to asynchronous variational integrators [33] that preserve the multisymplectic structure of Hamiltonian partial differential equations. The discrete variational formulation of Hamiltonian mechanics was developed by Lall and West [29] as the dual, in the sense of optimization, to discrete Lagrangian mechanics. Discrete analogues of the Hamilton–Pontryagin principle were introduced in [8, 26] for particular choices of discrete Lagrangians. Discrete Lagrangian, Hamiltonian, and nonholonomic mechanics have also been generalized to Lie groupoids [24, 34, 41, 49].

Contributions of this paper. In this paper, we introduce discrete analogues of Tulczyjew’s triple and induced Dirac structures, and show how they describe discrete Lagrange–Dirac and nonholonomic Hamiltonian systems. The construction relies on the observation that Tulczyjew’s triple arises from symplectic maps between the iterated tangent and cotangent bundles T^*TQ , TT^*Q , and T^*T^*Q . By analogy, we construct discrete analogues of Tulczyjew’s triple that are derived from properties of symplectic maps between discrete analogues of the iterated tangent and cotangent bundles. We then demonstrate that they yield discrete Lagrange–Dirac and nonholonomic Hamiltonian systems, and recover nonholonomic integrators that are typically derived from a discrete Lagrange–d’Alembert principle.

We also introduce discrete analogues of the Lagrange–d’Alembert–Pontryagin and Hamilton–d’Alembert variational principles, which provide a variational characterization of discrete Lagrange–Dirac and nonholonomic Hamiltonian systems that we previously described in terms of the discrete analogues of Tulczyjew’s triple and induced Dirac structures. The discrete Lagrange–Dirac and nonholonomic Hamiltonian systems recover the standard Lagrangian variational integrators (see, e.g., Marsden and West [36]), Hamiltonian variational integrators of Lall and West [29], and nonholonomic integrators (see, e.g., Cortés and Martínez [11] and McLachlan and Perlmutter [38]).

Discrete Hamiltonian mechanics [29] is not intrinsic, due to its dependence on Type 2 or 3 generating functions of symplectic maps. Since discrete Dirac mechanics encompasses discrete Hamiltonian mechanics, we first limit our discussions to the cases where the configuration manifold Q is a vector space. We then introduce a retraction, a map from TQ to Q , to extend the ideas to the more general case where Q is a manifold. Specifically, we extend the Lagrange–d’Alembert–Pontryagin principle to this case, and show that it yields, using a certain class of coordinate charts specified by the retraction, the same coordinate expressions for Lagrange–Dirac systems as in the linear case. This gives a firm theoretical foundation and a prescription for performing computations with Lagrange–Dirac systems on manifolds.

Outline of this paper. The paper is organized as follows. In Section 2, we review induced Dirac structures, Tulczyjew’s triple, and Lagrange–Dirac systems with an LC circuit as a motivating example. In Sections 3 and 4, we construct discrete analogues of Tulczyjew’s triple and induced Dirac structures. These discrete analogues lead us to the development of discrete Dirac mechanics, i.e., discrete Lagrange–Dirac and nonholonomic Hamiltonian systems, in Section 5. We then come back to the LC circuit example in Section 6: We discretize the LC circuit and describe it as a discrete Lagrange–Dirac system to obtain a numerical method; we also test the method numerically and compare the result with an exact solution. In Section 7, we briefly come back to the continuous-time setting to review the Lagrange–d’Alembert–Pontryagin and Hamilton–d’Alembert principles for Lagrange–Dirac and nonholonomic Hamiltonian systems. Then, in Section 8, we define the discrete analogues of the variational principles. In Section 9, we extend our results to computations on manifolds.

2. DIRAC STRUCTURES, TULCZYJEV'S TRIPLE, AND LAGRANGE–DIRAC SYSTEMS

We first briefly review the induced Dirac structures that give rise to Lagrange–Dirac systems, taking an LC circuit as an example (see [50, 51, 53]). Lagrange–Dirac systems are particularly useful in formulating systems with degenerate Lagrangians and/or constraints. LC circuits are a class of examples that is particularly well suited for the formulation as Lagrange–Dirac systems, since they often involve degenerate Lagrangians and also constraints arising from the Kirchhoff laws.

2.1. LC Circuit—Example of Degenerate Lagrangian System with Constraints. Following Yoshimura and Marsden [50], consider the LC circuit with an inductor ℓ and three capacitors c_1, c_2 , and c_3 shown in Fig. 1. The configuration space is the 4-dimensional vector

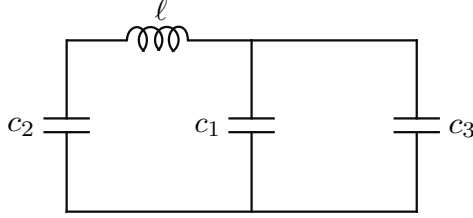


FIGURE 1. LC circuit—Example of degenerate Lagrangian system with constraints (see [50]).

space $Q = \{(q^\ell, q^{c_1}, q^{c_2}, q^{c_3})\}$, which represents charges in the circuit elements. Then, an element $f_q = (f^\ell, f^{c_1}, f^{c_2}, f^{c_3})$ in the tangent space $T_q Q$ represents the currents in the corresponding circuit elements; hence the tangent bundle TQ is a charge-current space. The Lagrangian $L : TQ \rightarrow \mathbb{R}$ is given by

$$L(q, f) = \frac{\ell}{2}(f^\ell)^2 - \frac{(q^{c_1})^2}{2c_1} - \frac{(q^{c_2})^2}{2c_2} - \frac{(q^{c_3})^2}{2c_3}. \quad (2.1)$$

The Lagrangian is clearly degenerate:

$$\det \left(\frac{\partial^2 L}{\partial f^i \partial f^j} \right) = 0,$$

which corresponds to the fact that not every circuit component has inductance. Therefore, the Legendre transformation $\mathbb{F}L : TQ \rightarrow T^*Q$, with T^*Q being the cotangent bundle of Q , defined by

$$\mathbb{F}L : f \mapsto \frac{\partial L}{\partial f^i} dq^i$$

is not invertible, and hence it is impossible to write the system as a Hamiltonian system in the conventional sense. Notice also that the Kirchhoff current law imposes the constraints $-f^\ell + f^{c_2} = 0$ and $-f^{c_1} + f^{c_2} - f^{c_3} = 0$. This defines the constraint distribution $\Delta_Q \subset TQ$ given by

$$\Delta_Q = \{f \in TQ \mid \omega^a(f) = 0, a = 1, 2\}, \quad (2.2)$$

with the constraint one-forms $\{\omega^1, \omega^2\}$ defined as

$$\omega^1 = -dq^\ell + dq^{c_2}, \quad \omega^2 = -dq^{c_1} + dq^{c_2} - dq^{c_3}. \quad (2.3)$$

Then, one can write the constraints simply as $f \in \Delta_Q$. If we introduce the annihilator distribution (or codistribution) $\Delta_Q^\circ \subset T^*Q$ of $\Delta_Q \subset TQ$ by

$$\Delta_Q^\circ(q) := \{\alpha_q \in T_q^*Q \mid \forall v_q \in \Delta_Q, \langle \alpha_q, v_q \rangle = 0\}, \quad (2.4)$$

then we have $\Delta_Q^\circ = \text{span}\{\omega^1, \omega^2\}$.

2.2. Induced Dirac Structures. The key idea in formulating Lagrange–Dirac systems for systems with constraints like the above LC circuits is to introduce a Dirac structure induced by the above constraints. Let us first recall the basic definitions and results following Yoshimura and Marsden [50].

Definition 2.1 (Dirac Structures on Vector Spaces). Let V be a vector space and V^* be its dual. For a subspace $D \subset V \oplus V^*$, we define

$$D^\perp := \{(v, \alpha) \in V \oplus V^* \mid \langle \alpha', v \rangle + \langle \alpha, v' \rangle = 0 \text{ for any } (v', \alpha') \in D\}, \quad (2.5)$$

where $\langle \cdot, \cdot \rangle : V^* \times V \rightarrow \mathbb{R}$ is the natural pairing. A subspace D of $V \oplus V^*$ is called a *Dirac structure* on V if $D^\perp = D$.

This definition naturally extends to manifolds:

Definition 2.2 (Dirac Structures on Manifolds). Let M be a manifold and TM and T^*M be its tangent and cotangent bundles. For a subbundle $D \subset TM \oplus T^*M$, we define

$$D^\perp := \{(v, \alpha) \in TM \oplus T^*M \mid \langle \alpha', v \rangle + \langle \alpha, v' \rangle = 0 \text{ for any } (v', \alpha') \in D\}, \quad (2.6)$$

where \oplus is the Whitney sum, and $\langle \cdot, \cdot \rangle : T^*M \times TM \rightarrow \mathbb{R}$ is the natural pairing. A subbundle D over M of $TM \oplus T^*M$ is called a (*generalized*) *Dirac structure* on M if $D^\perp = D$.

A particularly important class of Dirac structures is the *induced Dirac structure* on a cotangent bundle defined in the following way: Let Q be a manifold, $\pi_Q : T^*Q \rightarrow Q$ be the cotangent bundle projection, and $\Omega^b : TT^*Q \rightarrow T^*T^*Q$ be the flat map associated with the standard symplectic structure Ω on T^*Q .

Proposition 2.3 (The Induced Dirac Structure on T^*Q ; see [14, 44, 50]). *Given a constant-dimensional distribution $\Delta_Q \subset TQ$ on Q , define the lifted distribution*

$$\Delta_{T^*Q} := (T\pi_Q)^{-1}(\Delta_Q) \subset TT^*Q, \quad (2.7)$$

and let $\Delta_{T^*Q}^\circ \subset T^*T^*Q$ be its annihilator, which is also given by $\Delta_{T^*Q}^\circ = \pi_Q^*(\Delta_Q^\circ)$. Then, the subbundle $D_{\Delta_Q} \subset TT^*Q \oplus T^*T^*Q$ defined by

$$D_{\Delta_Q} := \left\{ (v, \alpha) \in TT^*Q \oplus T^*T^*Q \mid v \in \Delta_{T^*Q}, \alpha - \Omega^b(v) \in \Delta_{T^*Q}^\circ \right\} \quad (2.8)$$

is a Dirac structure on T^*Q .

In the above LC circuit example, the Kirchhoff current law constraints Δ_Q in Eq. (2.2) induce the Dirac structure D_{Δ_Q} . In coordinates, we write an element in T^*Q as (q, p) with $p = (p_\ell, p_{c_1}, p_{c_2}, p_{c_3})$ and then by noting that $\Omega = dq \wedge dp$, we have

$$D_{\Delta_Q}(q, p) = \{(\dot{q}, \dot{p}, \alpha_q, \alpha_p) \in TT^*Q \oplus T^*T^*Q \mid \dot{q} \in \Delta_Q, \dot{q} = \alpha_p, \dot{p} + \alpha_q \in \Delta_Q^\circ\},$$

where $\Delta_Q^\circ \subset T^*Q$ is the annihilator of Δ_Q defined in Eq. (2.4).

2.3. Tulczyjew's Triple. Following Tulczyjew [42, 43] and Yoshimura and Marsden [50], let us introduce Tulczyjew's triple, i.e., the diffeomorphisms Ω^b , κ_Q , and $\gamma_Q := \Omega^b \circ \kappa_Q^{-1}$ defined between the iterated tangent and cotangent bundles as follows.

$$\begin{array}{ccccc}
 & & \xrightarrow{\gamma_Q} & & \\
 T^*TQ & \xleftarrow{\kappa_Q} & TT^*Q & \xrightarrow{\Omega^b} & T^*T^*Q \\
 \searrow \pi_{TQ} & & \searrow T\pi_Q & & \searrow \tau_{T^*Q} \\
 & & TQ & & T^*Q \\
 & & \swarrow \pi_{T^*Q} & & \swarrow \pi_{T^*Q}
 \end{array} \quad (2.9a)$$

$$\begin{array}{ccccc}
 (q, \delta q, \delta p, p) & \longleftarrow & (q, p, \delta q, \delta p) & \longrightarrow & (q, p, -\delta p, \delta q) \\
 & \swarrow & \nearrow & \swarrow & \nearrow \\
 & (q, \delta q) & & (q, p) &
 \end{array} \tag{2.9b}$$

The maps Ω^b and κ_Q induce symplectic forms on TT^*Q in the following way: Let $\Theta_{T^*T^*Q}$ and Θ_{T^*TQ} be standard symplectic one-forms on the cotangent bundles T^*T^*Q and T^*TQ , respectively. One defines one-forms χ and λ on TT^*Q by

$$\chi := (\Omega^b)^* \Theta_{T^*T^*Q} = -\delta p dq + \delta q dp, \quad \lambda := (\kappa_Q)^* \Theta_{T^*TQ} = \delta p dq + p d(\delta q),$$

and, using these one-forms, define the two-form Ω_{TT^*Q} on TT^*Q by

$$\Omega_{TT^*Q} := -d\lambda = d\chi = dq \wedge d(\delta p) + d(\delta q) \wedge dp.$$

Then, this gives a symplectic form on TT^*Q .

2.4. Lagrange–Dirac Systems. To define a Lagrange–Dirac system, it is necessary to introduce the Dirac differential of a Lagrangian function: Given a Lagrangian $L : TQ \rightarrow \mathbb{R}$, we define the *Dirac differential* $\mathfrak{D}L : TQ \rightarrow T^*T^*Q$ by

$$\mathfrak{D}L := \gamma_Q \circ dL.$$

In local coordinates,

$$\mathfrak{D}L(q, v) = \left(q, \frac{\partial L}{\partial v}, -\frac{\partial L}{\partial q}, v \right).$$

Now we are ready to define a Lagrange–Dirac system:

Definition 2.4 (Lagrange–Dirac Systems). Suppose that a Lagrangian $L : TQ \rightarrow \mathbb{R}$ and a Dirac structure $D \subset TT^*Q \oplus T^*T^*Q$ are given. Let $X \in \mathfrak{X}(T^*Q)$ be a vector field on T^*Q . Then a *Lagrange–Dirac system* is defined by

$$(X, \mathfrak{D}L) \in D. \tag{2.10}$$

In particular, if D is the induced Dirac structure D_{Δ_Q} given in Eq. (2.8), the Lagrange–Dirac system can be written as follows:

$$T\pi_Q(X) \in \Delta_Q, \quad \Omega^b(X) - \mathfrak{D}L \in \Delta_{T^*Q}^\circ,$$

or in local coordinates, by setting $X = \dot{q} \partial_q + \dot{p} \partial_p$,

$$\dot{q} \in \Delta_Q, \quad \dot{q} = v, \quad p = \frac{\partial L}{\partial v}, \quad \dot{p} - \frac{\partial L}{\partial q} \in \Delta_Q^\circ. \tag{2.11}$$

Example 2.5 (LC circuit). With the Dirac structure D_{Δ_Q} in Eq. (2.8) induced by the constraints Δ_Q in Eq. (2.2), the Lagrange–Dirac system $(X, \mathfrak{D}L) \in D_{\Delta_Q}$ gives

$$\dot{q} \in \Delta_Q, \quad \dot{q} = f, \quad p = \frac{\partial L}{\partial f}, \quad \dot{p} - \frac{\partial L}{\partial q} = \mu_1 \omega^1 + \mu_2 \omega^2 \tag{2.12a}$$

with the Lagrange multipliers $\mu_1, \mu_2 \in \mathbb{R}$; to be more explicit,

$$\begin{aligned}
 \dot{q}^\ell &= \dot{q}^{c_2}, & \dot{q}^{c_1} &= \dot{q}^{c_2} - \dot{q}^{c_3}, \\
 \dot{q}^\ell &= f^\ell, & \dot{q}^{c_1} &= f^{c_1}, & \dot{q}^{c_2} &= f^{c_2}, & \dot{q}^{c_3} &= f^{c_3}, \\
 p_\ell &= \ell f^\ell, & p_{c_1} &= p_{c_2} = p_{c_3} = 0, \\
 \dot{p}_\ell &= -\mu_1, & \dot{p}_{c_1} + \frac{q^{c_1}}{c_1} &= -\mu_2, & \dot{p}_{c_2} + \frac{q^{c_2}}{c_2} &= \mu_1 + \mu_2, & \dot{p}_{c_3} + \frac{q^{c_3}}{c_3} &= -\mu_2.
 \end{aligned} \tag{2.12b}$$

This formulation recovers the equations given by circuit theory.

Remark 2.6. Notice that this formulation by Yoshimura and Marsden [50] does not use the Kirchhoff voltage law; it instead uses the Kirchhoff current law with the symplectic structure on T^*Q to define the Dirac structure $D_{\Delta_Q} \subset TT^*Q \oplus T^*T^*Q$. On the other hand, the formulation by Bloch and Crouch [7] and van der Schaft [44] uses the Dirac structure $D \subset TP \oplus T^*P$, with a different configuration space P , defined by *both* the Kirchhoff voltage and current laws, without using any additional geometric (symplectic) structure.

2.5. Implicit and Nonholonomic Hamiltonian Systems. One can define an implicit Hamiltonian system in an analogous way as shown by van der Schaft [44] and Dalsmo and van der Schaft [14]:

Definition 2.7. Suppose that a Hamiltonian $H : T^*Q \rightarrow \mathbb{R}$ and a Dirac structure $D \subset TT^*Q \oplus T^*T^*Q$ are given. Let $X \in \mathfrak{X}(T^*Q)$ be a vector field on T^*Q . Then an *implicit Hamiltonian system (IHS)* is defined by

$$(X, dH) \in D.$$

In particular, if D is the induced Dirac structure D_{Δ_Q} given in Eq. (2.8), the IHS gives the *nonholonomic Hamilton's equations* (see, e.g., Bates and Sniatycki [4], van der Schaft and Maschke [46], and Koon and Marsden [27]):

$$T\pi_Q(X) \in \Delta_Q, \quad \Omega^b(X) - dH \in \Delta_{T^*Q}^\circ,$$

or in local coordinates, by setting $X = \dot{q} \partial_q + \dot{p} \partial_p$,

$$\dot{q} \in \Delta_Q, \quad \dot{q} = \frac{\partial H}{\partial p}, \quad \dot{p} + \frac{\partial H}{\partial q} \in \Delta_Q^\circ.$$

To keep the exposition in this section concise, we will not go into details about IHS here. We would like to point the reader to the references cited above for details and examples of IHS.

3. DISCRETE ANALOGUES OF TULCZYJEW'S TRIPLE

In this section, we construct discrete analogues of Tulczyjew's triple shown in Eq. (2.9) that retain the key geometric properties, especially the symplecticity of the maps involved. This makes it possible to formulate a natural structure-preserving discrete analogue of Lagrange–Dirac systems. The discussion here is limited to the case where the configuration space Q is a vector space.

To give the big picture of what we would like to do in this section, constructing a discrete analogue of Tulczyjew's triple involves replacing, for example, the tangent bundle TQ in Eq. (2.9) by the product $Q \times Q$ in accordance with the basic idea of discrete mechanics (see, e.g., [36]); likewise TT^*Q is replaced by $T^*Q \times T^*Q$; the role of T^*Q in discrete mechanics is quite subtle in general, but since Q is assumed to be a vector space, we can replace it with $Q \times Q^*$. Fig. 2 gives a rough picture of a discrete analogue of Tulczyjew's triple. We work out the details of how to obtain the maps κ_Q^d and Ω_d^b in the sections to follow. The guiding principle here is to make use of

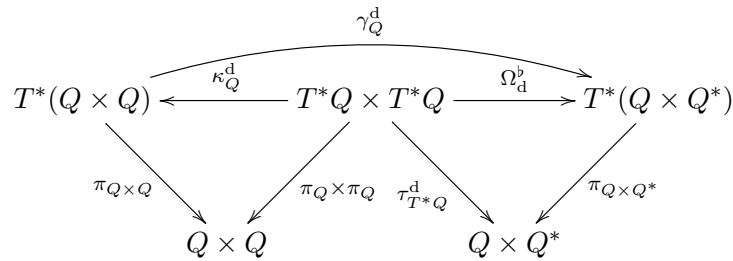


FIGURE 2. A rough picture of a discrete analogue of Tulczyjew's triple.

symplectic maps associated with generating functions instead of smooth symplectic flows.

3.1. Discrete Mechanics and Generating Functions. Let us first review some basic facts on generating functions. Consider a map $F : T^*Q \rightarrow T^*Q$ written as $(q_0, p_0) \mapsto (q_1, p_1)$. Note that, since Q is assumed to be a vector space here, the cotangent bundle is trivial, i.e., $T^*Q \cong Q \times Q^*$, and so one can write $F : Q \times Q^* \rightarrow Q \times Q^*$ as well. One then considers the following four maps associated with F :

- (i) $F_1 : Q \times Q \rightarrow Q^* \times Q^*$; $(q_0, q_1) \mapsto (p_0, p_1)$,
- (ii) $F_2 : Q \times Q^* \rightarrow Q^* \times Q$; $(q_0, p_1) \mapsto (p_0, q_1)$,
- (iii) $F_3 : Q^* \times Q \rightarrow Q \times Q^*$; $(p_0, q_1) \mapsto (q_0, p_1)$,
- (iv) $F_4 : Q^* \times Q^* \rightarrow Q \times Q$; $(p_0, p_1) \mapsto (q_0, q_1)$.

The Type i generating function with $i = 1, 2, 3, 4$ (using the terminology set by Goldstein et al. [19]) is a scalar function S_i defined on the range of the map F_i that exists if and only if the map F is symplectic. Let us look at the first three cases (the fourth one is not important here) and their relationship to discrete analogues of the map κ_Q and Ω^b in the sections to follow.

3.2. Generating Function of Type 1 and the Map κ_Q^d . This section relates the Type 1 generating function with a discrete analogue κ_Q^d of the map κ_Q in Tulczyjew's triple, Eq. (2.9).

First, we regard (p_0, p_1) as functions of (q_0, q_1) as indicated in the definition of the map F_1 above, and then define $i_{F_1} : Q \times Q \rightarrow T^*Q \times T^*Q$ by

$$i_{F_1} : (q_0, q_1) \mapsto ((q_0, p_0), (q_1, p_1)) \quad \text{where} \quad (p_0, p_1) = F_1(q_0, q_1).$$

Now recall that the map $F : (q_0, p_0) \mapsto (q_1, p_1)$ is symplectic if and only if $dq_0 \wedge dp_0 = dq_1 \wedge dp_1$, or equivalently $d(-p_0 dq_0 + p_1 dq_1) = 0$. Then, the Poincaré lemma states that this is true if and only if there exists some function $S_1 : Q \times Q \rightarrow \mathbb{R}$, a *Type 1 generating function*, such that

$$-p_0 dq_0 + p_1 dq_1 = dS_1(q_0, q_1).$$

This relates the (p_0, p_1) with the generating function S_1 :

$$p_0 = -D_1 S_1(q_0, q_1), \quad p_1 = D_2 S_1(q_0, q_1). \quad (3.1)$$

Then, this gives rise to the map $\kappa_Q^d : T^*Q \times T^*Q \rightarrow T^*(Q \times Q)$ so that the diagram

$$\begin{array}{ccc} T^*Q \times T^*Q & \xrightarrow{\kappa_Q^d} & T^*(Q \times Q) \\ \swarrow i_{F_1} & & \nearrow dS_1 \\ Q \times Q & & \end{array} \quad \begin{array}{ccc} ((q_0, p_0), (q_1, p_1)) & \mapsto & (q_0, q_1, -p_0, p_1) \\ \swarrow & & \nearrow \\ (q_0, q_1) & & \end{array} \quad (3.2)$$

commutes, i.e., we obtain

$$\kappa_Q^d : ((q_0, p_0), (q_1, p_1)) \mapsto (q_0, q_1, -p_0, p_1). \quad (3.3)$$

3.3. Generating Function of Type 2 and the Map Ω_{d+}^b . Next, we would like to relate the Type 2 generating function with one of the two discrete analogues of the map Ω^b in Tulczyjew's triple, Eq. (2.9).

First, we regard (p_0, q_1) as functions of (q_0, p_1) as indicated in the definition of the map F_2 above, and then define $i_{F_2} : Q \times Q^* \rightarrow T^*Q \times T^*Q$ by

$$i_{F_2} : (q_0, p_1) \mapsto ((q_0, p_0), (q_1, p_1)) \quad \text{where} \quad (p_0, q_1) = F_2(q_0, p_1).$$

The map $F : (q_0, p_0) \mapsto (q_1, p_1)$ is symplectic if and only if $dq_0 \wedge dp_0 = dq_1 \wedge dp_1$, or equivalently $d(p_0 dq_0 + q_1 dp_1) = 0$. Then, the Poincaré lemma states that this is true if and only if there exists some function $S_2 : Q \times Q^* \rightarrow \mathbb{R}$, a *Type 2 generating function*, such that

$$p_0 dq_0 + q_1 dp_1 = dS_2(q_0, p_1).$$

This relates the (p_0, q_1) with the generating function S_2 :

$$p_0 = D_1 S_2(q_0, p_1), \quad q_1 = D_2 S_2(q_0, p_1). \quad (3.4)$$

Then, this gives rise to the map $\Omega_{d+}^b : T^*Q \times T^*Q \rightarrow T^*(Q \times Q^*)$ so that the diagram

$$\begin{array}{ccc} T^*Q \times T^*Q & \xrightarrow{\Omega_{d+}^b} & T^*(Q \times Q^*) & ((q_0, p_0), (q_1, p_1)) \mapsto & (q_0, p_1, p_0, q_1) \\ & \swarrow i_{F_2} & \nearrow dS_2 & & \swarrow \searrow \\ & & Q \times Q^* & & (q_0, p_1) \end{array} \quad (3.5)$$

commutes, i.e., we obtain

$$\Omega_{d+}^b : ((q_0, p_0), (q_1, p_1)) \mapsto (q_0, p_1, p_0, q_1). \quad (3.6)$$

3.4. Generating Function of Type 3 and the Map Ω_{d-}^b . The other discrete analogue of the map Ω^b follows from the Type 3 generating function.

In this case, we regard (q_0, p_1) as functions of (p_0, q_1) as indicated in the definition of the map F_3 above, and then define $i_{F_3} : Q^* \times Q \rightarrow T^*Q \times T^*Q$ by

$$i_{F_3} : (p_0, q_1) \mapsto ((q_0, p_0), (q_1, p_1)) \quad \text{where} \quad (q_0, p_1) = F_3(p_0, q_1).$$

The map $F : (q_0, p_0) \mapsto (q_1, p_1)$ is symplectic if and only if $dq_0 \wedge dp_0 = dq_1 \wedge dp_1$, or equivalently $d(-q_0 dp_0 - p_1 dq_1) = 0$. Then, again by the Poincaré lemma, this is true if and only if there exists some function $S_3 : Q^* \times Q \rightarrow \mathbb{R}$ such that

$$-q_0 dp_0 - p_1 dq_1 = dS_3(p_0, q_1).$$

This relates the (q_0, p_1) with the generating function S_3 :

$$q_0 = -D_1 S_3(p_0, q_1), \quad p_1 = -D_2 S_3(p_0, q_1). \quad (3.7)$$

Then, this gives rise to the map $\Omega_{d-}^b : T^*Q \times T^*Q \rightarrow T^*(Q^* \times Q)$ so that the diagram

$$\begin{array}{ccc} T^*Q \times T^*Q & \xrightarrow{\Omega_{d-}^b} & T^*(Q^* \times Q) & ((q_0, p_0), (q_1, p_1)) \mapsto & (p_0, q_1, -q_0, -p_1) \\ & \swarrow i_{F_3} & \nearrow dS_3 & & \swarrow \searrow \\ & & Q^* \times Q & & (p_0, q_1) \end{array} \quad (3.8)$$

commutes, i.e., we obtain

$$\Omega_{d-}^b : ((q_0, p_0), (q_1, p_1)) \mapsto (p_0, q_1, -q_0, -p_1). \quad (3.9)$$

3.5. (+)-Discrete Tulczyjew Triple. Combining the diagrams in Eqs. (3.2) and (3.5), we obtain the following (+)-discrete Tulczyjew triple.

$$\begin{array}{ccccc} & & \gamma_Q^{d+} & & \\ & & \curvearrowright & & \\ T^*(Q \times Q) & \xleftarrow{\kappa_Q^d} & T^*Q \times T^*Q & \xrightarrow{\Omega_{d+}^b} & T^*(Q \times Q^*) \\ & \searrow \pi_{Q \times Q} & \swarrow \pi_{Q \times \pi_Q} & \searrow \tau_{T^*Q}^{d+} & \swarrow \pi_{Q \times Q^*} \\ & & Q \times Q & & Q \times Q^* \end{array} \quad (3.10a)$$

$$\begin{array}{ccccc}
 (q_0, q_1, -p_0, p_1) & \longleftarrow & ((q_0, p_0), (q_1, p_1)) & \longrightarrow & (q_0, p_1, p_0, q_1) \\
 \swarrow & & \swarrow & & \swarrow \\
 & & (q_0, q_1) & & (q_0, p_1)
 \end{array} \tag{3.10b}$$

The maps κ_Q^d and Ω_{d+}^b inherit the properties of κ_Q and Ω^b discussed in Section 2.3 in the following sense: Let $\Theta_{T^*(Q \times Q^*)}$ and $\Theta_{T^*(Q \times Q)}$ be the symplectic one-forms on $T^*(Q \times Q^*)$ and $T^*(Q \times Q)$, respectively. The maps κ_Q^d and Ω_{d+}^b induce two symplectic one-forms on $T^*Q \times T^*Q$. One is

$$\chi_{d+} := (\Omega_{d+}^b)^* \Theta_{T^*(Q \times Q^*)} = p_0 dq_0 + q_1 dp_1,$$

and the other is

$$\lambda_{d+} := (\kappa_Q^d)^* \Theta_{T^*(Q \times Q)} = -p_0 dq_0 + p_1 dq_1.$$

Then, using these one-forms, define the two-form $\Omega_{T^*Q \times T^*Q}$ by

$$\Omega_{T^*Q \times T^*Q} = -d\lambda_{d+} = d\chi_{d+} = dq_1 \wedge dp_1 - dq_0 \wedge dp_0.$$

This is a natural symplectic form defined on the product of two cotangent bundles (see Abraham and Marsden [1, Proposition 5.2.1 on p. 379]).

3.6. (-)-Discrete Tulczyjew Triple. Combining the diagrams in Eqs. (3.2) and (3.8), we obtain the following (-)-discrete Tulczyjew triple.

$$\begin{array}{ccccc}
 & & \gamma_Q^{d-} & & \\
 & \xrightarrow{\kappa_Q^d} & & \xrightarrow{\Omega_{d-}^b} & \\
 T^*(Q \times Q) & \longleftarrow & T^*Q \times T^*Q & \longrightarrow & T^*(Q^* \times Q) \\
 \swarrow \pi_{Q \times Q} & & \swarrow \pi_Q \times \pi_Q & & \swarrow \pi_{Q^* \times Q} \\
 & & Q \times Q & & Q^* \times Q
 \end{array} \tag{3.11a}$$

$$\begin{array}{ccccc}
 (q_0, q_1, -p_0, p_1) & \longleftarrow & ((q_0, p_0), (q_1, p_1)) & \longrightarrow & (p_0, q_1, -q_0, -p_1) \\
 \swarrow & & \swarrow & & \swarrow \\
 & & (q_0, q_1) & & (p_0, q_1)
 \end{array} \tag{3.11b}$$

As in the (+)-discrete case, the maps κ_Q^d and Ω_{d-}^b inherit the properties of κ_Q and Ω^b : Let $\Theta_{T^*(Q^* \times Q)}$ be the symplectic one-form on $T^*(Q^* \times Q)$. Then, we have

$$\chi_{d-} := (\Omega_{d-}^b)^* \Theta_{T^*(Q^* \times Q)} = -p_1 dq_1 - q_0 dp_0,$$

and

$$\lambda_{d-} := (\kappa_Q^d)^* \Theta_{T^*(Q \times Q)} = -p_0 dq_0 + p_1 dq_1.$$

Then, they induce the same symplectic form $\Omega_{T^*Q \times T^*Q}$ as above:

$$\Omega_{T^*Q \times T^*Q} := -d\lambda_{d-} = d\chi_{d-} = dq_1 \wedge dp_1 - dq_0 \wedge dp_0.$$

4. DISCRETE ANALOGUES OF INDUCED DIRAC STRUCTURES

Recall from Section 2.2 that, given a constraint distribution $\Delta_Q \subset TQ$, we first defined the distribution $\Delta_{T^*Q} \subset TT^*Q$ and then constructed the induced Dirac structure $D_{\Delta_Q} \subset TT^*Q \oplus T^*T^*Q$. This section develops a discrete analogue of this construction.

4.1. Discrete constraint distributions. Given the fact that the tangent bundle TQ is replaced by the product $Q \times Q$ in the discrete setting, a natural discrete analogue of a constraint distribution $\Delta_Q \subset TQ$ is a subset $\Delta_Q^d \subset Q \times Q$. We follow the approach of Cortés and Martínez [11] (see also McLachlan and Perlmutter [38]) to construct discrete constraints $\Delta_Q^d \subset Q \times Q$ based on given (continuous) constraints $\Delta_Q \subset TQ$.

Let $\Delta_Q^\circ \subset T^*Q$ be the annihilator distribution (or codistribution) of $\Delta_Q \subset TQ$ and $m := \dim T_q Q - \dim \Delta_Q(q)$ for each $q \in Q$. Then, one can find a set of m constraint one-forms $\{\omega^a\}_{a=1}^m$ that spans the annihilator:

$$\Delta_Q^\circ = \text{span}\{\omega^a\}_{a=1}^m.$$

In local coordinates, we may write

$$\omega^a(q, v) = A_i^a(q)v^i, \quad (4.1)$$

where $(A_i^a(q))$ is an $m \times n$ full-rank matrix for each $q \in Q$, i.e., $\text{rank } A(q) = m$.

Then, using the one-forms ω^a and a retraction $\mathcal{R} : TQ \rightarrow Q$ (see Section 9.1), we define functions $\omega_{d\pm}^a : Q \times Q \rightarrow \mathbb{R}$ by

$$\omega_{d+}^a(q_0, q_1) := \omega^a(q_0, \mathcal{R}_{q_0}^{-1}(q_1)), \quad \omega_{d-}^a(q_0, q_1) := \omega^a(q_1, -\mathcal{R}_{q_1}^{-1}(q_0)), \quad (4.2)$$

and then define the discrete constraints $\Delta_Q^{d\pm} \subset Q \times Q$ as follows:

$$\Delta_Q^{d\pm} := \{(q_0, q_1) \in Q \times Q \mid \omega_{d\pm}^a(q_0, q_1) = 0, a = 1, 2, \dots, m\}. \quad (4.3)$$

The following proposition suggests that it is natural to think of q_1 as a discrete analogue of the velocity $v_{q_0} \in T_{q_0}Q$ when imposing the constraint $(q_0, q_1) \in \Delta_Q^{d+}$, and q_0 a discrete analogue of $v_{q_1} \in T_{q_1}Q$ when imposing $(q_0, q_1) \in \Delta_Q^{d-}$:

Proposition 4.1. *The discrete constraints defined by $(q_0, q_1) \in \Delta_Q^{d\pm} \subset Q \times Q$ are constraints only on the variable q_1 and q_0 , respectively; i.e., $\text{pr}_1(\Delta_Q^{d+}) = Q$ and $\text{pr}_2(\Delta_Q^{d-}) = Q$, where $\text{pr}_i : Q \times Q \rightarrow Q$ with $i = 1, 2$ is the projection to the i -th component.*

Proof. Let $\omega : TQ \rightarrow \mathbb{R}^m$ be the map defined by

$$\omega(q, v) := (\omega^1(q, v), \dots, \omega^m(q, v)),$$

and $\omega_{d+} : Q \times Q \rightarrow \mathbb{R}^m$ be the map defined by

$$\omega_{d+}(q_0, q_1) := (\omega_{d+}^1(q_0, q_1), \dots, \omega_{d+}^m(q_0, q_1)).$$

In the first equation in Eq. (4.2), take the derivative respect to q_1 to obtain

$$\begin{aligned} D_2\omega_{d+}(q_0, q_1) &= D_2\omega(q_0, \mathcal{R}_{q_0}^{-1}(q_1)) \cdot D\mathcal{R}_{q_0}^{-1}(q_1) \\ &= A(q_0) \cdot D\mathcal{R}_{q_0}^{-1}(q_1), \end{aligned}$$

where we used the coordinate expression for ω in Eq. (4.1). Since $D\mathcal{R}_{q_0}^{-1}$ is an invertible matrix (see Remark 9.2) and $\text{rank } A = m$, we find that $\text{rank } D_2\omega_{d+} = m$. Therefore, by the implicit function theorem, we may (locally) rewrite the constraints $\omega_{d+}(q_0, q_1) = 0$ as $q_1^{i_l} = f^l(q_0, q_1^{j_1}, \dots, q_1^{j_{n-m}})$ with some function $f^l : \mathbb{R}^n \times \mathbb{R}^{n-m} \rightarrow \mathbb{R}^m$ for $l = 1, \dots, m$, where $\{i_1, \dots, i_m\} \cup \{j_1, \dots, j_{n-m}\} = \{1, 2, \dots, n\}$ and $\{i_1, \dots, i_m\} \cap \{j_1, \dots, j_{n-m}\} = \emptyset$. Hence q_0 is a free variable and so the claim follows. Similarly for ω_{d-} . \square

Next, we introduce discrete analogues of the distribution $\Delta_{T^*Q} \subset TT^*Q$ using the discrete constraint $\Delta_Q^{d\pm}$ defined above. Natural discrete analogues of Δ_{T^*Q} would be $\Delta_{T^*Q}^{d\pm} \subset T^*Q \times T^*Q$ defined by

$$\Delta_{T^*Q}^{d\pm} := (\pi_Q \times \pi_Q)^{-1}(\Delta_Q^{d\pm}) = \left\{ ((q_0, p_0), (q_1, p_1)) \in T^*Q \times T^*Q \mid (q_0, q_1) \in \Delta_Q^{d\pm} \right\},$$

which is analogous to the continuous distribution $\Delta_{T^*Q} := (T\pi_Q)^{-1}(\Delta_Q)$ in Eq. (2.7).

We will also need discrete analogues of the annihilator $\Delta_{T^*Q}^\circ$ defined in Eq. (2.7); natural discrete analogues of it would be annihilator distributions on $Q \times Q^*$ and $Q^* \times Q$. We use the projections $\pi_Q^{\text{d}+} : Q \times Q^* \rightarrow Q$ and $\pi_Q^{\text{d}-} : Q^* \times Q \rightarrow Q$ to define annihilator distributions $\Delta_{Q \times Q^*}^\circ \subset T^*(Q \times Q^*)$ and $\Delta_{Q^* \times Q}^\circ \subset T^*(Q^* \times Q)$ as follows:

$$\begin{aligned}\Delta_{Q \times Q^*}^\circ &:= (\pi_Q^{\text{d}+})^*(\Delta_Q^\circ) = \{(q, p, \alpha_q, 0) \in T^*(Q \times Q^*) \mid \alpha_q dq \in \Delta_Q^\circ(q)\}, \\ \Delta_{Q^* \times Q}^\circ &:= (\pi_Q^{\text{d}-})^*(\Delta_Q^\circ) = \{(p, q, 0, \alpha_q) \in T^*(Q^* \times Q) \mid \alpha_q dq \in \Delta_Q^\circ(q)\},\end{aligned}$$

which is analogous to the expression for the continuous annihilator distribution $\Delta_{T^*Q}^\circ = \pi_Q^*(\Delta_Q^\circ)$.

4.2. Discrete Induced Dirac Structures. Now we are ready to define discrete analogues of the induced Dirac structures D_{Δ_Q} shown in Proposition 2.3.

Definition 4.2 (Discrete Induced Dirac Structures). Given a discrete constraint distribution $\Delta_Q^{\text{d}+} \subset Q \times Q$, we define the (+)-discrete induced Dirac structure as follows:

$$\begin{aligned}D_{\Delta_Q}^{\text{d}+} &:= \left\{ ((z, z^+), \alpha_{\hat{z}}) \in (T^*Q \times T^*Q) \times T^*(Q \times Q^*) \mid \right. \\ &\quad \left. (z, z^+) \in \Delta_{T^*Q}^{\text{d}+}, \alpha_{\hat{z}} - \Omega_{\text{d}+}^{\text{b}}(z, z^+) \in \Delta_{Q \times Q^*}^\circ \right\},\end{aligned}$$

where if $z = (q, p)$ and $z^+ = (q^+, p^+)$ then $\hat{z} := (q, p^+) \in Q \times Q^*$. Likewise, given a discrete constraint distribution $\Delta_Q^{\text{d}-} \subset Q \times Q$, we define the (-)-discrete induced Dirac structure as follows:

$$\begin{aligned}D_{\Delta_Q}^{\text{d}-} &:= \left\{ ((z^-, z), \alpha_{\tilde{z}}) \in (T^*Q \times T^*Q) \times T^*(Q^* \times Q) \mid \right. \\ &\quad \left. (z^-, z) \in \Delta_{T^*Q}^{\text{d}-}, \alpha_{\tilde{z}} - \Omega_{\text{d}-}^{\text{b}}(z^-, z) \in \Delta_{Q^* \times Q}^\circ \right\},\end{aligned}$$

where if $z = (q, p)$ and $z^- = (q^-, p^-)$ then $\tilde{z} := (p^-, q) \in Q^* \times Q$.

5. DISCRETE DIRAC MECHANICS

Now that we have discrete analogues of both Tulczyjew's triple and induced Dirac structures at our disposal, we are ready to define discrete analogues of Lagrange–Dirac and nonholonomic Hamiltonian systems. As we shall see, two types of discrete Lagrange–Dirac/nonholonomic Hamiltonian systems will follow from the (\pm)-discrete Tulczyjew triples and (\pm)-discrete induced Dirac structures.

5.1. (+)-Discrete Dirac Mechanics.

5.1.1. (+)-Discrete Lagrange–Dirac Systems. Let us first introduce a discrete analogue of the Dirac differential: Define $\gamma_Q^{\text{d}+} : T^*(Q \times Q) \rightarrow T^*(Q \times Q^*)$ by

$$\gamma_Q^{\text{d}+} := \Omega_{\text{d}+}^{\text{b}} \circ (\kappa_Q^{\text{d}})^{-1},$$

and, for a given discrete Lagrangian $L_{\text{d}} : Q \times Q \rightarrow \mathbb{R}$, define the (+)-discrete Dirac differential $\mathfrak{D}^+ L_{\text{d}} : Q \times Q \rightarrow T^*(Q \times Q^*)$ by

$$\mathfrak{D}^+ L_{\text{d}} := \gamma_Q^{\text{d}+} \circ dL_{\text{d}}.$$

In coordinates, we have

$$\mathfrak{D}^+ L_{\text{d}}(q_k, q_k^+) = (q_k, D_2 L_{\text{d}}, -D_1 L_{\text{d}}, q_k^+).$$

Definition 5.1 ((+)-Discrete Lagrange–Dirac System). Suppose that a discrete Lagrangian $L_d : Q \times Q \rightarrow \mathbb{R}$ and the constraint distribution $\Delta_Q \subset TQ$ are given; and so Eq. (4.3) gives the discrete constraint distribution $\Delta_Q^{d+} \subset Q \times Q$. Let

$$X_d^k = ((q_k, p_k), (q_{k+1}, p_{k+1})) \in T^*Q \times T^*Q \quad (5.1)$$

be a discrete analogue of a vector field on T^*Q . Then, a (+)-discrete Lagrange–Dirac system is a triple (L_d, Δ_Q, X_d) with

$$\left(X_d^k, \mathfrak{D}^+ L_d(q_k, q_k^+) \right) \in D_{\Delta_Q}^{d+}. \quad (5.2)$$

Remark 5.2. The variable q_k^+ in Eq. (5.2) is a discrete analogue of v in Eq. (2.11). See Proposition 4.1.

Let us find a coordinate expression for a (+)-discrete Lagrange–Dirac system: Eq. (5.2) gives

$$(q_k, q_{k+1}) \in \Delta_Q^{d+}, \quad \mathfrak{D}^+ L_d - \Omega_{d+}^b(X_d^k) \in \Delta_{Q \times Q^*}^{\circ},$$

where

$$\Omega_{d+}^b(X_d^k) = (q_k, p_{k+1}, p_k, q_{k+1}).$$

Thus, we obtain the following set of equations:

$$\begin{aligned} (q_k, q_{k+1}) &\in \Delta_Q^{d+}, & q_{k+1} &= q_k^+, \\ p_{k+1} &= D_2 L_d(q_k, q_k^+), & p_k + D_1 L_d(q_k, q_k^+) &\in \Delta_Q^{\circ}(q_k), \end{aligned} \quad (5.3a)$$

or more explicitly, with the Lagrange multipliers μ_a ,

$$\begin{aligned} \omega_{d+}^a(q_k, q_{k+1}) &= 0, & q_{k+1} &= q_k^+, \\ p_{k+1} &= D_2 L_d(q_k, q_k^+), & p_k + D_1 L_d(q_k, q_k^+) &= \mu_a \omega^a(q_k), \end{aligned} \quad (5.3b)$$

where $a = 1, 2, \dots, m$. We shall call them the (+)-discrete Lagrange–Dirac equations; they recover the nonholonomic integrator of Cortés and Martínez [11] (see also McLachlan and Perlmutter [38]).

Consider the special case $\Delta_Q = TQ$. In this case, $\Delta_Q^{d+} = Q \times Q$ and $\Delta_Q^{\circ} = 0$, and so the above equations reduce to

$$q_{k+1} = q_k^+, \quad p_{k+1} = D_2 L_d(q_k, q_k^+), \quad p_k = -D_1 L_d(q_k, q_k^+). \quad (5.4)$$

These are equivalent to the discrete Euler–Lagrange equations (see Marsden and West [36]).

5.1.2. (+)-Discrete Nonholonomic Hamiltonian System. A nonholonomic discrete Hamiltonian system is defined analogously:

Definition 5.3 ((+)-Discrete Nonholonomic Hamiltonian System). Suppose that a (+)-discrete Hamiltonian (referred to as the right discrete Hamiltonian in [29]) $H_{d+} : Q \times Q^* \rightarrow \mathbb{R}$ and the constraint distribution $\Delta_Q \subset TQ$ are given; and so Eq. (4.3) gives the discrete constraint distribution $\Delta_Q^{d+} \subset Q \times Q$. Let X_d^k be a discrete analogue of a vector field on T^*Q as in Eq. (5.1). Then, a (+)-discrete nonholonomic Hamiltonian system is a triple (H_{d+}, Δ_Q, X_d) with

$$\left(X_d^k, dH_{d+}(q_k, p_{k+1}) \right) \in D_{\Delta_Q}^{d+}. \quad (5.5)$$

A coordinate expression is obtained in a similar way:

$$(q_k, q_{k+1}) \in \Delta_Q^{d+}, \quad q_{k+1} = D_2 H_{d+}(q_k, p_{k+1}), \quad p_k - D_1 H_{d+}(q_k, p_{k+1}) \in \Delta_Q^{\circ}(q_k), \quad (5.6a)$$

or more explicitly

$$\omega_{d+}^a(q_k, q_{k+1}) = 0, \quad q_{k+1} = D_2 H_{d+}(q_k, p_{k+1}), \quad p_k - D_1 H_{d+}(q_k, p_{k+1}) = \mu_a \omega^a(q_k), \quad (5.6b)$$

where $a = 1, 2, \dots, m$. We shall call them the (+)-discrete nonholonomic Hamilton's equations.

If $\Delta_Q = TQ$, then $\Delta_Q^{\text{d}+} = Q \times Q$ and $\Delta_Q^\circ = 0$; and so the above equations reduce to

$$q_{k+1} = D_2 H_{\text{d}+}(q_k, p_{k+1}), \quad p_k = D_1 H_{\text{d}+}(q_k, p_{k+1}), \quad (5.7)$$

which are the right discrete Hamilton's equations in Lall and West [29].

5.2. (-)-Discrete Dirac Mechanics.

5.2.1. *(-)-Discrete Lagrange–Dirac Systems.* Let us first introduce the (-)-version of the Dirac differential: Define $\gamma_Q^{\text{d}-} : T^*(Q \times Q) \rightarrow T^*(Q^* \times Q)$ by

$$\gamma_Q^{\text{d}-} := \Omega_{\text{d}-}^{\text{b}} \circ (\kappa_Q^{\text{d}})^{-1},$$

and, for a given discrete Lagrangian $L_{\text{d}} : Q \times Q \rightarrow \mathbb{R}$, define the (-)-discrete Dirac differential $\mathfrak{D}^- L_{\text{d}} : Q \times Q \rightarrow T^*(Q^* \times Q)$ by

$$\mathfrak{D}^- L_{\text{d}} := \gamma_Q^{\text{d}-} \circ dL_{\text{d}}.$$

In coordinates, we have

$$\mathfrak{D}^- L_{\text{d}}(q_{k+1}^-, q_{k+1}) = (-D_1 L_{\text{d}}, q_{k+1}, -q_{k+1}^-, -D_2 L_{\text{d}}).$$

Definition 5.4 ((-)-Discrete Lagrange–Dirac System). Suppose that a discrete Lagrangian $L_{\text{d}} : Q \times Q \rightarrow \mathbb{R}$ and the constraint distribution $\Delta_Q \subset TQ$ are given; and so Eq. (4.3) gives the discrete constraint distribution $\Delta_Q^{\text{d}-} \subset Q \times Q$. Let X_{d}^k be a discrete analogue of a vector field on T^*Q as in Eq. (5.1). Then, a *(-)-discrete Lagrange–Dirac system* is a triple $(L_{\text{d}}, \Delta_Q, X_{\text{d}})$ with

$$\left(X_{\text{d}}^k, \mathfrak{D}^- L_{\text{d}}(q_{k+1}^-, q_{k+1}) \right) \in D_{\Delta_Q^{\text{d}-}}^{\text{d}-}. \quad (5.8)$$

Remark 5.5. The variable q_{k+1}^- in Eq. (5.8) is a discrete analogue of v in Eq. (2.11). See Proposition 4.1.

Let us find a coordinate expression for a (-)-discrete Lagrange–Dirac system: Eq. (5.8) gives

$$(q_k, q_{k+1}) \in \Delta_Q^{\text{d}-}, \quad \mathfrak{D}^- L_{\text{d}} - \Omega_{\text{d}-}^{\text{b}}(X_{\text{d}}^k) \in \Delta_{Q^* \times Q}^\circ,$$

where

$$\Omega_{\text{d}-}^{\text{b}}(X_{\text{d}}^k) = (p_k, q_{k+1}, -q_k, -p_{k+1}).$$

Thus, we obtain the following set of equations:

$$\begin{aligned} (q_k, q_{k+1}) &\in \Delta_Q^{\text{d}-}, & q_k &= q_{k+1}^-, \\ p_k &= -D_1 L_{\text{d}}(q_{k+1}^-, q_{k+1}), & p_{k+1} - D_2 L_{\text{d}}(q_{k+1}^-, q_{k+1}) &\in \Delta_Q^\circ(q_{k+1}), \end{aligned} \quad (5.9\text{a})$$

or more explicitly

$$\begin{aligned} \omega_{\text{d}-}^a(q_k, q_{k+1}) &= 0, & q_k &= q_{k+1}^-, \\ p_k &= -D_1 L_{\text{d}}(q_{k+1}^-, q_{k+1}), & p_{k+1} - D_2 L_{\text{d}}(q_{k+1}^-, q_{k+1}) &= \mu_a \omega^a(q_{k+1}), \end{aligned} \quad (5.9\text{b})$$

where $a = 1, 2, \dots, m$. We shall call them the *(-)-discrete Lagrange–Dirac equations*; they again recover the nonholonomic integrator of Cortés and Martínez [11] (see also McLachlan and Perlmutter [38]).

If $\Delta_Q = TQ$, then $\Delta_Q^{\text{d}-} = Q \times Q$ and $\Delta_Q^\circ = 0$; and so the above equations reduce to

$$q_k = q_{k+1}^-, \quad p_k = -D_1 L_{\text{d}}(q_{k+1}^-, q_{k+1}), \quad p_{k+1} = D_2 L_{\text{d}}(q_{k+1}^-, q_{k+1}). \quad (5.10)$$

This is a slightly different (but equivalent) expression for Eq. (5.4).

5.2.2. *(-)-Discrete Nonholonomic Hamiltonian System.* The corresponding discrete nonholonomic Hamiltonian system is defined analogously:

Definition 5.6 ((-)-Discrete Nonholonomic Hamiltonian System). Suppose that a (-)-discrete Hamiltonian (referred to as the left discrete Hamiltonian in [29]) $H_{d-} : Q^* \times Q \rightarrow \mathbb{R}$ and the constraint distribution $\Delta_Q \subset TQ$ are given; and so Eq. (4.3) gives the discrete constraint distribution $\Delta_Q^{d-} \subset Q \times Q$. Let X_d^k be a discrete analogue of a vector field on T^*Q as in Eq. (5.1). Then, a *(-)-discrete nonholonomic Hamiltonian system* is a triple (H_{d-}, Δ_Q, X_d) with

$$\left(X_d^k, dH_{d-}(p_k, q_{k+1}) \right) \in D_{\Delta_Q}^{d-}. \quad (5.11)$$

A coordinate expression is obtained in a similar way: We obtain the following set of equations, which we shall call the *(-)-discrete nonholonomic Hamilton's equations*:

$$(q_k, q_{k+1}) \in \Delta_Q^{d-}, \quad q_k = -D_1 H_{d-}(p_k, q_{k+1}), \quad p_{k+1} + D_2 H_{d-}(p_k, q_{k+1}) \in \Delta_Q^\circ(q_{k+1}), \quad (5.12a)$$

or more explicitly

$$\omega_{d-}^a(q_k, q_{k+1}) = 0, \quad q_k = -D_1 H_{d-}(p_k, q_{k+1}), \quad p_{k+1} + D_2 H_{d-}(p_k, q_{k+1}) = \mu_a \omega^a(q_{k+1}), \quad (5.12b)$$

where $a = 1, 2, \dots, m$.

If $\Delta_Q = TQ$, then $\Delta_Q^{d-} = Q \times Q$ and $\Delta_Q^\circ = 0$; and so the above equations reduce to

$$q_k = -D_1 H_{d-}(p_k, q_{k+1}), \quad p_{k+1} = -D_2 H_{d-}(p_k, q_{k+1}), \quad (5.13)$$

which are the left discrete Hamilton's equations in Lall and West [29].

6. EXAMPLE OF DISCRETE LAGRANGE–DIRAC SYSTEM—LC CIRCUIT

6.1. **Formulation.** We apply the above formulation of discrete Dirac mechanics, in particular discrete Lagrange–Dirac systems, to the LC circuit example from Section 2.

Choose the retraction $\mathcal{R} : TQ \rightarrow Q$ (see Section 9.1 for more details) defined by

$$\mathcal{R}_q(v) := q + vh, \quad (6.1)$$

where h is the time step; hence we have

$$\mathcal{R}_{q_0}^{-1}(q_1) = \frac{q_1 - q_0}{h}.$$

Then, we define the discrete Lagrangian $L_d : Q \times Q \rightarrow \mathbb{R}$ in terms of the continuous Lagrangian, Eq. (2.1), as follows:

$$\begin{aligned} L_d(q_k, q_k^+) &:= h L(q_k, \mathcal{R}_{q_k}^{-1}(q_k^+)) \\ &= h \left[\frac{\ell}{2} \left(\frac{q_k^{+, \ell} - q_k^\ell}{h} \right)^2 - \sum_{i=1}^3 \frac{(q_k^{c_i})^2}{2c_i} \right]. \end{aligned} \quad (6.2)$$

This is a discretization that corresponds to the symplectic Euler method (see, e.g., [36]).

We also introduce the discrete constraints Δ_Q^{d+} using Eq. (4.2) with the original constraint one-forms $\{\omega^1, \omega^2\}$ given in Eq. (2.3):

$$\omega_{d+}^a(q_k, q_{k+1}) := \langle \omega^a(q_k), \mathcal{R}_{q_k}^{-1}(q_{k+1}) \rangle.$$

Simple computations show that

$$\begin{aligned} \omega_{d+}^1(q_k, q_{k+1}) &= \frac{1}{h} \left[-(q_{k+1}^\ell - q_k^\ell) + (q_{k+1}^{c_2} - q_k^{c_2}) \right], \\ \omega_{d+}^2(q_k, q_{k+1}) &= \frac{1}{h} \left[-(q_{k+1}^{c_1} - q_k^{c_1}) + (q_{k+1}^{c_2} - q_k^{c_2}) - (q_{k+1}^{c_3} - q_k^{c_3}) \right]. \end{aligned}$$

Then, Eq. (4.3) gives

$$\begin{aligned} \Delta_Q^{d+} &:= \{(q_k, q_{k+1}) \in Q \times Q \mid \omega_{d+}^a(q_k, q_{k+1}) = 0, a = 1, 2\} \\ &= \{(q_k, q_{k+1}) \in Q \times Q \mid -q_{k+1}^\ell + q_{k+1}^{c_2} = -q_k^\ell + q_k^{c_2}, \\ &\quad -q_{k+1}^{c_1} + q_{k+1}^{c_2} - q_{k+1}^{c_3} = -q_k^{c_1} + q_k^{c_2} - q_k^{c_3}\}. \end{aligned}$$

Note that the original constraints are holonomic, i.e., the one-forms ω^a are exact, and the above expression for the discrete constraints are the integral form of the original constraints.

Then the (+)-discrete Lagrange–Dirac equations (5.3) give

$$\begin{aligned} q_{k+1}^\ell - q_k^\ell &= q_{k+1}^{c_2} - q_k^{c_2}, & q_{k+1}^{c_1} - q_k^{c_1} &= (q_{k+1}^{c_2} - q_k^{c_2}) - (q_{k+1}^{c_3} - q_k^{c_3}), \\ q_{k+1}^\ell &= q_k^{+, \ell}, & q_{k+1}^{c_i} &= q_k^{+, c_i} \quad (i = 1, 2, 3), \\ p_{\ell, k+1} &= \ell \frac{q_k^{+, \ell} - q_k^\ell}{h}, & p_{c_i, k+1} &= 0 \quad (i = 1, 2, 3), \\ p_{\ell, k} - \ell \frac{q_k^{+, \ell} - q_k^\ell}{h} &= -\mu_1, \\ p_{c_i, k} - \frac{h q_k^{+, c_i}}{2c_i} &= -\mu_2 \quad (i = 1, 3), & p_{c_2, k} - \frac{h q_k^{+, c_2}}{2c_2} &= \mu_1 + \mu_2, \end{aligned} \tag{6.3}$$

where μ_a are Lagrange multipliers, and we used the fact that $\Delta_Q^\circ = \text{span}\{\omega^1, \omega^2\}$ with ω^1 and ω^2 defined in Eq. (2.3).

6.2. Numerical Result. Assume the initial condition

$$q^\ell(0) = q^{c_1}(0) = q^{c_2}(0) = q^{c_3}(0) = 0, \quad \dot{q}^\ell(0) = \dot{q}^{c_2}(0) = 10, \quad \dot{q}^{c_1}(0) = \dot{q}^{c_3}(0) = 0.$$

Applying elementary circuit theory to the example, we obtain the exact solution

$$q_{\text{ex}}^\ell(t) = \frac{10}{c} \sin ct,$$

where

$$c := \sqrt{\frac{c_1 + c_2 + c_3}{c_2(c_1 + c_3)L}},$$

and thus the period of the solution is $T := 2\pi/c$. With the choice of the parameters

$$\ell = \frac{3}{4}, \quad c_1 = 1, \quad c_2 = 2, \quad c_3 = 3,$$

we have $c = 1$, and so the period T becomes 2π .

Fig. 3 compares the exact solution with the numerical solution for time step size $h = 2\pi/40 \simeq 0.157$, i.e., 40 time intervals per period.

Table 1 shows how the error at $t = 5T = 10\pi$ converges as N , the number of time intervals per period, increases. The method clearly exhibits second-order convergence behavior, whereas the discretization corresponds to the symplectic Euler method, which is first-order accurate.

TABLE 1. Convergence of numerical method: Number of time intervals per period N vs. Error at $t = 5T = 10\pi$.

N	20	40	80	160
$ q_{5N}^\ell - q_{\text{ex}}^\ell(5T) $	1.31915	0.324829	0.0808631	0.0201938

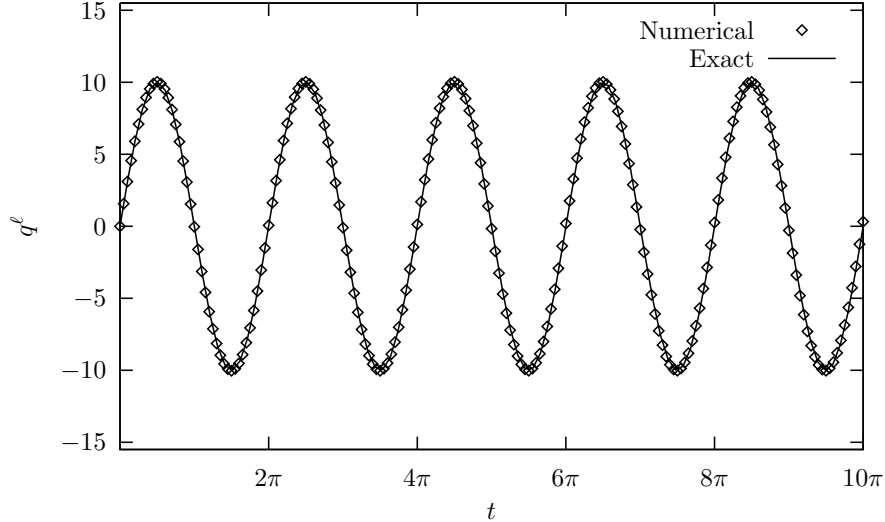


FIGURE 3. Comparison of exact and numerical solutions (40 points per period) for LC circuit.

Remark 6.1. One possible explanation for the second-order convergence rate is the following: As one can see from Eq. (6.3), the $\{q_k^\ell\}$ are the only variables explicitly involved with the time evolution¹ and the other variables could be determined from the constraints. Since $\{q_k^\ell\}$ are not present in the potential term in the discrete Lagrangian, Eq. (6.2), only the first term (that corresponds to the inductance energy or “kinetic energy” with the electrical-mechanical analogy) is relevant to the time evolution. However, since the coefficient of this term is constant, the approximation of the “kinetic energy” term in the discrete Lagrangian, Eq. (6.2), is the same as that of the midpoint rule, i.e., the approximation given by the discrete Lagrangian of the form

$$L_d^{\text{MP}}(q_k, q_k^+) = h L \left(\frac{q_k + q_k^+}{2}, \frac{q_k^+ - q_k}{h} \right),$$

which yields a second-order accurate method.

Remark 6.2. Eliminating p and μ from Eq. (2.12), we obtain

$$\ell \ddot{q}^\ell = -\frac{q^{c_3}}{c_3} - \frac{q^{c_2}}{c_2}, \quad \dot{q}^{c_2} = \dot{q}^\ell, \quad (c_1 + c_3) \dot{q}^{c_3} = c_3 \dot{q}^{c_2},$$

If we apply the central difference approximation to \ddot{q}^ℓ and forward difference to all the first-order derivatives in the above equations, we obtain the same numerical method defined by Eq. (6.3) (after p_k and μ are eliminated).

In this paper, we do not delve into the issue of accuracy of the numerical methods defined by discrete Lagrange–Dirac systems, instead, we leave it as a topic for future studies.

7. VARIATIONAL STRUCTURE FOR LAGRANGE–DIRAC AND NONHOLONOMIC HAMILTONIAN SYSTEMS

In this section we briefly come back to the continuous setting discussed in Section 2 to review variational formulations of Lagrange–Dirac and nonholonomic Hamiltonian systems, again following Yoshimura and Marsden [51]. This section is a precursor to the development of the corresponding discrete analogues to follow in the next section.

¹This is due to the fact that the original Lagrangian, Eq. (2.1), is degenerate, i.e., its f -dependence is only through ℓ -component f^ℓ .

7.1. Lagrange–d’Alembert–Pontryagin Principle and Lagrange–Dirac Systems.

Definition 7.1. Suppose that a Lagrangian $L : TQ \rightarrow \mathbb{R}$ and a constraint distribution $\Delta_Q \subset TQ$ are given. The *Lagrange–d’Alembert–Pontryagin principle* is the augmented variational principle on the *Pontryagin bundle* $TQ \oplus T^*Q$ defined by

$$\delta \int_a^b [L(q, v) + p(\dot{q} - v)] dt = 0, \quad (7.1)$$

with the constraint $\dot{q} \in \Delta_Q$; we assume that the variation δq vanishes at the endpoints, i.e., $\delta q(a) = \delta q(b) = 0$, and also impose $\delta q \in \Delta_Q$ *after* taking the variations inside the integral sign.

The Lagrange–Dirac system follows from the Lagrange–d’Alembert–Pontryagin principle: In a local trivialization, Q is represented by an open set U in a linear space E , so the Pontryagin bundle is represented by $(U \times E) \oplus (U \times E^*) \cong U \times E \times E^*$, with local coordinates (q, v, p) . If we consider q, v , and p as independent variables, we have that,

$$\begin{aligned} \delta \int_a^b [L(q, v) + p(\dot{q} - v)] dt &= \int_a^b \left[\frac{\partial L}{\partial q} \delta q + \left(\frac{\partial L}{\partial v} - p \right) \delta v + (\dot{q} - v) \delta p + p \delta \dot{q} \right] dt \\ &= \int_a^b \left[\left(\frac{\partial L}{\partial q} - \dot{p} \right) \delta q + \left(\frac{\partial L}{\partial v} - p \right) \delta v + (\dot{q} - v) \delta p \right] dt, \end{aligned}$$

where we used integration by parts, and the fact that the variation δq vanishes at the endpoints. Taking account of the constraints $\delta q \in \Delta_Q$, Eq. (7.1) gives the Lagrange–Dirac equation (2.11):

$$\dot{q} \in \Delta_Q, \quad \dot{q} = v, \quad p = \frac{\partial L}{\partial v}, \quad \dot{p} - \frac{\partial L}{\partial q} \in \Delta_Q^\circ. \quad (7.2)$$

7.2. Hamilton–d’Alembert Principle in Phase Space and Nonholonomic Hamiltonian Systems.

Definition 7.2. Suppose that a Hamiltonian $H : T^*Q \rightarrow \mathbb{R}$ and a constraint distribution $\Delta_Q \subset TQ$ are given. The *Hamilton–d’Alembert principle in phase space* is the variational principle defined by

$$\delta \int_a^b [p \dot{q} - H(q, p)] dt = 0, \quad (7.3)$$

with the constraint $\dot{q} \in \Delta_Q$; we assume that the variation δq vanishes at the endpoints, i.e., $\delta q(a) = \delta q(b) = 0$, and also impose $\delta q \in \Delta_Q$ *after* taking the variations inside the integral sign.

The nonholonomic Hamiltonian system follows from the Hamilton–d’Alembert principle in phase space: Eq. (7.3) gives

$$\begin{aligned} 0 &= \delta \int_a^b [p \dot{q} - H(q, p)] dt = \int_a^b \left(\dot{q} \delta p + p \delta \dot{q} - \frac{\partial H}{\partial q} \delta q - \frac{\partial H}{\partial p} \delta p \right) dt \\ &= \int_a^b \left[\left(-\dot{p} - \frac{\partial H}{\partial q} \right) \delta q + \left(\dot{q} - \frac{\partial H}{\partial p} \right) \delta p \right] dt, \end{aligned}$$

which, under the constraints $\delta q \in \Delta_Q$, yields

$$\dot{q} \in \Delta_Q, \quad \dot{q} = \frac{\partial H}{\partial p}, \quad \dot{p} + \frac{\partial H}{\partial q} \in \Delta_Q^\circ. \quad (7.4)$$

8. DISCRETE VARIATIONAL STRUCTURE FOR DISCRETE LAGRANGE–DIRAC AND NONHOLONOMIC HAMILTONIAN SYSTEMS

This section develops discrete analogues of the variational structure discussed in the last section. It is shown that the discrete versions of Lagrange–d’Alembert–Pontryagin principle and Hamilton–d’Alembert principle in phase space yield discrete Lagrange–Dirac and nonholonomic Hamiltonian systems, respectively.

8.1. Discrete Pontryagin Bundles. Let us first introduce discrete analogues of the Pontryagin bundle $TQ \oplus T^*Q$:

Definition 8.1 ((\pm)-Discrete Pontryagin Bundles). The ($+$)-discrete Pontryagin bundle is defined by

$$(Q \times Q) \oplus (Q \times Q^*) = \{((q_k, q_k^+), (q_k, p_{k+1}))\},$$

or, by identifying the first Q of each, we have

$$(Q \times Q) \oplus (Q \times Q^*) \cong Q \times Q \times Q^* = \{(q_k, q_k^+, p_{k+1})\}.$$

Similarly, the ($-$)-discrete Pontryagin bundle is defined by

$$(Q \times Q) \oplus (Q^* \times Q) = \{((q_{k+1}^-, q_{k+1}), (p_k, q_{k+1}))\},$$

or, by identifying the second Q of each, we have

$$(Q \times Q) \oplus (Q^* \times Q) \cong Q \times Q^* \times Q = \{(q_{k+1}^-, p_k, q_{k+1})\}.$$

8.2. Discrete Lagrange–d’Alembert–Pontryagin Principle and Discrete Lagrange–Dirac Systems.

Definition 8.2 ((\pm)-Discrete Lagrange–d’Alembert–Pontryagin Principle). Suppose that a discrete Lagrangian $L_d : Q \times Q \rightarrow \mathbb{R}$ and the constraint distribution $\Delta_Q \subset TQ$ are given; and so Eq. (4.3) gives the discrete constraint distributions $\Delta_Q^{\text{d}\pm} \subset Q \times Q$. Then, the (\pm)-discrete Lagrange–d’Alembert–Pontryagin principle is the discrete augmented variational principle defined by

$$\delta \sum_{k=0}^{N-1} [L_d(q_k, q_k^+) + p_{k+1}(q_{k+1} - q_k^+)] = 0 \quad (8.1)$$

or

$$\delta \sum_{k=0}^{N-1} [L_d(q_{k+1}^-, q_{k+1}) - p_k(q_k - q_{k+1}^-)] = 0, \quad (8.2)$$

with the constraint $(q_k, q_{k+1}) \in \Delta_Q^{\text{d}\pm}$ respectively; we assume that the variations δq_k vanish at the endpoints, i.e., $\delta q_0 = \delta q_N = 0$, and also impose $\delta q_k \in \Delta_Q(q_k)$ after taking the variations inside the summation.

Proposition 8.3. *The (\pm)-discrete Lagrange–d’Alembert–Pontryagin principles yield the (\pm)-discrete Lagrange–Dirac equations (5.3) and (5.9), respectively.*

Proof. First taking the variations in Eqs. (8.1) and (8.2), we have

$$\begin{aligned} 0 &= \delta \sum_{k=0}^{N-1} [L_d(q_k, q_k^+) + p_{k+1}(q_{k+1} - q_k^+)] \\ &= \sum_{k=1}^{N-1} [D_1 L_d(q_k, q_k^+) + p_k] \delta q_k + \sum_{k=0}^{N-1} \{ [D_2 L_d(q_k, q_k^+) - p_{k+1}] \delta q_k^+ + (q_{k+1} - q_k^+) \delta p_{k+1} \}, \end{aligned}$$

and

$$\begin{aligned}
 0 &= \delta \sum_{k=0}^{N-1} [L_d(q_{k+1}^-, q_{k+1}) - p_k(q_k - q_{k+1}^-)] \\
 &= \sum_{k=0}^{N-2} [D_2 L_d(q_{k+1}^-, q_{k+1}) - p_{k+1}] \delta q_{k+1} \\
 &\quad + \sum_{k=0}^{N-1} \{ [D_1 L_d(q_{k+1}^-, q_{k+1}) + p_k] \delta q_{k+1}^- + (q_{k+1}^- - q_k) \delta p_k \},
 \end{aligned}$$

where we used $\delta q_0 = 0$ and $\delta q_N = 0$. Taking account of the corresponding constraints on the variations in each of the above equations, we obtain Eqs. (5.3) and (5.9), respectively. \square

8.3. Discrete Hamilton–d’Alembert Principle in Phase Space and Discrete Nonholonomic Hamiltonian Systems.

Definition 8.4 ((\pm)-Discrete Hamilton–d’Alembert Principle in Phase Space). Suppose that a (\pm)-discrete Hamiltonian $H_{d+} : Q \times Q^* \rightarrow \mathbb{R}$ or $H_{d-} : Q^* \times Q \rightarrow \mathbb{R}$ and the constraint distribution $\Delta_Q \subset TQ$ are given; and so Eq. (4.3) gives the discrete constraint distributions $\Delta_Q^{d\pm} \subset Q \times Q$. Then, the (\pm)-discrete Hamilton–d’Alembert principle in phase space is the discrete variational principle defined by

$$\delta \sum_{k=0}^{N-1} [p_{k+1} q_{k+1} - H_{d+}(q_k, p_{k+1})] = 0 \tag{8.3}$$

or

$$\delta \sum_{k=0}^{N-1} [-p_k q_k - H_{d-}(p_k, q_{k+1})] = 0, \tag{8.4}$$

with the constraint $(q_k, q_{k+1}) \in \Delta_Q^{d\pm}$ respectively; we assume that the variations δq_k vanish at the endpoints, i.e., $\delta q_0 = \delta q_N = 0$, and also impose $\delta q_k \in \Delta_Q(q_k)$ after taking the variations inside the summation.

Proposition 8.5. *The (\pm)-discrete Hamilton–d’Alembert principles yield the (\pm)-discrete nonholonomic Hamilton’s equations (5.6) and (5.12), respectively.*

Proof. First taking the variations in Eqs. (8.3) and (8.4), we have

$$\begin{aligned}
 0 &= \delta \sum_{k=0}^{N-1} [p_{k+1} q_{k+1} - H_{d+}(q_k, p_{k+1})] \\
 &= \sum_{k=0}^{N-1} [q_{k+1} - D_2 H_{d+}(q_k, p_{k+1})] \delta p_{k+1} + \sum_{k=1}^{N-1} [p_k - D_1 H_{d+}(q_k, p_{k+1})] \delta q_k
 \end{aligned}$$

and

$$\begin{aligned}
 0 &= \delta \sum_{k=0}^{N-1} [-p_k q_k - H_{d-}(p_k, q_{k+1})] \\
 &= - \sum_{k=0}^{N-1} [q_k + D_1 H_{d-}(p_k, q_{k+1})] \delta p_k - \sum_{k=0}^{N-2} [p_{k+1} + D_2 H_{d-}(p_k, q_{k+1})] \delta q_{k+1},
 \end{aligned}$$

where we used $\delta q_0 = 0$ and $\delta q_N = 0$. Taking account of the constraints on the variations δq_k in each of the above equations, we obtain Eqs. (5.6) and (5.12), respectively. \square

9. EXTENSION TO COMPUTATIONS ON MANIFOLDS

This section presents a means to apply the preceding theory to computations for the case when Q is a manifold. We do not attempt a full extension of the theory to manifolds since discrete Hamiltonian mechanics [29] is not intrinsic: Recall that the (+)-discrete Hamiltonian H_{d+} is a Type 2 generating function (see Lall and West [29] and also Section 3.1), which is based on the idea of generating the pair (p_0, q_1) with the pair (q_0, p_1) fixed. However, this does not make intrinsic sense, since fixing p_1 in T^*Q requires that its corresponding base point q_1 is fixed as well.

Instead, we make use of the idea of retractions and introduce the notion of retraction compatible coordinate charts to provide a means of applying the results in the linear theory to computations on manifolds, in a semi-globally compatible fashion. Retraction compatible coordinate charts provide a generalization of the canonical coordinates of the first kind on Lie groups (see, e.g., Varadarajan [48, Section 2.10] and also Example 9.5 below) to more general configuration manifolds. By semi-global, we mean that the discrete flow is well-defined on a neighborhood of the diagonal of $Q \times Q$, which corresponds to a restriction on the size of the time step.

In particular, on a retraction compatible coordinate chart, the discrete flow is described, in local coordinates, by the vector space expressions. This has non-trivial implications for geometric numerical integration, since naïvely applying a linear space numerical integrator on different charts may lead to poor global properties, as discussed in [5]. By restricting ourselves to retraction compatible coordinate charts, we ensure that the local conservation properties of the geometric numerical integrators we introduce in this paper persist globally as well.

9.1. Retractions. Let us first recall the definition of a retraction:

Definition 9.1 (Absil et al. [2, Definition 4.1.1 on p. 55]). A retraction on a manifold Q is a smooth mapping $\mathcal{R} : TQ \rightarrow Q$ with the following properties: Let $\mathcal{R}_q : T_qQ \rightarrow Q$ be the restriction of \mathcal{R} to T_qQ for an arbitrary $q \in Q$; then,

- (i) $\mathcal{R}_q(0_q) = q$, where 0_q denotes the zero element of T_qQ ;
- (ii) with the identification $T_{0_q}T_qQ \simeq T_qQ$, \mathcal{R}_q satisfies

$$T_{0_q}\mathcal{R}_q = \text{id}_{T_qQ}, \quad (9.1)$$

where $T_{0_q}\mathcal{R}_q$ is the tangent map of \mathcal{R}_q at $0_q \in T_qQ$.

Remark 9.2. Eq. (9.1) implies that the map $\mathcal{R}_q : T_qQ \rightarrow Q$ is invertible in some neighborhood of 0_q in T_qQ .

It is convenient to introduce $\tilde{\mathcal{R}} : TQ \rightarrow Q \times Q$ defined by

$$\tilde{\mathcal{R}}(v_q) := (q, \mathcal{R}_q(v_q)). \quad (9.2)$$

It is easy to see from the above expression and the above remark that $\tilde{\mathcal{R}} : TQ \rightarrow Q \times Q$ is also invertible in some neighborhood of $0_q \in TQ$ for any $q \in Q$.

Let us introduce a special class of coordinate charts that are convenient to work with:

Definition 9.3 (Retraction compatible coordinate charts and atlas). Let Q be an n -dimensional manifold equipped with a retraction $\mathcal{R} : TQ \rightarrow Q$. A coordinate chart (U, φ) with U an open subset in Q and $\varphi : U \rightarrow \mathbb{R}^n$ is said to be *retraction compatible at $q \in U$* if

- (i) φ is centered at q , i.e., $\varphi(q) = 0$;
- (ii) the compatibility condition

$$\mathcal{R}(v_q) = \varphi^{-1} \circ T_q\varphi(v_q) \quad (9.3)$$

holds, where we identify $T_0\mathbb{R}^n$ with \mathbb{R}^n as follows: Let $\varphi = (x^1, \dots, x^n)$ with $x^i : U \rightarrow \mathbb{R}$ for $i = 1, \dots, n$. Then

$$v^i \frac{\partial}{\partial x^i} \mapsto (v^1, \dots, v^n), \quad (9.4)$$

where $\partial/\partial x^i$ is the unit vector in the x^i -direction in $T_0\mathbb{R}^n$.

An atlas for the manifold Q is *retraction compatible* if it consists of retraction compatible coordinate charts.

Remark 9.4. In Eq. (9.3), we assumed that $T_q\varphi(v_q) \in \varphi(U) \subset \mathbb{R}^n$ and so strictly speaking \mathcal{R}_q is defined on $(T_q\varphi)^{-1}(\varphi(U)) \subset T_qQ$. However, it is always possible to define a coordinate chart such that $\varphi(U) = \mathbb{R}^n$ by “stretching out” the open set $\varphi(U)$ to \mathbb{R}^n so that Eq. (9.3) is defined for any $v_q \in T_qQ$.

Example 9.5 (Retraction and canonical coordinates of the first kind on a Lie group). Let G be a (finite-dimensional) Lie group and \mathfrak{g} be its Lie algebra. The exponential map $\exp : \mathfrak{g} \rightarrow G$ (see, e.g., Marsden and Ratiu [35, Section 9.1] and Varadarajan [48, Section 2.10]) is a diffeomorphism on an open neighborhood \mathfrak{u} of the origin of \mathfrak{g} . Let U be the neighborhood of the identity e in G defined by $U := \exp(\mathfrak{u}) \subset G$, and restrict the domain of the exponential map to redefine $\exp : \mathfrak{u} \rightarrow U$ for notational simplicity. Then, it is a diffeomorphism and so we have the inverse $\exp^{-1} : U \rightarrow \mathfrak{u}$.

Now let us define $\mathcal{R}_g : T_gG \rightarrow G$ for any $g \in G$ by²

$$\mathcal{R}_g := L_g \circ \exp \circ T_gL_{g^{-1}},$$

where $L_g : G \rightarrow G$ is the left translation by g . This indeed gives a retraction: Since $\exp(0) = e$, we have $\mathcal{R}_g(0_g) = g$; we also have, with the identification $T_0gT_gG \simeq T_gG$,

$$\begin{aligned} T_0g\mathcal{R}_g &= T_eL_g \circ T_0\exp \circ T_0gT_gL_{g^{-1}} \\ &= T_eL_g \circ T_gL_{g^{-1}} \\ &= \text{id}_{T_gG}, \end{aligned}$$

where we used the fact that $T_0\exp : T\mathfrak{u} \simeq \mathfrak{g} \rightarrow \mathfrak{g}$ is the identity (see [48, Eq. (2.10.17) on p. 88]), and also that $T_0gT_gL_{g^{-1}} = T_gL_{g^{-1}}$ with the above identification³.

The exponential map also induces the *canonical coordinates of the first kind* on the Lie group G as follows (see, e.g., Varadarajan [48, Section 2.10] and Marsden et al. [37]): For any $g \in G$, let $U_g := L_g(U)$ and define a chart $\varphi_g : U_g \rightarrow \mathfrak{g}$ by

$$\varphi_g := \exp^{-1} \circ L_{g^{-1}}.$$

Then, the chart φ_g is retraction compatible: We have

$$\varphi_g(g) = \exp^{-1} \circ L_{g^{-1}}(g) = \exp^{-1}(e) = 0,$$

and also, with the identification $T\mathfrak{u} \simeq \mathfrak{g}$,

$$\begin{aligned} \varphi_g^{-1} \circ T_g\varphi_g &= L_g \circ \exp \circ T_e\exp^{-1} \circ T_gL_{g^{-1}} \\ &= L_g \circ \exp \circ T_gL_{g^{-1}} \\ &= \mathcal{R}_g, \end{aligned}$$

where we used the fact that $T_e\exp^{-1} = \text{id}_{\mathfrak{g}}$, which follows from $T_0\exp = \text{id}_{\mathfrak{g}}$ mentioned above.

Calculations involving a retraction are particularly simple with a retraction compatible chart:

Proposition 9.6. *Let (U, φ) be a retraction compatible chart at a point $q \in U$. Take an arbitrary point r in U and let $(r^1, \dots, r^n) := \varphi(r) \in \mathbb{R}^n$. Then*

$$\mathcal{R}_q^{-1}(r) = r^i \frac{\partial}{\partial x^i} \Big|_q \tag{9.5}$$

²Strictly speaking, \mathcal{R}_g is defined only on $T_eL_g(\mathfrak{u}) \subset T_gG$.

³The derivative of a linear map at the origin is the linear map itself.

where

$$\left. \frac{\partial}{\partial x^i} \right|_q := T_0 \varphi^{-1} \left(\frac{\partial}{\partial x^i} \right) \in T_q Q.$$

Furthermore, let $dx^i|_q \in T_q^* Q$ be the dual basis to $\partial/\partial x^i|_q \in T_q Q$, i.e., $dx^i|_q(\partial/\partial x^j|_q) = \delta_j^i$. Then, for any $p_q = p_i dx^i|_q \in T_q^* Q$, we have

$$\langle p_q, \mathcal{R}_q^{-1}(r) \rangle = \langle p_q, \tilde{\mathcal{R}}^{-1}(q, r) \rangle = p_i r^i, \quad (9.6)$$

where $\langle \cdot, \cdot \rangle$ is the natural pairing between elements in $T^* Q$ and TQ .

Proof. Follows from straightforward calculations. \square

9.2. Discrete Lagrange–d’Alembert–Pontryagin Principles with Retraction. Let us use a retraction to reformulate the (\pm) -discrete Lagrange–d’Alembert–Pontryagin principle, Eq. (8.1), as follows:

Definition 9.7 ((\pm) -Discrete Lagrange–d’Alembert–Pontryagin Principle with Retraction). Suppose that a discrete Lagrangian $L_d : Q \times Q \rightarrow \mathbb{R}$ and the constraint distribution $\Delta_Q \subset TQ$ are given; and so Eq. (4.3) gives the discrete constraint distributions $\Delta_Q^{\pm} \subset Q \times Q$. Then, the (\pm) -discrete Lagrange–d’Alembert–Pontryagin principle is the discrete augmented variational principle defined by

$$\delta S_{d+}^N = \delta \sum_{k=0}^{N-1} \left[L_d(q_k, q_k^+) + \left\langle p_{k+1}, \mathcal{R}_{q_{k+1}}^{-1}(q_{k+1}) - \mathcal{R}_{q_{k+1}}^{-1}(q_k^+) \right\rangle \right] \quad (9.7)$$

or

$$\delta S_{d-}^N = \delta \sum_{k=0}^{N-1} \left[L_d(q_{k+1}^-, q_{k+1}) - \left\langle p_k, \mathcal{R}_{q_k}^{-1}(q_k) - \mathcal{R}_{q_k}^{-1}(q_{k+1}^-) \right\rangle \right], \quad (9.8)$$

with the constraint $(q_k, q_{k+1}) \in \Delta_Q^{\pm}$ respectively; we assume that the variations δq_k vanish at the endpoints, i.e., $\delta q_0 = \delta q_N = 0$, and also impose $\delta q_k \in \Delta_Q(q_k)$ after taking the variations inside the summation.

With a retraction compatible coordinate chart, Lemma 9.6 implies that Eqs. (9.7) and (9.8) become

$$S_{d+}^N = \sum_{k=0}^{N-1} \left[L_d(q_k, q_k^+) + p_{k+1} \cdot (q_{k+1} - q_k^+) \right]$$

and

$$S_{d-}^N = \sum_{k=0}^{N-1} \left[L_d(q_{k+1}^-, q_{k+1}) - p_k \cdot (q_k - q_{k+1}^-) \right],$$

where we slightly abused the notation, i.e., q_{k+1} , q_k^+ , q_{k+1}^- are interpreted as both points in Q as well as their coordinate representations. Therefore the (\pm) -discrete Lagrange–d’Alembert–Pontryagin principle in Definition 9.7, written in terms of retraction compatible charts, reduce to those in the linear theory, i.e., Definition 8.2.

Remark 9.8. Note that $\mathcal{R}_{q_k}^{-1}(q_k) = 0$ by definition, and so the terms of the form

$$\langle p_k, \mathcal{R}_{q_k}^{-1}(q_k) \rangle = p_k \cdot q_k$$

vanish.

The above discussion implies that the discrete Lagrange–Dirac equations (5.3) and (5.9) in the linear theory are coordinate representations (using a retraction compatible chart) of the systems defined by the discrete Lagrange–d’Alembert–Pontryagin principles in Definition 9.7. Therefore, if we have a retraction compatible atlas on Q , then we may use the coordinate expression, Eq. (5.3), in the linear theory to perform a computation in a single chart, and, if necessary, transform the system to another chart in the atlas, which again has the same form as Eq. (5.3), to continue the computation.

10. CONCLUSION

In this paper, we developed the theoretical foundations of discrete Dirac mechanics from two different perspectives: One through discrete analogues of Tulczyjew’s triple and induced Dirac structures, and the other from the variational point of view.

We exploited the discrete Tulczyjew triples to define discrete analogues of the Dirac differential, which is a key in defining the discrete Lagrange–Dirac systems, particularly those with degenerate Lagrangians; and we employed the discrete induced Dirac structures to incorporate discrete constraints. We also introduced extended discrete variational principles, i.e., the discrete Lagrange–d’Alembert–Pontryagin and Hamilton–d’Alembert principles that give variational formulations of discrete Lagrange–Dirac and nonholonomic Hamiltonian systems.

An LC circuit is taken as an example of a system with a degenerate Lagrangian and constraints, and is modeled as a discrete Lagrange–Dirac system. We performed numerical computations with the resulting scheme and obtained numerical solutions that converge to the exact solution obtained by elementary circuit theory.

Several interesting topics for future work are suggested by the theoretical developments introduced in this paper:

- *Application to inter-connected systems.* Port-Hamiltonian systems [45] provide a natural description of modular and interconnected systems, but this does not naturally lead to geometric structure-preserving discretizations of interconnected systems. It is therefore desirable to develop a unified port-Lagrangian framework for modeling and simulating interconnected systems based on extensions of Lagrange–Dirac mechanics and variational discrete Dirac mechanics.
- *Hamilton–Jacobi theory for Lagrange–Dirac systems* (Leok et al. [32]). Since Dirac structures are related to Lagrangian submanifolds, which in turn describe the geometry of the Hamilton–Jacobi equation, it is natural to explore the Dirac description of Hamilton–Jacobi theory. The resulting theory is expected to give insights into discrete Dirac mechanics as the classical Hamilton–Jacobi theory does to discrete mechanics [36, Sections 1.8 and 4.8]; it is also natural to expect it to specialize to nonholonomic Hamilton–Jacobi theory [9, 15, 25, 39, 40].
- *Discrete reduction theory for discrete Dirac mechanics with symmetry.* The Dirac formulation of reduction (see Yoshimura and Marsden [52, 54]) provides a means of unifying symplectic, Poisson, nonholonomic, Lagrangian, and Hamiltonian reduction theory, as well as addressing the issue of reduction by stages. The discrete analogue of Dirac reduction will proceed by considering the issue of quotient discrete Dirac structures, and constructing a category containing discrete Dirac structures, that is closed under quotients.
- *Discrete multi-Dirac mechanics for Hamiltonian partial differential equations.* Dirac generalizations of multisymplectic field theory (see Vankerschaver et al. [47]), and their corresponding discretizations will provide important insights into the construction of geometric numerical methods for degenerate field theories, such as the Einstein equations of general relativity.

- *Variational error analysis of discrete Lagrange–Dirac systems.* It is natural, and desirable, to extend the variational error analysis techniques developed by Marsden and West [36] for discrete Lagrangian mechanics to the case of discrete Lagrange–Dirac systems. In particular, this may provide insight into the rather unexpected convergence behavior observed in Section 6.2.

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