A Discrete-Time Formulation of Hamiltonian Dynamics

Yosi Shibberu
Mathematics Department
Rose-Hulman Institute of Technology
Terre Haute, IN 47803
email: Yosi.Shibberu@Rose-Hulman.Edu

June 28, 1997

Abstract

An energy conserving, symplectic discretization of Hamiltonian dynamics is obtained by discretizing the principle of least action in extended phase space. The resulting piecewise-linear, continuous trajectories exactly conserve the Hamiltonian at the midpoints of each linear segment. The discrete action generates symplectic transformations between the vertices of the trajectories. Conserved quadratic functions are exactly conserved at the vertices. As in the discrete mechanics of T.D. Lee, time is a dependent dynamic variable. Existence and uniqueness results are presented as well as some preliminary results on coordinate invariance.

1 Introduction

For both theoretical and computational reasons, discrete models have received increased attention in recent years. Dilemmas that the concept of infinity can introduce in continuous models are described by Greenspan [4],[5]. Horzela *et al.* [6] discuss discrete models of space-time and their associated properties. Because Hamiltonian dynamical systems arise naturally in classical mechanics, quantum mechanics and statistical mechanics, as well as in other areas such as optimal control theory, discrete models of Hamiltonian dynamical systems are of considerable interest.

Hamiltonian dynamics has several very distinctive properties which ideally should be reproduced by discrete models. The Hamiltonian function is always conserved. (Note that, when formulated in extended phase space, this property holds true even for nonautonomous systems.) The trajectory flow in phase space is always a symplectic transformation of the initial conditions. (For systems with one-degree of freedom, this property is equivalent to the requirement that the trajectory flow always preserve the phase space area of any set of initial conditions.) Often, Hamiltonian systems have symmetries which give rise to conserved quantities such as linear and angular momentum. Ideally, discrete models should reproduce these symmetries whenever they are present. Hamiltonian dynamics is invariant under symplectic coordinate transformations. Ideally, discrete models should exhibit some similar form of coordinate invariance.

Discrete models which are symplectic can be represented exactly by a Hamiltonian function. This property of symplectic models is useful for proving theoretical results about computer simulations of Hamiltonian dynamics. (An excellent introduction to symplectic methods for Hamiltonian systems is given by Sanz-Serna and Calvo [11].) A theorem due to Ge [2] illustrates the difficulty of formulating a general discrete model which is both symplectic and which exactly conserves the Hamiltonian. We will discuss this theorem in more detail in section 3.

Since Hamiltonian dynamics has a variational formulation, discrete models can be constructed by discretizing variational principles. A recent survey of models based on discrete variational principles is given in [14]. The discrete model proposed in this paper is similar to one proposed by T.D. Lee [9],[8] and later modified by D'Innocenzo *et al.* [1]. A distinctive feature of these models is that time is a dependent dynamic variable. This feature is in contrast with the continuous theory where time is an independent parameter. In fact, T.D. Lee suggests that the discrete model may be more fundamental than the continuous one. The discrete models have an asymptotic distribution for time which can not be recovered from the continuous model alone. We describe this property in more detail in section 3.

The discrete models developed by Lee and D'Innocenzo *et al.* are for Newtonian potential systems and are constructed in a Lagrangian framework. The discretization we describe in this paper is applicable to arbitrary Hamiltonian systems and is constructed by discretizing a version of the principle of least action in extended phase space. We will refer to the discretization as "DTH dynamics", DTH being an abbreviation of "Discrete-Time Hamiltonian."

The principle of least action has several equivalent formulations [3],[7],[13]. Once discretized however, these different formulations may no longer be equivalent to one another. DTH dynamics is based on a discretization of an extended phase space formulation of the principle of least action described below. Additional motivation for choosing this particular formulation is given in [13].

Consider an n-degree of freedom Hamiltonian system with Hamiltonian function $H(t, q_1, \ldots q_n, p_1, \ldots p_n)$ where t represents time and $(q_1, \ldots q_n)^\top$ and $(p_1, \ldots p_n)^\top$ are position and momentum coordinates respectively. Let $\mathbf{q} = (q_1, \ldots q_n, t)^\top$ and $\mathbf{p} = (p_1, \ldots p_n, p_t)^\top$ where p_t is the momentum of time. (See [3],[7],[13] for a description of p_t.) Define $\mathbf{z} = (\mathbf{q}, \mathbf{p})^\top$ to be coordinates in extended phase space. The extended phase space Hamiltonian function corresponding to $H(t, q_1, \ldots q_n, p_1, \ldots p_n)$ is defined by

$$\mathcal{H}(\mathbf{z}) = p_t + H(t, q_1, \ldots q_n, p_1, \ldots p_n)$$

Consider the extended phase space action integral defined by

$$\mathcal{A}[\mathbf{z}(\tau)] = \int_{\tau_o}^{\tau_f} \frac{1}{2}\, \mathbf{z}(\tau)^\top \, \mathbf{J}\, \mathbf{z}'(\tau)\, d\tau \qquad (1)$$

where J is the skew-symmetric matrix

$$\mathrm{J} = \begin{pmatrix} \mathbf{0} & \mathrm{I} \\ -\mathrm{I} & \mathbf{0} \end{pmatrix}$$

and I is the $n+1$ by $n+1$ identity matrix.

Definition 1 (Principle of Least Action) *The trajectory* $\mathrm{z}(\tau)$ *of a Hamiltonian dynamical system with Hamiltonian function* $\mathcal{H}(\mathrm{z})$ *causes the action integral* $\mathcal{A}[\mathrm{z}(\tau)]$ *to be stationary under the boundary constraints* $\mathrm{q}(\tau_o) = \mathrm{q}_0,\ \mathrm{p}(\tau_f) = \mathrm{p}_f$ *and the Hamiltonian constraint* $\mathcal{H}(\mathrm{z}(\tau)) = 0$.

We can obtain Hamilton's equations of motion from Definition 1 by introducing Lagrange multipliers for the Hamiltonian constraint $\mathcal{H}(\mathrm{z}(\tau)) = 0$ and writing down the appropriate Euler-Lagrange equations.

$$\mathcal{A}[\lambda(\tau), \mathrm{z}(\tau)] = \int_{\tau_o}^{\tau_f} \left(\frac{1}{2} \mathrm{z}(\tau)^\top \mathrm{J}\, \mathrm{z}'(\tau) + \lambda(\tau)\, \mathcal{H}(\mathrm{z}(\tau)) \right) d\tau$$

The Lagrangian is given by

$$L(\lambda, \mathrm{z}, \mathrm{z}') = \frac{1}{2} \mathrm{z}(\tau)^\top \mathrm{J}\, \mathrm{z}'(\tau) + \lambda(\tau)\, \mathcal{H}(\mathrm{z}(\tau))$$

and the Euler-Lagrange equations are

$$\frac{d}{d\tau}\left(\frac{\partial L}{\partial \mathrm{z}'}\right) - \frac{\partial L}{\partial \mathrm{z}} = 0 \qquad (2)$$

$$\frac{d}{d\tau}\left(\frac{\partial L}{\partial \lambda'}\right) - \frac{\partial L}{\partial \lambda} = 0. \qquad (3)$$

Equation (2) yields Hamilton's equations of motion

$$\mathrm{z}'(\tau) = \lambda(\tau)\, \mathrm{J}\, \mathrm{H}_{\mathrm{z}}(\mathrm{z}(\tau)). \qquad (4)$$

Equation (3) yield the Hamiltonian constraint

$$\mathcal{H}(\mathrm{z}(\tau)) = 0 \qquad (5)$$

Equation (5) is not independent from equation (4) since Hamilton's equations of motion independently conserve the Hamiltonian. Thus, $\lambda(\tau)$ is indeterminate. Since the equation for time is $t'(\tau) = \lambda(\tau)\mathcal{H}_{p_t}(\mathrm{z}(\tau)) = \lambda(\tau)$, the "velocity" of time is indeterminate in the continuous formulation of Hamiltonian dynamics. This is not the case for the discretization described below. We will discretize the principle of least action given in Definition 1 by replacing the trajectory $\mathrm{z}(\tau)$ by a piecewise-linear, continuous trajectory $\hat{\mathrm{z}}(\tau)$ and enforcing the Hamiltonian constraint only at the midpoints of the piecewise-linear trajectory.

We begin in section 2 by introducing notation for describing piecewise-linear trajectories. Then we state the DTH principle of stationary action, the discrete variational principle used to define DTH dynamics. Equations of motion are derived and existence and uniqueness results are presented. In section 3 we describe several properties of DTH dynamics. First, we show that the discrete action in Definition 2 generates symplectic transformations between vertices of DTH trajectories. We describe Ge's theorem and explain why the theorem does not preclude DTH dynamics from exactly conserving energy. We describe the asymptotic behavior of time in DTH dynamics. The preservation of quadratic conservation laws is proved. Finally, invariance with respect to linear, symplectic coordinate transformations is demonstrated.

2 Foundations of DTH Dynamics

Assume the points $\tau_k,\ k = 0, 1, \cdots N$ partition the interval $[\tau_0, \tau_N]$ into N equal intervals of length $\Delta\tau = (\tau_N - \tau_0)/N$. Assume $\hat{\mathbf{z}} : [\tau_0, \tau_N] \longrightarrow \Re^{2n+2}$ is a piecewise-linear, continuous function of τ as shown in Figure 1 where $\mathbf{z}^{(k)} = \hat{\mathbf{z}}(\tau_k)$ are the vertices of $\hat{\mathbf{z}}(\tau)$. Clearly, $\hat{\mathbf{z}}(\tau)$ is completely determined by its

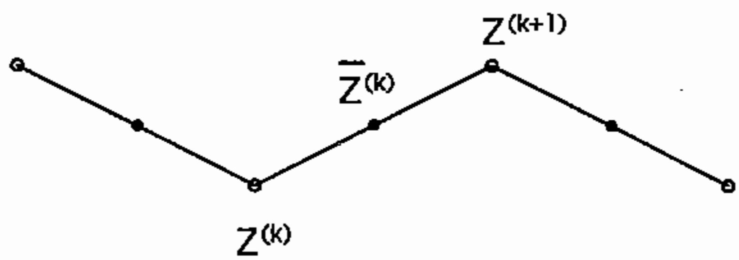

Figure 1: A piecewise-linear, continuous trajectory $\hat{\mathbf{z}}(\tau)$.

vertices $\mathbf{z}^{(k)}$. Define

$$\overline{\mathbf{z}}^{(k)} = \overline{\mathbf{z}}^{(k)}(\mathbf{z}^{(k+1)}, \mathbf{z}^{(k)}) = \frac{\mathbf{z}^{(k+1)} + \mathbf{z}^{(k)}}{2} \quad (6)$$

$$\overline{\mathbf{z}}'^{(k)} = \overline{\mathbf{z}}'^{(k)}(\mathbf{z}^{(k+1)}, \mathbf{z}^{(k)}) = \frac{\mathbf{z}^{(k+1)} - \mathbf{z}^{(k)}}{\Delta\tau} \quad (7)$$

where $k = 0, 1, \cdots N-1$. Since $\hat{\mathbf{z}}(\tau)$ is piecewise-linear, it can be expressed in terms of the values of $\overline{\mathbf{z}}^{(k)}$ and $\overline{\mathbf{z}}'^{(k)}$ in the following way.

$$\hat{\mathbf{z}}(\tau) = \begin{cases} \overline{\mathbf{z}}^{(k)} + \overline{\mathbf{z}}'^{(k)}(\tau - \overline{\tau}_k) & \tau_k \le \tau < \tau_{k+1} \quad k = 0, 1, \cdots N-1 \\ \mathbf{z}^{(N)} & \tau = \tau_N \end{cases} \quad (8)$$

where

$$\overline{\tau}_k = \frac{\tau_{k+1} + \tau_k}{2}.$$

The following lemmas will be used in the proof of Theorem 1. The continuity of $\hat{z}(\tau)$ implies that $\overline{z}^{(k)}$ and $\overline{z}'^{(k)}$ must satisfy the following continuity constraint.

Lemma 1 (Continuity Constraint) *A piecewise-linear function $\hat{z}(\tau)$ is continuous if and only if*

$$\frac{\overline{z}^{(k+1)} - \overline{z}^{(k)}}{\Delta\tau} = \frac{\overline{z}'^{(k+1)} + \overline{z}'^{(k)}}{2}$$

The proof of Lemma 1 is given in [12].

Lemma 2 *From (6) and (7) it follows that for $k = 0, 1, \cdots N-1$*

$$\frac{\partial\overline{z}^{(k)}}{\partial z^{(k)}} = \frac{1}{2}\,\mathrm{I}_{2n+2} \quad \frac{\partial\overline{z}'^{(k)}}{\partial z^{(k)}} = -\frac{1}{\Delta\tau}\,\mathrm{I}_{2n+2}$$

$$\frac{\partial\overline{z}^{(k)}}{\partial z^{(k+1)}} = \frac{1}{2}\,\mathrm{I}_{2n+2} \quad \frac{\partial\overline{z}'^{(k)}}{\partial z^{(k+1)}} = \frac{1}{\Delta\tau}\,\mathrm{I}_{2n+2}$$

where I_{2n+2} is the $2n+2$ by $2n+2$ identity matrix.

The following discrete variational principle is used as the definition of DTH dynamics.

Definition 2 (DTH Principle of Stationary Action) *A DTH trajectory is a piecewise-linear, continuous function $\hat{z} : [\tau_0, \tau_N] \longrightarrow \Re^{2n+2}$ for which the sum:*

$$\begin{aligned} \mathcal{A}\left[\Delta\tau, \lambda_0, \cdots \lambda_{N-1}, \hat{z}(\cdot)\right] \;=\; & \frac{1}{2}\left(q^{(0)}\right)^T p^{(0)} \;+ \\ & \sum_{j=0}^{N-1}\left[\frac{1}{2}\left(\overline{z}^{(j)}\right)^T \mathrm{J}\left(\overline{z}'^{(j)}\right) + \lambda_j \mathcal{H}(\overline{z}^{(j)})\right]\Delta\tau \;+ \\ & \frac{1}{2}\left(q^{(N)}\right)^T p^{(N)} \end{aligned}$$

is stationary. The endpoints $q^{(0)}$ and $p^{(N)}$ are assumed fixed. For a Hamiltonian system with a Hamiltonian function $H(t, q_1, \ldots q_n, p_1, \ldots p_n)$, the function $\mathcal{H}(z)$ is defined to be

$$\mathcal{H}(z) = p_t + H(t, q_1, \ldots q_n, p_1, \ldots p_n)$$

The variable λ_j in Definition 2 is a Lagrange multiplier for the Hamiltonian constraint $\mathcal{H}(\overline{z}^{(j)}) = 0$. Observe that the discretization enforces this constraint only at the midpoints $\overline{z}^{(j)}$. The equations of motion for DTH dynamics are given by the following theorem.

Theorem 1 (DTH Equations of Motion) *A piecewise-linear, continuous function $\hat{z} : [\tau_0, \tau_N] \longrightarrow \Re^{2n+2}$ is a DTH trajectory if and only if $\overline{z}^{(k)}$ and $\overline{z}'^{(k)}$ satisfy the following equations:*

$$\frac{\overline{z}^{(k+1)} - \overline{z}^{(k)}}{\Delta\tau} = \frac{1}{2}\mathrm{J}\left[\lambda_{k+1}\frac{\partial\mathcal{H}(\overline{z}^{(k+1)})}{\partial\overline{z}^{(k+1)}} + \lambda_k\frac{\partial\mathcal{H}(\overline{z}^{(k)})}{\partial\overline{z}^{(k)}}\right] \quad k = 0, 1, \cdots N-2 \quad (9)$$

$$\overline{z}'^{(k)} = \lambda_k J \frac{\partial \mathcal{H}(\overline{z}^{(k)})}{\partial \overline{z}^{(k)}} \quad k = 0, 1, \cdots N-1 \tag{10}$$

$$\mathcal{H}(\overline{z}^{(k)}) = 0 \quad k = 0, 1, \cdots N-1 \tag{11}$$

Theorem 1 says that Definition 2 completely determines the values of $\overline{z}^{(k)}$ and $\overline{z}'^{(k)}$ for $k = 0, 1, \cdots N-1$ which, by equation (8) implies $\hat{z}(\tau)$ is completely determined also. (Existence and uniqueness questions will be addressed later.) It is important to note that the initial value of $z_{2n+2}^{(k)} = p_t^{(k)}$ (the momentum of time) must be chosen so that equation (11) is satisfied at $k = 0$. Theorem 1 is proved by equating the appropriate partial derivatives of $\mathcal{A}[\Delta\tau, \lambda_0, \cdots \lambda_{N-1}, \hat{z}(\cdot)]$ to zero and simplifying the resulting equations. Apart from the algebraic manipulations involved, the proof is straight forward.

Proof: Assume $\hat{z}(\tau)$ is a DTH trajectory. From Definition 2, we have that for fixed endpoints $q^{(0)}$ and $p^{(0)}$, $\mathcal{A}[\cdot]$ is stationary at $\hat{z}(\tau)$. Thus, the following derivatives of $\mathcal{A}[\cdot]$ are equal to zero.

$$\frac{\partial \mathcal{A}}{\partial z^{(k+1)}} = 0, \; k = 0, 1, \ldots N-2 \tag{12}$$

$$\frac{\partial \mathcal{A}}{\partial p^{(0)}} = 0 \tag{13}$$

$$\frac{\partial \mathcal{A}}{\partial q^{(N)}} = 0 \tag{14}$$

$$\frac{\partial \mathcal{A}}{\partial \lambda_k} = 0, \; k = 0, 1, \ldots N-1 \tag{15}$$

where we have used the notation

$$\frac{\partial \mathcal{A}}{\partial z^{(k+1)}} = \begin{pmatrix} \frac{\partial \mathcal{A}}{\partial z_1^{(k+1)}} \\ \vdots \\ \frac{\partial \mathcal{A}}{\partial z_{2n+2}^{(k+1)}} \end{pmatrix} \quad \frac{\partial \mathcal{A}}{\partial p^{(0)}} = \begin{pmatrix} \frac{\partial \mathcal{A}}{\partial p_1^{(0)}} \\ \vdots \\ \frac{\partial \mathcal{A}}{\partial p_{n+1}^{(0)}} \end{pmatrix} \quad \frac{\partial \mathcal{A}}{\partial q^{(N)}} = \begin{pmatrix} \frac{\partial \mathcal{A}}{\partial q_1^{(N)}} \\ \vdots \\ \frac{\partial \mathcal{A}}{\partial q_{n+1}^{(N)}} \end{pmatrix}$$

Equation (12) implies equation (9) as follows. For $k = 0, 1, \cdots N-2$ we have from Definition 2 that

$$\begin{aligned} \frac{\partial \mathcal{A}}{\partial z^{(k+1)}} &= \frac{\partial}{\partial z^{(k+1)}} \left[\frac{1}{2} \left(\overline{z}^{(k)}\right)^{\mathsf{T}} J \left(\overline{z}'^{(k)}\right) + \lambda_k \mathcal{H}(\overline{z}^{(k)}) \right. \\ &+ \left. \frac{1}{2} \left(\overline{z}^{(k+1)}\right)^{\mathsf{T}} J \left(\overline{z}'^{(k+1)}\right) + \lambda_{k+1} \mathcal{H}(\overline{z}^{(k+1)}) \right] \Delta\tau \end{aligned}$$

since only the kth and $k+1$st terms of $\mathcal{A}[\cdot]$ depend on $z^{(k+1)}$. Using Lemma 2 to evaluate the derivatives of $\overline{z}^{(k)}$, $\overline{z}'^{(k)}$, $\overline{z}^{(k+1)}$ and $\overline{z}'^{(k+1)}$ with respect to $z^{(k+1)}$ and using the fact that $J^{\mathsf{T}} = -J$, we have

$$\frac{\partial \mathcal{A}}{\partial z^{(k+1)}} =$$

$$\Delta\tau\left[\frac{1}{2}\left(\frac{1}{2}\mathbf{I}\right)^{\top}\mathbf{J}\overline{\mathbf{z}}'^{(k)}+\frac{1}{2}\left(\frac{1}{\Delta\tau}\mathbf{I}\right)^{\top}(-\mathbf{J})\overline{\mathbf{z}}^{(k)}+\lambda_k\left(\frac{1}{2}\mathbf{I}\right)^{\top}\frac{\partial\mathcal{H}(\overline{\mathbf{z}}^{(k)})}{\partial\overline{\mathbf{z}}^{(k)}}+\right.$$

$$\left.\frac{1}{2}\left(\frac{1}{2}\mathbf{I}\right)^{\top}\mathbf{J}\overline{\mathbf{z}}'^{(k+1)}+\frac{1}{2}\left(-\frac{1}{\Delta\tau}\mathbf{I}\right)^{\top}(-\mathbf{J})\overline{\mathbf{z}}^{(k+1)}+\lambda_{k+1}\left(\frac{1}{2}\mathbf{I}\right)^{\top}\frac{\partial\mathcal{H}(\overline{\mathbf{z}}^{(k+1)})}{\partial\overline{\mathbf{z}}^{(k+1)}}\right]=$$

$$\Delta\tau\left[\frac{1}{2}\mathbf{J}\left(\frac{\overline{\mathbf{z}}'^{(k+1)}+\overline{\mathbf{z}}'^{(k)}}{2}\right)+\frac{1}{2}\mathbf{J}\left(\frac{\overline{\mathbf{z}}^{(k+1)}-\overline{\mathbf{z}}^{(k)}}{\Delta\tau}\right)+\frac{1}{2}\left(\lambda_{k+1}\frac{\partial\mathcal{H}(\overline{\mathbf{z}}^{(k+1)})}{\partial\overline{\mathbf{z}}^{(k+1)}}+\lambda_k\frac{\partial\mathcal{H}(\overline{\mathbf{z}}^{(k)})}{\partial\overline{\mathbf{z}}^{(k)}}\right)\right].$$

Using the continuity constraint on $\hat{\mathbf{z}}(\tau)$ (Lemma 1) and the fact that $\mathbf{J}^2=-\mathbf{I}$ we can simplify the above expression to

$$\begin{aligned}\frac{\partial\mathcal{A}}{\partial\mathbf{z}^{(k+1)}} &= \Delta\tau\left[\mathbf{J}\left(\frac{\overline{\mathbf{z}}^{(k+1)}-\overline{\mathbf{z}}^{(k)}}{\Delta\tau}\right)+\frac{1}{2}\left(\lambda_{k+1}\frac{\partial\mathcal{H}(\overline{\mathbf{z}}^{(k+1)})}{\partial\overline{\mathbf{z}}^{(k+1)}}+\lambda_k\frac{\partial\mathcal{H}(\overline{\mathbf{z}}^{(k)})}{\partial\overline{\mathbf{z}}^{(k)}}\right)\right]\\ &= \Delta\tau\mathbf{J}\left[\left(\frac{\overline{\mathbf{z}}^{(k+1)}-\overline{\mathbf{z}}^{(k)}}{\Delta\tau}\right)-\frac{1}{2}\mathbf{J}\left(\lambda_{k+1}\frac{\partial\mathcal{H}(\overline{\mathbf{z}}^{(k+1)})}{\partial\overline{\mathbf{z}}^{(k+1)}}+\lambda_k\frac{\partial\mathcal{H}(\overline{\mathbf{z}}^{(k)})}{\partial\overline{\mathbf{z}}^{(k)}}\right)\right]\end{aligned}$$

Since $\mathbf{J}$ is nonsingular, $\partial\mathcal{A}/\partial\mathbf{z}^{(k+1)}=0$ implies that

$$\frac{\overline{\mathbf{z}}^{(k+1)}-\overline{\mathbf{z}}^{(k)}}{\Delta\tau}=\frac{1}{2}\mathbf{J}\left(\lambda_{k+1}\frac{\partial\mathcal{H}(\overline{\mathbf{z}}^{(k+1)})}{\partial\overline{\mathbf{z}}^{(k+1)}}+\lambda_k\frac{\partial\mathcal{H}(\overline{\mathbf{z}}^{(k)})}{\partial\overline{\mathbf{z}}^{(k)}}\right)\quad k=0,1,\cdots N-2$$

which is equation (9).

Next we use an induction argument to show that equations (13) and (14) imply (10). Recall that $\overline{\mathbf{z}}^{(k)}=(\overline{\mathbf{q}}^{(k)},\overline{\mathbf{p}}^{(k)})$ where $\overline{\mathbf{q}}^{(k)}$ and $\overline{\mathbf{p}}^{(k)}$ are position and momentum coordinates respectively. From Definition 2,

$$\frac{\partial\mathcal{A}}{\partial\mathbf{p}^{(0)}}=\frac{\partial}{\partial\mathbf{p}^{(0)}}\left[\frac{1}{2}\left(\mathbf{q}^{(0)}\right)^{\top}\mathbf{p}^{(0)}+\frac{\Delta\tau}{2}\left(\overline{\mathbf{z}}^{(0)}\right)^{\top}\mathbf{J}\left(\overline{\mathbf{z}}'^{(0)}\right)+\Delta\tau\lambda_0\mathcal{H}(\overline{\mathbf{z}}^{(0)})\right]=$$

$$\frac{1}{2}\mathbf{q}^{(0)}+\frac{\Delta\tau}{2}\frac{\partial}{\partial\mathbf{p}^{(0)}}\left[\left(\overline{\mathbf{q}}^{(0)}\right)^{\top}\overline{\mathbf{p}}'^{(0)}-\left(\overline{\mathbf{p}}^{(0)}\right)^{\top}\overline{\mathbf{q}}'^{(0)}\right]+\Delta\tau\lambda_0\frac{\partial\overline{\mathbf{p}}^{(0)}}{\partial\mathbf{p}^{(0)}}\frac{\partial\mathcal{H}}{\partial\overline{\mathbf{p}}^{(0)}}=$$

$$\frac{1}{2}\mathbf{q}^{(0)}-\frac{1}{2}\overline{\mathbf{q}}^{(0)}-\frac{\Delta\tau}{4}\overline{\mathbf{q}}'^{(0)}+\frac{\Delta\tau}{2}\lambda_0\frac{\partial\mathcal{H}}{\partial\overline{\mathbf{p}}^{(0)}}=$$

$$-\frac{\mathbf{q}^{(1)}-\mathbf{q}^{(0)}}{4}-\frac{\Delta\tau}{4}\overline{\mathbf{q}}'^{(0)}+\frac{\Delta\tau}{2}\lambda_0\frac{\partial\mathcal{H}}{\partial\overline{\mathbf{p}}^{(0)}}=$$

$$-\frac{\Delta\tau}{2}\left[\overline{\mathbf{q}}'^{(0)}-\lambda_0\frac{\partial\mathcal{H}}{\partial\overline{\mathbf{p}}^{(0)}}\right].$$

Thus

$$\frac{\partial\mathcal{A}}{\partial\mathbf{p}^{(0)}}=-\frac{\Delta\tau}{2}\left[\overline{\mathbf{q}}'^{(0)}-\lambda_0\frac{\partial\mathcal{H}}{\partial\overline{\mathbf{p}}^{(0)}}\right].$$

Therefore, $\partial \mathcal{A}/\partial \mathrm{p}^{(0)} = 0$ implies

$$\overline{\mathrm{q}}'^{(0)} = \lambda_0 \frac{\partial \mathcal{H}}{\partial \overline{\mathrm{p}}^{(0)}} \tag{16}$$

In a similar fashion we can show that $\partial \mathcal{A}/\partial \mathrm{q}^{(N)} = 0$ implies

$$\overline{\mathrm{p}}'^{(N-1)} = -\lambda_{N-1} \frac{\partial \mathcal{H}}{\partial \overline{\mathrm{q}}^{(N-1)}} \tag{17}$$

Now equation (9) which we have shown to hold true for $k = 0, 1, \cdots N-1$, can be expressed as two equations

$$\frac{\overline{\mathrm{q}}^{(k+1)} - \overline{\mathrm{q}}^{(k)}}{\Delta\tau} = \frac{1}{2}\left(\lambda_{k+1}\frac{\partial \mathcal{H}}{\partial \overline{\mathrm{p}}^{(k+1)}} + \lambda_k \frac{\partial \mathcal{H}}{\partial \overline{\mathrm{p}}^{(k)}}\right) \tag{18}$$

$$\frac{\overline{\mathrm{p}}^{(k+1)} - \overline{\mathrm{p}}^{(k)}}{\Delta\tau} = -\frac{1}{2}\left(\lambda_{k+1}\frac{\partial \mathcal{H}}{\partial \overline{\mathrm{q}}^{(k+1)}} + \lambda_k \frac{\partial \mathcal{H}}{\partial \overline{\mathrm{q}}^{(k)}}\right) \tag{19}$$

Using the continuity constraints on $\hat{\mathrm{q}}(\tau)$ and $\hat{\mathrm{p}}(\tau)$ (Lemma 1) equations (18) and (19) can be expressed as

$$\frac{\overline{\mathrm{q}}'^{(k+1)} + \overline{\mathrm{q}}'^{(k)}}{2} = \frac{1}{2}\left(\lambda_{k+1}\frac{\partial \mathcal{H}}{\partial \overline{\mathrm{p}}^{(k+1)}} + \lambda_k \frac{\partial \mathcal{H}}{\partial \overline{\mathrm{p}}^{(k)}}\right) \tag{20}$$

$$\frac{\overline{\mathrm{p}}'^{(k+1)} + \overline{\mathrm{p}}'^{(k)}}{2} = -\frac{1}{2}\left(\lambda_{k+1}\frac{\partial \mathcal{H}}{\partial \overline{\mathrm{q}}^{(k+1)}} + \lambda_k \frac{\partial \mathcal{H}}{\partial \overline{\mathrm{q}}^{(k)}}\right) \tag{21}$$

Assume for some k, $0 \le k \le N-2$ that

$$\overline{\mathrm{q}}'^{(k)} = \lambda_k \frac{\partial \mathcal{H}}{\partial \overline{\mathrm{p}}^{(k)}} \tag{22}$$

Equation (20) implies

$$\overline{\mathrm{q}}'^{(k+1)} = \lambda_{k+1} \frac{\partial \mathcal{H}}{\partial \overline{\mathrm{p}}^{(k+1)}} \tag{23}$$

Equation (16) shows (22) holds for $k = 0$. Therefore, by induction

$$\overline{\mathrm{q}}'^{(k)} = \lambda_k \frac{\partial \mathcal{H}}{\partial \overline{\mathrm{p}}^{(k)}} \quad k = 0, 1, \cdots N-1 \tag{24}$$

Now assume for some k, $0 \le k \le N-2$ that

$$\overline{\mathrm{p}}'^{(k+1)} = -\lambda_{k+1} \frac{\partial \mathcal{H}}{\partial \overline{\mathrm{q}}^{(k+1)}} \tag{25}$$

Equation (21) implies

$$\overline{\mathrm{p}}'^{(k)} = -\lambda_k \frac{\partial \mathcal{H}}{\partial \overline{\mathrm{q}}^{(k)}} \tag{26}$$

Since by (17) equation (25) holds true for $k = N - 2$, we have by induction (k decreasing) that

$$\overline{\mathrm{p}}'^{(k)} = -\lambda_k \frac{\partial \mathcal{H}}{\partial \overline{\mathrm{q}}^{(k)}} \quad k = 0, 1, \cdots N-1 \tag{27}$$

Using symplectic notation, equations (24) and (27) can be combined into the following equation, which is equation (10).

$$\overline{\mathrm{z}}'^{(k)} = \lambda_k \mathrm{J} \frac{\partial \mathcal{H}}{\partial \overline{\mathrm{z}}'^{(k)}} \quad k = 0, 1, \cdots N-1$$

Finally, equation (11) follows easily from $\partial \mathcal{A}/\partial \lambda_k = 0$ since

$$\frac{\partial \mathcal{A}}{\partial \lambda_k} = \mathcal{H}(\overline{\mathrm{z}}^{(k)}), \quad k = 0, 1, \cdots N-1.$$

To conclude the proof, we observe that each step used in the proof is reversible and thus equations (9)–(11) not only are necessary but are also sufficient conditions for a piecewise-linear, continuous function to be a DTH trajectory.

□

For autonomous systems, the DTH equations of motion can be simplified to the following equations. We use the notation $\mathrm{x} = (q_1, \ldots q_n, p_1, \ldots p_n)^{\mathsf{T}}$. Time and the momentum of time are not included. We point out, however, that the time $\widehat{t}(\tau)$ must still be determined from the equations $(\overline{t}_{k+1} - \overline{t}_k)/\Delta\tau = (\lambda_{k+1} + \lambda_k)/2$ and $\overline{t}'_k = \lambda_k$.

Corollary 1 (DTH Equations for Autonomous Systems) *A piecewise-linear, continuous function $\hat{\mathrm{x}} : [\tau_0, \tau_N] \longrightarrow \Re^{2n}$ is a DTH trajectory of an autonomous Hamiltonian system $H(\mathrm{x})$, if and only if $\overline{\mathrm{x}}^{(k)}$ and $\overline{\mathrm{x}}'^{(k)}$ satisfy the following equations:*

$$\frac{\overline{\mathrm{x}}^{(k+1)} - \overline{\mathrm{x}}^{(k)}}{\Delta\tau} = \frac{1}{2}\mathrm{J}\left[\lambda_{k+1}\frac{\partial H(\overline{\mathrm{x}}^{(k+1)})}{\partial \overline{\mathrm{x}}^{(k+1)}} + \lambda_k \frac{\partial H(\overline{\mathrm{x}}^{(k)})}{\partial \overline{\mathrm{x}}^{(k)}}\right] \quad k = 0, 1, \cdots N-2 \tag{28}$$

$$\overline{\mathrm{x}}'^{(k)} = \lambda_k \mathrm{J} \frac{\partial H(\overline{\mathrm{x}}^{(k)})}{\partial \overline{\mathrm{x}}^{(k)}} \quad k = 0, 1, \cdots N-1 \tag{29}$$

$$H(\overline{\mathrm{x}}^{(k)}) - H(\overline{\mathrm{x}}^{(0)}) = 0 \quad k = 0, 1, \cdots N-1 \tag{30}$$

Proof: Equations (28) and (29) follow directly from equations (9) and (10) of Theorem 1. Since $H(\mathrm{x})$ is autonomous, $\partial H/\partial t = \partial H/\partial z_{n+1} = 0$ and therefore the momentum of time, $\overline{z}^{(k)}_{2n+2} = p_t^{(k)}$ is constant. Equation (11) $\mathcal{H}(\overline{\mathrm{z}}^{(k)}) = p_t^{(k)} + H(\overline{\mathrm{x}}^{(k)}) = 0, \quad k = 0, 1, \cdots N-1$ then implies equation (30).

□

The constant trajectory $\lambda_{k+1} = -\lambda_k$, $\overline{z}^{(k+1)} = \overline{z}^{(k)}$ is always a solution to equations (9)–(11). For such trajectories, time stands still. The following theorem gives sufficient conditions for the existence and local uniqueness of nonconstant DTH trajectories.

Theorem 2 (Existence and Uniqueness of DTH Trajectories) *Assume* $\mathcal{H} \in C^3(U)$ *where* $U \subset \Re^{2n+2}$ *is open. Assume also that* $\lambda_o > 0$ *and that there exists a* $\overline{z}^{(0)} \in U$ *such that* $\mathcal{H}(\overline{z}^{(0)}) = 0$ *and* $\psi(\overline{z}^{(0)}) \neq 0$ *where*

$$\psi(z) = (J\mathcal{H}_z)^T \mathcal{H}_{zz} (J\mathcal{H}_z).$$

Then for any positive integer N*, there exists a time step* $\Delta\tau$ *and a locally unique piecewise-linear, continuous trajectory determined by* $\overline{z}^{(k)}$, $k = 0, 1, \ldots N-1$ *where* $\overline{z}^{(k)}$ *satisfies the DTH equations of dynamics for locally unique* $\lambda_k > 0$, $k = 0, 1, \ldots N-1$.

The proof, which is constructive, is based on the Newton-Kantorovich Theorem and is given in [12]. We provide an interpretation of the quantity $\psi(z)$ in section 3.

Theorem 2 proves, as has already been observed by T.D. Lee [9], that a discrete-time formulation can be fundamentally different from the continuous one. Recall that in the continuous formulation of the principle of least action, $\lambda(\tau)$ is indeterminate. Since $t'(\tau) = \lambda(\tau)$, there is no preferred parametrization of time. The local uniqueness of λ_j by Theorem 2 demonstrates that there is a preferred parametrization of time in DTH dynamics.

3 Properties of DTH Dynamics

DTH dynamics has the interesting property of being both symplectic (at the vertices $z^{(k)}$) and energy conserving (at the midpoints $\overline{z}^{(k)}$). The importance of preserving both symplecticness and energy conservation in discretizing Hamiltonian systems is illustrated by a theorem due to Ge [2]. Roughly speaking, Ge's theorem says that a general, energy conserving, symplectic discretization of Hamiltonian dynamics will yield, up to a reparametrization of time, the exact dynamics. Unfortunately, because symplecticness and energy conservation do not occur at the same point, DTH dynamics does not satisfy the requirements of Ge's theorem.

The reasoning behind Ge's theorem is as follows [2]. Assume that $H(x)$ is a Hamiltonian system which does not have any independent first integrals other than $H(x)$ itself. (This means that if $I(x)$ is conserved along the flow of $H(x)$ then there exists a function such that $I(x) = f(H(x))$). Now assume there exists an energy conserving, symplectic discretization which approximates the flow of $H(x)$. Since the discretization is symplectic, it can be represented as the exact flow of a time dependent Hamiltonian $\widetilde{H}(h, x)$ where h is the time step of the discretization [11]. (We assume that the discretization gives rise to a one parameter family of symplectic transformations parametrized by the time step h.) Since the discretization exactly conserves energy $dH(\widetilde{\mathbf{x}}(h))/dh = 0$. But

$$\frac{d}{dh}H(\widetilde{\mathbf{x}}(h)) = \mathbf{H_x}(\widetilde{\mathbf{x}}(h))^\top \frac{d}{dh}\widetilde{\mathbf{x}}(h) = \mathbf{H_x}(\widetilde{\mathbf{x}}(h))^\top \mathbf{J}\,\widetilde{\mathbf{H}}_\mathbf{x}(h, \widetilde{\mathbf{x}}(h))$$

Therefore $\mathbf{H_x}(\mathbf{x})^\top \mathbf{J}\,\widetilde{\mathbf{H}}_\mathbf{x}(h, \mathbf{x}) = 0$. Along the exact flow, for fixed h, we have

$$\frac{d}{dt}\widetilde{H}(h, \mathbf{x}(t)) = \widetilde{\mathbf{H}}_\mathbf{x}(h, \mathbf{x}(t))^\top \frac{d}{dt}\mathbf{x}(t) = \widetilde{\mathbf{H}}_\mathbf{x}(h, \mathbf{x}(t))\,\mathbf{J}\,\mathbf{H_x}(\mathbf{x}(t)) = 0$$

and $\widetilde{H}(h, \mathbf{x})$ is a first integral of $H(\mathbf{x})$. But then $\widetilde{H}(h, \mathbf{x}) = f(h, H(\mathbf{x}))$ which implies that $\widetilde{\mathbf{H}}_\mathbf{x} = (\partial f/\partial H)\ \mathbf{H_x}$. The vector fields of $\widetilde{\mathbf{H}}_\mathbf{x}$ and $\mathbf{H_x}$ are parallel and so their integral curves must be reparametrizations of one another.

Even though DTH dynamics does not satisfy the requirements of Ge's theorem, the theorem, nevertheless illustrates the desirability of preserving both symplecticness and energy conservation. In the following theorem we construct a generating function which generates symplectic transformations between vertices of a DTH trajectory.

Theorem 3 (Generating Function for DTH Trajectories) *Define*

$$S(\Delta\tau, \mathbf{q}^{(0)}, \mathbf{p}^{(N)}) = \mathcal{A}[\Delta\tau, \lambda_0, \cdots \lambda_{N-1}, \hat{\mathbf{z}}(\cdot)]$$

where the action $\mathcal{A}[\cdot]$ is evaluated along DTH trajectories which satisfies the boundary conditions $\hat{\mathbf{q}}(\tau_0) = \mathbf{q}^{(0)}$ and $\hat{\mathbf{p}}(\tau_N) = \mathbf{p}^{(N)}$. Then

$$\frac{\partial S}{\partial \mathbf{q}^{(0)}} = \mathbf{p}^{(0)} \tag{31}$$

$$\frac{\partial S}{\partial \mathbf{p}^{(N)}} = \mathbf{q}^{(N)} \tag{32}$$

where $\mathbf{p}^{(0)} = \hat{\mathbf{p}}(\tau_0)$ and $\mathbf{q}^{(N)} = \hat{\mathbf{q}}(\tau_N)$.

<u>Proof:</u> For sufficiently small step sizes $\Delta\tau$, the boundary conditions $\hat{\mathbf{q}}(\tau_0) = \mathbf{q}^{(0)}$ and $\hat{\mathbf{p}}(\tau_N) = \mathbf{p}^{(N)}$ determine a DTH trajectory $\hat{\mathbf{z}}(\tau)$. By the DTH Principle of Stationary Action, along $\hat{\mathbf{z}}(\tau)$ we have

$$\frac{\partial \mathcal{A}}{\partial \mathbf{p}^{(0)}} = \frac{\partial \mathcal{A}}{\partial \mathbf{q}^{(N)}} = 0$$

$$\frac{\partial \mathcal{A}}{\partial \lambda_k} = 0, \quad k = 0, 1, \cdots N-1$$

$$\frac{\partial \mathcal{A}}{\partial \mathbf{z}^{(k)}} = 0, \quad k = 1, 2, \cdots N-1$$

Thus $S(\Delta\tau, \mathbf{q}^{(0)}, \mathbf{p}^{(N)})$ is a well defined function depending only on $\mathbf{q}^{(0)}$ and $\mathbf{p}^{(N)}$. Now we evaluate $\partial S/\partial \mathbf{q}^{(0)}$. From the above definition we have that

$$\frac{\partial S}{\partial \mathbf{q}^{(0)}} = \frac{\partial \mathcal{A}}{\partial \mathbf{q}^{(0)}}\ |_{\hat{\mathbf{z}}(\cdot)}$$

$$
\begin{aligned}
&= \frac{1}{2}\mathbf{p}^{(0)} + \frac{\partial}{\partial \mathbf{q}^{(0)}}\left[\frac{1}{2}\left(\overline{\mathbf{z}}^{(0)}\right)^T \mathbf{J}\left(\overline{\mathbf{z}}'^{(0)}\right) + \lambda_0\,\mathcal{H}(\overline{\mathbf{z}}^{(0)})\right]\Delta\tau \\
&= \frac{1}{2}\mathbf{p}^{(0)} + \frac{\partial}{\partial \mathbf{q}^{(0)}}\left[\frac{1}{2}\left[\left(\overline{\mathbf{q}}^{(0)}\right)^T\left(\overline{\mathbf{p}}'^{(0)}\right) - \left(\overline{\mathbf{p}}^{(0)}\right)^T\left(\overline{\mathbf{q}}'^{(0)}\right)\right] + \lambda_0\mathcal{H}(\overline{\mathbf{q}}^{(0)}, \overline{\mathbf{p}}^{(0)})\right]\Delta\tau \\
&= \frac{1}{2}\mathbf{p}^{(0)} + \frac{\Delta\tau}{2}\left[\left(\frac{\partial\overline{\mathbf{q}}^{(0)}}{\partial\mathbf{q}^{(0)}}\right)\overline{\mathbf{p}}'^{(0)} - \left(\frac{\partial\overline{\mathbf{q}}'^{(0)}}{\partial\mathbf{q}^{(0)}}\right)\overline{\mathbf{p}}^{(0)}\right] + \lambda_0\left(\frac{\partial\overline{\mathbf{q}}^{(0)}}{\partial\mathbf{q}^{(0)}}\right)\frac{\partial\mathcal{H}}{\partial\overline{\mathbf{q}}^{(0)}}\Delta\tau \\
&= \frac{1}{2}\mathbf{p}^{(0)} + \frac{\Delta\tau}{2}\left[\left(\frac{1}{2}\mathbf{I}\right)\overline{\mathbf{p}}'^{(0)} - \left(-\frac{1}{\Delta\tau}\mathbf{I}\right)\overline{\mathbf{p}}^{(0)}\right] + \lambda_0\left(\frac{1}{2}\mathbf{I}\right)\frac{\partial\mathcal{H}}{\partial\overline{\mathbf{q}}^{(0)}}\Delta\tau \qquad (33)
\end{aligned}
$$

Since $\mathcal{A}[\cdot]$ is evaluated along a DTH trajectory, $\hat{\mathbf{z}}(\tau)$ must satisfy the DTH equations of motion. Thus, from equation (10) of Theorem 1 we have that

$$
\overline{\mathbf{p}}'^{(0)} = -\lambda_0\frac{\partial\mathcal{H}}{\partial\overline{\mathbf{q}}^{(0)}} \qquad (34)
$$

Substituting (34) into (33) and simplifying we have

$$
\begin{aligned}
\frac{\partial S}{\partial \mathbf{q}^{(0)}} &= \frac{1}{2}\mathbf{p}^{(0)} + \frac{1}{2}\left[\frac{\Delta\tau}{2}\overline{\mathbf{p}}'^{(0)} + \overline{\mathbf{p}}^{(0)}\right] - \frac{\Delta\tau}{2}\overline{\mathbf{p}}'^{(0)} \\
&= \frac{1}{2}\mathbf{p}^{(0)} + \frac{1}{2}\left[\overline{\mathbf{p}}^{(0)} - \frac{\Delta\tau}{2}\overline{\mathbf{p}}'^{(0)}\right] \\
&= \frac{1}{2}\mathbf{p}^{(0)} + \frac{1}{2}\mathbf{p}^{(0)} \\
&= \mathbf{p}^{(0)}
\end{aligned}
$$

Similarly,

$$
\frac{\partial S}{\partial \mathbf{p}^{(N)}} = \frac{\partial\mathcal{A}}{\partial\mathbf{p}^{(N)}}\,|_{\hat{\mathbf{z}}(\cdot)}
$$

$$
\begin{aligned}
&= \frac{\partial}{\partial\mathbf{p}^{(N)}}\left[\frac{1}{2}\left(\overline{\mathbf{z}}^{(N-1)}\right)^T\mathbf{J}\left(\overline{\mathbf{z}}'^{(N-1)}\right) + \lambda_{N-1}\,\mathcal{H}(\overline{\mathbf{z}}^{(N-1)})\right]\Delta\tau + \frac{1}{2}\mathbf{q}^{(N)} \\
&= \frac{\Delta\tau}{2}\frac{\partial}{\partial\mathbf{p}^{(N)}}\left[\left(\overline{\mathbf{q}}^{(N-1)}\right)^T\left(\overline{\mathbf{p}}'^{(N-1)}\right) - \left(\overline{\mathbf{p}}^{(N-1)}\right)^T\left(\overline{\mathbf{q}}'^{(N-1)}\right)\right] + \\
&\quad \lambda_{N-1}\left(\frac{\partial\overline{\mathbf{p}}^{(N-1)}}{\partial\mathbf{p}^{(N)}}\right)\frac{\partial\mathcal{H}}{\partial\overline{\mathbf{p}}^{(N-1)}}\Delta\tau + \frac{1}{2}\mathbf{q}^{(N)} \\
&= \frac{\Delta\tau}{2}\left[\frac{1}{\Delta\tau}\overline{\mathbf{q}}^{(N-1)} - \frac{1}{2}\overline{\mathbf{q}}'^{(N-1)}\right] + \frac{\Delta\tau}{2}\lambda_{N-1}\frac{\partial\mathcal{H}}{\partial\overline{\mathbf{p}}^{(N-1)}} + \frac{1}{2}\mathbf{q}^{(N)} \qquad (35)
\end{aligned}
$$

Along a DTH trajectory we have that

$$
\overline{\mathbf{q}}'^{(N-1)} = \lambda_{N-1}\frac{\partial\mathcal{H}}{\partial\overline{\mathbf{p}}^{(N-1)}} \qquad (36)
$$

Substituting (36) into (35) and simplifying we have

$$\begin{aligned}
\frac{\partial S}{\partial \mathbf{p}^{(N)}} &= \frac{1}{2}\left[\overline{\mathbf{q}}^{(N-1)} - \frac{\Delta\tau}{2}\overline{\mathbf{q}}'^{(N-1)}\right] + \frac{\Delta\tau}{2}\overline{\mathbf{q}}'^{(N-1)} + \frac{1}{2}\mathbf{q}^{(N)} \\
&= \frac{1}{2}\left[\overline{\mathbf{q}}^{(N-1)} + \frac{\Delta\tau}{2}\overline{\mathbf{q}}'^{(N-1)}\right] + \frac{1}{2}\mathbf{q}^{(N)} \\
&= \frac{1}{2}\mathbf{q}^{(N)} + \frac{1}{2}\mathbf{q}^{(N)} \\
&= \mathbf{q}^{(N)}
\end{aligned}$$

□

In the next theorem, we show that DTH trajectories exactly conserve the Hamiltonian function at the midpoints of each linear segment. Note that the theorem applies even to nonautonomous systems because for such systems the extended phase space Hamiltonian function $\mathcal{H}(\mathbf{z})$ continues to be conserved at zero even when the Hamiltonian function $H(t, \mathbf{x})$ is no longer conserved.

Theorem 4 (Conservation of Energy) *The extended phase space Hamiltonian function $\mathcal{H}(\mathbf{z}) = z_{2n+2} + H(\mathbf{z})$ is exactly conserved along DTH trajectories at the midpoints $\overline{\mathbf{z}}^{(k)}$. For autonomous Hamiltonian systems, the Hamiltonian function $H(\mathbf{x})$ is also exactly conserved at the midpoint $\overline{\mathbf{x}}^{(k)}$ of DTH trajectories.*

Proof: By equation (11) of Theorem 1, a necessary condition for a trajectory to be a DTH trajectory is that $\mathcal{H}(\overline{\mathbf{z}}^{(k)}) = 0$ and so $\mathcal{H}(\mathbf{z})$ is conserved at $\overline{\mathbf{z}}^{(k)}$. By equation (30) of Corollary 1, a necessary condition for a trajectory to be a DTH trajectory is that $H(\overline{\mathbf{x}}^{(k+1)}) - H(\overline{\mathbf{x}}^{(0)}) = 0$ and so $H(\mathbf{x})$ is conserved at $\overline{\mathbf{x}}^{(k)}$.

□

As described earlier, in the continuous time formulation of Hamiltonian dynamics, there is no preferred parameterization of time. In DTH dynamics, the behavior of time is determined by conservation of the Hamiltonian. The following theorem characterizes the "velocity" of time in DTH dynamics.

Theorem 5 (Asymptotic Behavior of Time) *The asymptotic ($\Delta\tau \to 0$) behavior of time in DTH dynamics is invariant under linear symplectic coordinate transformations and is characterized by the following relationship.*

$$\frac{dt}{d\tau}\psi(\mathbf{z})^{\frac{1}{3}} = const$$

where

$$\psi(\mathbf{z}) = (\mathrm{J}\mathcal{H}_{\mathbf{z}})^{\top}\,\mathcal{H}_{\mathbf{zz}}\,(\mathrm{J}\mathcal{H}_{\mathbf{z}})$$

(The proof will be published elsewhere.)

We show that it is possible to relate $\psi(z)$ to the "acceleration" of the Hamiltonian function $\mathcal{H}(z)$ at the midpoints of a DTH trajectory. Assume $\widehat{z}(\tau)$ is a DTH trajectory. Then for $\tau_k < \tau < \tau_{k+1}$ we have

$$\frac{d}{d\tau}\mathcal{H}(\widehat{z}(\tau)) = \mathcal{H}_z(\widehat{z}(\tau))^{\mathsf{T}}\widehat{z}'(\tau) = \mathcal{H}_z(\widehat{z}(\tau))^{\mathsf{T}}\overline{z}'^{(k)} = \lambda_k \mathcal{H}_z(\widehat{z}(\tau))^{\mathsf{T}} \mathrm{J}\, \mathcal{H}_z\left(\overline{z}^{(k)}\right) \tag{37}$$

The "velocity" of the Hamiltonian $\mathcal{H}(z)$ at the midpoints $\tau = \overline{\tau}_k$ of a DTH trajectory is equal to zero since from equation (37)

$$\begin{aligned} \left.\frac{d}{d\tau}\mathcal{H}(\widehat{z}(\tau))\right|_{\tau=\overline{\tau}_k} &= \lambda_k \mathcal{H}_z(\widehat{z}(\overline{\tau}_k))^{\mathsf{T}} \mathrm{J}\, \mathcal{H}_z(\overline{z}^{(k)}) \\ &= \lambda_k \mathcal{H}_z(\overline{z}^{(k)})^{\mathsf{T}} \mathrm{J}\, \mathcal{H}_z(\overline{z}^{(k)}) = 0 \end{aligned}$$

Since, at the midpoints, $\mathcal{H}(\overline{z}^{(k)}) = 0$ also, this implies that a DTH trajectory is always tangent to the energy conserving manifold. Now since, $\widehat{z}''(\tau) = 0$, we have for $\tau_k < \tau < \tau_{k+1}$

$$\begin{aligned} \frac{d^2}{d\tau^2}\mathcal{H}(\widehat{z}(\tau)) &= (\widehat{z}'(\tau))^{\mathsf{T}} \mathcal{H}_{zz}(\widehat{z}(\tau))\,(\widehat{z}'(\tau)) + \mathcal{H}_z(\widehat{z}(\tau))^{\mathsf{T}}\widehat{z}''(\tau) \\ &= \left(\overline{z}'^{(k)}\right)^{\mathsf{T}} \mathcal{H}_{zz}(\widehat{z}(\tau))\left(\overline{z}'^{(k)}\right) \end{aligned}$$

At $\tau = \overline{\tau}_k$,

$$\begin{aligned} \left.\frac{d^2}{d\tau^2}\mathcal{H}(\widehat{z}(\tau))\right|_{\tau=\overline{\tau}_k} &= \left(\overline{z}'^{(k)}\right)^{\mathsf{T}} \mathcal{H}_{zz}\left(\overline{z}^{(k)}\right)\left(\overline{z}'^{(k)}\right) \\ &= \lambda_k^2 \left(\mathrm{J}\,\mathcal{H}_z(\overline{z}^{(k)})\right)^{\mathsf{T}} \mathcal{H}_{zz}(\overline{z}^{(k)})\left(\mathrm{J}\mathcal{H}_z(\overline{z}^{(k)})\right) \\ &= \lambda_k^2\, \psi(\overline{z}^{(k)}) \end{aligned}$$

Therefore, at the midpoints $\tau = \overline{\tau}_k$, the acceleration of the Hamiltonian is $\lambda_k^2\, \psi(\overline{z}^{(k)})$.

We may reinterpret the asymptotic expression $(dt/d\tau)\; \psi(z)^{\frac{1}{3}} = const$ of Theorem 5 in terms of the acceleration of the Hamiltonian function along DTH trajectories. Since $dt/d\tau = \lambda(\tau)$, we have

$$\frac{dt}{d\tau}\,\psi(z)^{\frac{1}{3}} = \left[\left(\frac{dt}{d\tau}\right)^3 \psi(z)\right]^{\frac{1}{3}} = \left[\left(\frac{dt}{d\tau}\right)\left(\frac{dt}{d\tau}\right)^2 \psi(z)\right]^{\frac{1}{3}} = \left[\left(\frac{dt}{d\tau}\right)\lambda^2\,\psi(z)\right]^{\frac{1}{3}}.$$

Therefore, in DTH dynamics, we have the following asymptotic relationship between the "velocity of time" and the "acceleration of energy".

$$\left(\frac{dt}{d\tau}\right)\left(\frac{d^2\mathcal{H}}{d\tau^2}\right) = const$$

That $\psi(z)$ is not coordinate invariant under nonlinear, symplectic coordinate transformations is troubling from a modeling point of view. This shortcoming makes it difficult to argue that discrete mechanics is more fundamental than continuous mechanics. It may be possible to overcome this shortcoming by considering piecewise-linear, continuous, symplectic transformations in place of nonlinear ones [12].

For autonomous systems, $\psi(\mathbf{z})$ does not depend on time or the momentum of time and $\psi(\mathbf{z})$ then reduces to

$$\psi(\mathbf{x}) = (\mathbf{J}\mathbf{H}_{\mathbf{x}})^{\top} \mathbf{H}_{\mathbf{x}\mathbf{x}} (\mathbf{J}\mathbf{H}_{\mathbf{x}})$$

For autonomous, linear Hamiltonian systems $H(\mathbf{x}) = \frac{1}{2}\mathbf{x}^{\top}\mathbf{A}\mathbf{x}$ where $\mathbf{A}$ is a symmetric matrix, $\psi(\mathbf{x}) = (\mathbf{J}\mathbf{A}\mathbf{x})^{\top} \mathbf{A}\ (\mathbf{J}\mathbf{A}\mathbf{x})$ is constant along Hamiltonian trajectories since

$$\begin{aligned} \frac{d}{dt}\psi(\mathbf{x}(t)) &= \psi_{\mathbf{x}}^{\top}\mathbf{x}' \\ &= 2\left((\mathbf{J}\mathbf{A})^{\top}\mathbf{A}\ (\mathbf{J}\mathbf{A}\mathbf{x})\right)^{\top}\mathbf{x}' \\ &= 2\left(\mathbf{x}^{\top}\mathbf{A}^{\top}\mathbf{J}^{\top}\mathbf{A}^{\top}\mathbf{J}\mathbf{A}\right)\mathbf{J}\mathbf{A}\mathbf{x} \\ &= 2\mathbf{x}^{\top}\mathbf{M}\mathbf{x} \end{aligned}$$

where $\mathbf{M} = -\mathbf{AJAJAJA}$ is a skew symmetric matrix. The skew-symmetry of $\mathbf{M}$ implies that $\mathbf{x}^{\top}\mathbf{M}\mathbf{x} = 0$ and therefore $\psi(\mathbf{x}(t))$ is constant. Theorem 5 suggests that for autonomous linear systems, the "velocity" of time in DTH dynamics should be nearly constant for small $\Delta\tau$. In the following theorem we show that if $\mathbf{A}$ is positive-definite, (e.g. simple harmonic oscillator) then the velocity of time in DTH dynamics must be constant.

Theorem 6 (Behavior of Time for Linear Systems) *Assume $H(\mathbf{x})$ is a quadratic Hamiltonian function given by*

$$H(\mathbf{x}) = \frac{1}{2}\mathbf{x}^{\top}\mathbf{A}\,\mathbf{x} + \mathbf{b}^{\top}\mathbf{x} + c$$

where $\mathbf{x} \in \Re^{2n}$ and $\mathbf{A}$ is symmetric and positive-definite. Assume $\lambda_0 \neq 0$, $\overline{\mathbf{x}}^{(0)} \neq 0$. If λ_1 and $\overline{\mathbf{x}}^{(1)}$ satisfy the DTH equations of motion, then $\lambda_1 = \pm\lambda_0$.

Proof: We may assume without loss in generality that

$$H(\mathbf{x}) = \frac{1}{2}\mathbf{x}^{\top}\mathbf{A}\,\mathbf{x} \tag{38}$$

since, given any positive-definite quadratic function $Q(\mathbf{y}) = \frac{1}{2}\mathbf{y}^{\top}\mathbf{A}\,\mathbf{y} + \mathbf{b}^{\top}\mathbf{y} + c$ we may use the translation $\mathbf{y} = \mathbf{x} - \mathbf{A}^{-1}\mathbf{b}$ to reduce $Q(\mathbf{y})$ to the form given above plus some constant $d = c - \frac{1}{2}\mathbf{b}^{\top}A^{-1}\mathbf{b}$. (Note that Hamiltonian functions differing by only a constant have the same equations. Therefore, without any loss in generality, d may be taken to be 0.)

For Hamiltonian functions of the form (38) one step of the reduced DTH equations of motion (equation (28)) is given by

$$\mathbf{x}^{(1)} - \mathbf{x}^{(0)} = \frac{\Delta\tau}{2}\mathbf{J}\mathbf{A}\left(\lambda_1\mathbf{x}^{(1)} + \lambda_0\mathbf{x}^{(0)}\right) \tag{39}$$

$$\frac{1}{2}(\mathbf{x}^{(1)})^\top \mathbf{A}(\mathbf{x}^{(1)}) - \frac{1}{2}(\mathbf{x}^{(0)})^\top \mathbf{A}(\mathbf{x}^{(0)}) = 0 \tag{40}$$

(Equation (29) will not be used in the proof.) Equation (39) implies the following.

$$\frac{1}{2}(\mathbf{x}^{(1)})^\top \mathbf{A}(\mathbf{x}^{(1)}) - \frac{1}{2}(\mathbf{x}^{(0)})^\top \mathbf{A}(\mathbf{x}^{(0)}) = \frac{1}{2}\left(\mathbf{x}^{(1)} + \mathbf{x}^{(0)}\right)^\top \mathbf{A}\left(\mathbf{x}^{(1)} - \mathbf{x}^{(0)}\right) =$$

$$\frac{1}{2}\left(\mathbf{x}^{(1)} + \mathbf{x}^{(0)}\right)^\top \mathbf{A}\left(\frac{\Delta\tau}{2}\mathbf{JA}(\lambda_1 \mathbf{x}^{(1)} + \lambda_0 \mathbf{x}^{(0)})\right) =$$

$$\frac{\Delta\tau}{4}(\lambda_1 - \lambda_0)\left(\mathbf{x}^{(0)}\right)^\top \mathbf{AJA}(\mathbf{x}^{(1)}).$$

(We have used the fact that $\mathbf{M} = \mathbf{AJA}$ is skew-symmetric, and therefore $\mathbf{x}^\top \mathbf{M}\,\mathbf{x} = 0$ for any $\mathbf{x}$.) Equation (40) implies that

$$\frac{\Delta\tau}{4}(\lambda_1 - \lambda_0)\left(\mathbf{x}^{(0)}\right)^\top \mathbf{AJA}\left(\mathbf{x}^{(1)}\right) = 0$$

Therefore, either $\lambda_1 = \lambda_0$ as claimed or

$$\left(\mathbf{x}^{(0)}\right)^\top \mathbf{AJA}\left(\mathbf{x}^{(1)}\right) = 0 \tag{41}$$

Using (39) and (41) we have

$$\left(\mathbf{x}^{(0)}\right)^\top \mathbf{A}\left(\mathbf{x}^{(1)}\right) - \left(\mathbf{x}^{(0)}\right)^\top \mathbf{A}\left(\mathbf{x}^{(0)}\right) = \left(\mathbf{x}^{(0)}\right)^\top \mathbf{A}\left(\mathbf{x}^{(1)} - \mathbf{x}^{(0)}\right) =$$

$$\left(\frac{\Delta\tau\,\lambda_1}{2}\right)\left(\mathbf{x}^{(0)}\right)^\top \mathbf{AJA}\left(\mathbf{x}^{(1)}\right) + \left(\frac{\Delta\tau\,\lambda_0}{2}\right)\left(\mathbf{x}^{(0)}\right)^\top \mathbf{AJA}\left(\mathbf{x}^{(0)}\right) = 0$$

Therefore

$$\left(\mathbf{x}^{(0)}\right)^\top \mathbf{A}\left(\mathbf{x}^{(1)}\right) = \left(\mathbf{x}^{(0)}\right)^\top \mathbf{A}\left(\mathbf{x}^{(0)}\right) \tag{42}$$

From (40)

$$\left(\mathbf{x}^{(1)}\right)^\top \mathbf{A}\left(\mathbf{x}^{(1)}\right) = \left(\mathbf{x}^{(0)}\right)^\top \mathbf{A}\left(\mathbf{x}^{(0)}\right) \tag{43}$$

Equations (42) and (43) imply that

$$\left(\mathbf{x}^{(1)} - \mathbf{x}^{(0)}\right)^\top \mathbf{A}\left(\mathbf{x}^{(1)} - \mathbf{x}^{(0)}\right) =$$

$$\left(\mathbf{x}^{(1)}\right)^\top \mathbf{A}\left(\mathbf{x}^{(1)}\right) - 2\left(\mathbf{x}^{(1)}\right)^\top \mathbf{A}\left(\mathbf{x}^{(0)}\right) + \left(\mathbf{x}^{(0)}\right)^\top \mathbf{A}\left(\mathbf{x}^{(0)}\right) = 0$$

Since $\mathbf{A}$ is positive-definite, we must have $\mathbf{x}^{(1)} = \mathbf{x}^{(0)}$. Substituting $\mathbf{x}^{(0)}$ for $\mathbf{x}^{(1)}$ in (39) we have

$$0 = \frac{\Delta\tau}{2}\mathbf{JA}\left(\lambda_1 \mathbf{x}^{(0)} + \lambda_0 \mathbf{x}^{(0)}\right) = \frac{\Delta\tau\,(\lambda_1 + \lambda_0)}{2}\mathbf{JAx}^{(0)}$$

Since $\mathbf{JA}$ is nonsingular and $\mathbf{x}^{(0)} \neq 0$ we must have $\lambda_1 = -\lambda_0$ as claimed.

□

For autonomous, positive-definite, linear systems, Theorem 6 states that the only nonconstant solution to the DTH equations is the one for which $\lambda_{k+1} = \lambda_k$. If we choose $\lambda_0 = 1$, then by induction, the nonconstant solution must have $\lambda_k \equiv 1$. If $\lambda_k \equiv 1$, equation (28) reduces to the trapezoid method and equation (29) reduces to the midpoint method. We conclude that for autonomous, positive-definite, linear Hamiltonian systems, such as the simple harmonic oscillator, DTH trajectories are given by the trapezoid and midpoint rules commonly used to integrating differential equations.

The following theorem shows that all quadratic conservation laws are reproduced exactly at the vertices of DTH trajectories.

Theorem 7 (Quadratic Conservation Laws) *Assume that $L(\mathbf{x})$ is a quadratic function given by*

$$L(\mathbf{x}) = \frac{1}{2}\mathbf{x}^\top \mathbf{A}\,\mathbf{x} + \mathbf{b}^\top \mathbf{x} + c$$

and assume the Poisson bracket $[L, H] = \mathbf{L}_\mathbf{x}^\top \mathbf{J}\,\mathbf{H}_\mathbf{x}$ is identically equal to zero. Then $L(\mathbf{x})$ is exactly conserved at the vertices of DTH trajectories.

Proof: We will show that

$$\frac{L(\mathbf{x}^{(k+1)}) - L(\mathbf{x}^{(k)})}{\Delta\tau} = 0$$

We have that

$$\frac{L(\mathbf{x}^{(k+1)}) - L(\mathbf{x}^{(k)})}{\Delta\tau} =$$

$$\frac{1}{\Delta\tau}\left(\frac{1}{2}\mathbf{x}^{(k+1)\top}\mathbf{A}\mathbf{x}^{(k+1)} - \frac{1}{2}\mathbf{x}^{(k)\top}\mathbf{A}\mathbf{x}^{(k)} + \mathbf{b}^\top\mathbf{x}^{(k+1)} - \mathbf{b}^\top\mathbf{x}^{(k)}\right) =$$

$$\left(\frac{\mathbf{x}^{(k+1)} + \mathbf{x}^{(k)}}{2}\right)^\top \mathbf{A}\left(\frac{\mathbf{x}^{(k+1)} - \mathbf{x}^{(k)}}{\Delta\tau}\right) + \mathbf{b}^\top\left(\frac{\mathbf{x}^{(k+1)} - \mathbf{x}^{(k)}}{\Delta\tau}\right) =$$

$$\left(\overline{\mathbf{x}}^{(k)}\right)^\top \mathbf{A}\left(\overline{\mathbf{x}}'^{(k)}\right) + \mathbf{b}^\top\left(\overline{\mathbf{x}}'^{(k)}\right) = \left[\left(\overline{\mathbf{x}}^{(k)}\right)^\top \mathbf{A} + \mathbf{b}^\top\right]\overline{\mathbf{x}}'^{(k)} =$$

$$\mathbf{L}_\mathbf{x}(\overline{\mathbf{x}}^{(k)})^\top \overline{\mathbf{x}}'^{(k)}.$$

Equation (29) implies that for DTH trajectories, $\overline{\mathbf{x}}'^{(k)} = \lambda_k \mathbf{J}\mathbf{H}_\mathbf{x}(\overline{\mathbf{x}}^{(k)})$. Therefore

$$\mathbf{L}_\mathbf{x}(\overline{\mathbf{x}}^{(k)})^\top \overline{\mathbf{x}}'^{(k)} = \lambda_k \mathbf{L}_\mathbf{x}(\overline{\mathbf{x}}^{(k)})^\top \mathbf{J}\mathbf{H}_\mathbf{x}(\overline{\mathbf{x}}^{(k)}) = 0$$

and thus $\left(L(\mathbf{x}^{(k+1)}) - L(\mathbf{x}^{(k)})\right)/\Delta\tau = \mathbf{L}_\mathbf{x}(\overline{\mathbf{x}}^{(k)})^\top \overline{\mathbf{x}}'^{(k)} = 0$.

□

Ge has shown that the midpoint scheme (among others) is invariant under linear symplectic coordinate transformations [2]. We show that DTH dynamics is also invariant under linear, symplectic coordinate transformations.

Theorem 8 (Linear Coordinate Invariance) *Consider the Hamiltonian function $\mathcal{H}(\mathbf{z})$ and the transformed Hamiltonian $\mathcal{K}(\mathbf{y}) = \mathcal{H}(\mathbf{T}\mathbf{y})$ where $\mathbf{z} = \mathbf{T}\mathbf{y}$ is a linear symplectic coordinate transformation. The DTH equations for $\mathcal{K}(\mathbf{y})$ are the same as the transformed equations of $\mathcal{H}(\mathbf{z})$.*

Proof: First, we note that since T is symplectic, $\mathbf{T}^{\top}\mathbf{J}\,\mathbf{T} = \mathbf{J}$??. This implies that $\mathbf{T}\mathbf{J}\,\mathbf{T}^{\top} = \mathbf{J}$ also since $\mathbf{T}^{\top}\mathbf{J}\,\mathbf{T} = \mathbf{J}$, $\mathbf{T}^{\top}\mathbf{J}\mathbf{T}\mathbf{J}\,\mathbf{T}^{\top} = \mathbf{J}^2\mathbf{T}^{\top}$, $\mathbf{T}^{\top}\mathbf{J}\mathbf{T}\mathbf{J}\,\mathbf{T}^{\top} = -\mathbf{T}^{\top}$, $\mathbf{J}(\mathbf{T}^{\top})^{-1}\mathbf{T}^{\top}\mathbf{J}\mathbf{T}\mathbf{J}\,\mathbf{T}^{\top} = -\mathbf{J}(\mathbf{T}^{\top})^{-1}\mathbf{T}^{\top}$, and therefore $\mathbf{T}\mathbf{J}\mathbf{T}^{\top} = \mathbf{J}$.

From Theorem 1 the DTH equations for $\mathcal{K}(\mathbf{y})$ are

$$\frac{\overline{\mathbf{y}}^{(k+1)} - \overline{\mathbf{y}}^{(k)}}{\Delta\tau} = \frac{1}{2}\mathbf{J}\left[\lambda_{k+1}\frac{\partial\mathcal{K}(\overline{\mathbf{y}}^{(k+1)})}{\partial\overline{\mathbf{y}}^{(k+1)}} + \lambda_k\frac{\partial\mathcal{K}(\overline{\mathbf{y}}^{(k)})}{\partial\overline{\mathbf{y}}^{(k)}}\right] \quad k = 0, 1, \cdots N-2 \tag{44}$$

$$\overline{\mathbf{y}}'^{(k)} = \lambda_k\mathbf{J}\frac{\partial\mathcal{K}(\overline{\mathbf{y}}^{(k)})}{\partial\overline{\mathbf{y}}^{(k)}} \quad k = 0, 1, \cdots N-1 \tag{45}$$

$$\mathcal{K}(\overline{\mathbf{y}}^{(k)}) = 0 \quad k = 0, 1, \cdots N-1 \tag{46}$$

Since $\mathbf{y} = \mathbf{T}^{-1}\mathbf{z}$, and $\partial\mathcal{K}(\mathbf{y})/\partial\mathbf{y} = \mathbf{T}^{\top}\partial\mathcal{H}(\mathbf{z})/\partial\mathbf{z}$ we have from (44) that

$$\frac{\overline{\mathbf{z}}^{(k+1)} - \overline{\mathbf{z}}^{(k)}}{\Delta\tau} = \frac{1}{2}\mathbf{T}\mathbf{J}\mathbf{T}^{\top}\left[\lambda_{k+1}\frac{\partial\mathcal{H}(\overline{\mathbf{z}}^{(k+1)})}{\partial\overline{\mathbf{z}}^{(k+1)}} + \lambda_k\frac{\partial\mathcal{H}(\overline{\mathbf{z}}^{(k)})}{\partial\overline{\mathbf{z}}^{(k)}}\right]$$

The symplecticness of $\mathbf{T}$ implies that $\mathbf{T}\mathbf{J}\mathbf{T}^{\top} = \mathbf{J}$. Similarly, since

$$\overline{\mathbf{y}}'^{(k)} = \frac{\mathbf{y}^{(k+1)} - \mathbf{y}^{(k)}}{\Delta\tau} = \mathbf{T}^{-1}\frac{\mathbf{z}^{(k+1)} - \mathbf{z}^{(k)}}{\Delta\tau} = \mathbf{T}^{-1}\overline{\mathbf{z}}'^{(k)}$$

equation (45) becomes

$$\overline{\mathbf{z}}'^{(k)} = \lambda_k\mathbf{T}\mathbf{J}\mathbf{T}^{\top}\frac{\partial\mathcal{H}(\overline{\mathbf{z}}^{(k)})}{\partial\overline{\mathbf{z}}^{(k)}}$$

and again the symplecticness of $\mathbf{T}$ implies $\mathbf{T}\mathbf{J}\mathbf{T}^{\top} = \mathbf{J}$. Finally, since

$$\mathcal{K}(\overline{\mathbf{y}}^{(k)}) = \mathcal{H}(\mathbf{T}\overline{\mathbf{y}}^{(k)}) = \mathcal{H}(\mathbf{T}\,\mathbf{T}^{-1}\overline{\mathbf{z}}^{(k)}) = \mathcal{H}(\overline{\mathbf{z}}^{(k)})$$

from equation (46) we have

$$\mathcal{H}(\overline{\mathbf{z}}^{(k)}) = 0$$

□

We remark that it is in fact possible (at least formally) to show that DTH dynamics (and the midpoint scheme) are coordinate invariant under a much larger class of piecewise-linear, continuous, symplectic coordinate transformations which are consistent with a special triangulation of phase space [12].

4 Concluding Remarks

We have seen that DTH dynamics reproduces, in some form, several of the distinctive properties of Hamiltonian dynamics. These include symplecticness, exact conservation of the Hamiltonian, preservation of quadratic conservation laws and coordinate invariance with respect to linear, symplectic coordinate transformations. A property of DTH dynamics not possessed by Hamiltonian dynamics is the dynamic behavior of time. This property needs to be explored further.

We have chosen in this paper to view DTH dynamics from a discrete modeling perspective, focusing on properties instead of error analysis or computational efficiency. Simulation results for the simple pendulum and a one-degree of freedom inverse-square-law system are given in [13]. Simulation results for Kepler's problem are given in [12]. A detailed error analysis and a computational efficiency study have not yet been completed.

For small time steps, the DTH equations are not as easy to solve as the equations of the implicit midpoint and trapezoid schemes. Computer simulations run to date have used a nested Newton iteration scheme, first to solve for $\overline{z}^{(k)}$ and then to solve for λ_k. Quadratic convergence of the nested iterations is proved in [12] and described in detail in [13]. Recently, Ander Murua [10] has suggested that more efficient solution techniques are possible. These are currently under study.

References

[1] A D'Innocenzo, L. Renna, and P. Rotelli. Some studies in discrete mechanics. *European Journal of Physics*, 8:245–252, 1987.

[2] Zhong Ge. Equivariant symplectic difference schemes and generating functions. *Physica D*, 49:376–386, 1991.

[3] Herbert Goldstein. *Classical Mechanics*. Addison-Wesley, Reading, MA, 1980.

[4] Donald Greenspan. *Discrete Models*. Addison-Wesley, Reading, MA, 1973.

[5] Donald Greenspan. *Discrete Numerical Methods in Physics and Engineering*. Academic Press, New York, NY, 1974.

[6] Andrzej Horzela, Edward Kapuscik, Jaroslaw Kempczynzki, and Charles Uzes. On discrete models of space-time. *Progress of Theoretical Physics*, 88(6):1065–1070, 1992.

[7] Cornelius Lanczos. *The Variational Principles of Mechanics*. Dover, Mineola, NY, 1970.

[8] T. D. Lee. Difference equations and conservation laws. *Journal of Statistical Physics*, 46(5/6):843–860, 1987.

[9] T.D. Lee. Can time be a discrete dynamic variable? *Physics Letters*, 122B(3/4):217–220, 1983.

[10] Ander Murua, 1997. private communication.

[11] J.M. Sanz-Serna and M.P. Calvo. *Numerical Hamiltonian Problems*. Chapman and Hall, New York, NY, 1994.

[12] Yosi Shibberu. *Discrete-Time Hamiltonian Dynamics*. PhD thesis, U. of Texas at Arlington, 1992.

[13] Yosi Shibberu. Time-discretization of hamiltonian dynamical systems. *Computers and Mathematics with Applications*, 28(10-12):123–145, 1994.

[14] Jeffrey M. Wendlandt and Jerrold E. Marsden. Mechanical integrators derived from a discrete variational principle. Technical Report CDS 96-013, California Institute of Technology, 1996.