Time-Discretization of Hamiltonian Dynamical Systems

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Abstract—Difference equations for Hamiltonian systems are derived from a discrete variational principle. The difference equations completely determine piecewise-linear, continuous trajectories which exactly conserve the Hamiltonian function at the midpoints of each linear segment. A generating function exists for transformations between the vertices of the trajectories. Existence and uniqueness results are present as well as simulation results for a simple pendulum and an inverse square law system.

1. INTRODUCTION

Hamiltonian systems are used in a wide variety of applications ranging in scope from quantum mechanics to optimal control theory. Computational methods which preserve their special structure are, therefore, of considerable interest.

Newtonian potential systems, a subclass of Hamiltonian systems, can be simulated by using the discrete mechanics equations developed by D. Greenspan [1,2]. These equations are equivariant with respect to rotation, translation, and uniform motion. For the Kepler problem, for example, the equations exactly conserve energy and angular momentum in Cartesian coordinates. R. Labudde [3] has extended the discrete mechanics of Greenspan to include a wide variety of Hamiltonian systems.

More recently, using a Lagrangian formulation, T. D. Lee developed a discrete mechanics in which trajectories in the configuration space of a system are assumed to be piecewise-linear and continuous [4]. The average value of the energy over each linear segment of the trajectory is conserved at each time step. A distinctive feature of this discrete mechanics is that time plays the role of a dynamic variable.

Symplectic integration schemes for Hamiltonian systems have received increased interest in recent years. Y.-H. Wu has shown that such schemes admit a natural, discrete variational principle [5]. In this way, symplectic schemes may be viewed as a type of discrete mechanics.

Discrete mechanics schemes are distinguished from conventional numerical schemes in that they are based on fundamental principles as opposed to approximations of differential equations derived from continuum mechanics. In fact, T. D. Lee suggests that discrete mechanics may be even more fundamental than continuum mechanics [4]. The finiteness of physical reality and the dilemmas that the concept of infinity can introduce in the continuum theory have been pointed out by Greenspan [1]. Such dilemmas do not occur in the discrete theory.

In this article, we describe a discrete-time theory for Hamiltonian dynamical systems which we call DTH dynamics [6]. ("DTH" is an abbreviation of "Discrete-Time Hamiltonian.") DTH dy-
namics is based on a variational principle which completely determines piecewise-linear, continuous trajectories in the extended phase space of a Hamiltonian system. In the spirit of Hamiltonian dynamics, DTH dynamics is completely symmetrical in the way position and momentum are treated. Like the discrete mechanics of Greenspan, DTH dynamics exactly conserves energy and conserved quadratic functions such as angular momentum. As in the discrete mechanics of T. D. Lee, time is treated as a dependent variable. For the simple harmonic oscillator, the DTH equations of motion reduce to the conventional trapezoidal and midpoint schemes commonly used to integrate differential equations.

We focus in this article on the basic ideas of DTH dynamics for the case of autonomous systems with one degree of freedom. (Generalizations to nonautonomous systems with n-degrees of freedom are given in [6].) We begin by reviewing the variational principles of mechanical systems in Section 2. In Section 3, we introduce notation for describing piecewise-linear, continuous functions. In Section 4, we motivate the “DTH principle of stationary action”—the variational principle on which DTH dynamics is based. Basic properties of DTH dynamics are described in Section 5 and simulation results for two Newtonian potential systems are presented in Section 6. Finally, in Section 7 we present, without proof, results for nonautonomous systems with n-degrees of freedom.

2. VARIATIONAL PRINCIPLES OF MECHANICS

Hamilton's principle is probably the most widely known variational principle of mechanics. This principle states that the integral \( I \) given by (1) is stationary for the trajectory \( q(t) \) of a dynamical system with Lagrangian function \( L(q, \dot{q}) \) (see [7]).

\[
I = \int_{t_0}^{t_f} L(q(t), \dot{q}(t)) \, dt. \tag{1}
\]

The principle of least action is another variational principle of mechanics. The following motivation for the principle of least action is based on [8]. Consider now the Legendre transformation \( \dot{q} \rightarrow p \) and \( L(q, \dot{q}) \rightarrow H(q, p) \), where \( p \) and \( H(q, p) \) are given by

\[
p = \frac{\partial L(q, \dot{q})}{\partial \dot{q}}, \tag{2}
\]

\[
H(q, p) = p\dot{q} - L(q, \dot{q}). \tag{3}
\]

(For the problems to be considered, \( \dot{q}(q, p) \) in (3) can be obtained by solving for \( \dot{q} \) in (2).) Under Legendre’s transformation, \( I \) can be expressed as

\[
I = \int_{t_0}^{t_f} (pq - H(q, p)) \, dt. \tag{4}
\]

Consider a reparametrization of time given by \( t = t(\tau) \). With this reparametrization, (4) becomes

\[
I = \int_{t_0}^{t_f} \left( p \frac{dq}{d\tau} + \frac{H(q, p)}{d\tau} \right) d\tau. \tag{5}
\]

Define \( \varphi = -H(q, p) \) and substitute \( \varphi \) in (5).

\[
I = \int_{t_0}^{t_f} \left( p \frac{dq}{d\tau} + \varphi \frac{dt}{d\tau} \right) d\tau. \tag{6}
\]

The integral (6) is called the action integral of a Hamiltonian dynamical system. The structure of (6) suggests that just as \( p \) is the momentum coordinate corresponding to the position coordinate \( q \), \( \varphi \) is the momentum coordinate corresponding to the time coordinate \( t \). (It is important to note that the variable \( t \) in (6) is a dependent variable, the independent variable being \( \tau \).)
DEFINITION 1. (Action Integral) Assume \( p(\tau), q(\tau), \varphi(\tau), \) and \( t(\tau) \) are differentiable functions of \( \tau \) on the interval \([\tau_0, \tau_T]\). The action integral of a Hamiltonian dynamical system is defined to be

\[
A(p(\tau), q(\tau), \varphi(\tau), t(\tau)) = \int_{\tau_0}^{\tau_T} \left( p(\tau) \frac{dq(\tau)}{d\tau} + \varphi(\tau) \frac{dt(\tau)}{d\tau} \right) d\tau.
\]

The trajectory of a Hamiltonian dynamical system can be obtained from the following principle.

DEFINITION 2. (Principle of Least Action) The trajectory of a Hamiltonian dynamical system with Hamiltonian function \( H(q, p) \) is given by functions \( p(t), q(t), \varphi(t), \) and \( t(\tau) \), which cause the action integral to be stationary under the constraint

\[
\varphi + H(q, p) = 0.
\]

The endpoints of \( q(T) \) and \( t(\tau) \) are assumed to be fixed.

The constraint (8) in Definition 2 is necessary because \( p \) is defined to be equal to \(-H(q, p)\) in (6), and thus, \( \varphi \) is not independent from \( p \) and \( q \).

The equations of motion for a Hamiltonian system can be obtained from the principle of least action as is shown in the following theorem. A discrete version of the principle of least action will be used in Theorem 3 to derive discrete-time equations.

THEOREM 1. The trajectory of a Hamiltonian dynamical system with the Hamiltonian function \( H(q, p) \) and initial conditions \( q(\tau_0) = q_0, p(\tau_0) = p_0, t(\tau_0) = 0, \) and \( \varphi(\tau_0) = -H(q_0, p_0) \) is a solution of the following system of differential equations.

\[
\frac{dq}{d\tau} = \lambda(\tau) \frac{\partial H(q, p)}{\partial p},
\]

\[
\frac{dp}{d\tau} = -\lambda(\tau) \frac{\partial H(q, p)}{\partial q},
\]

\[
\frac{dt}{d\tau} = \lambda(\tau),
\]

\[
\frac{d\varphi}{d\tau} = 0.
\]

The function \( \lambda(\tau) \) is an arbitrary function which determines the parametrization of the trajectory.

PROOF. The principle of least action states that the trajectory of a Hamiltonian system causes the action integral (7) to be stationary when subject to the constraint (8). Define

\[
g(q, p, \varphi) = \varphi + H(q, p)
\]

\[
f(p(\tau), q(\tau), \varphi(\tau), t(\tau), \lambda(\tau)) = A(p(\tau), q(\tau), \varphi(\tau), t(\tau)) - \int_{\tau_0}^{\tau_T} \lambda(\tau) g(q(\tau), p(\tau), \varphi(\tau)) d\tau,
\]

where \( \lambda(\tau) \) is a differentiable function of \( \tau \). From (7), (13), and (14),

\[
f(p(\tau), q(\tau), \varphi(\tau), t(\tau), \lambda(\tau)) = \int_{\tau_0}^{\tau_T} L(q(\tau), q'(\tau), p(\tau), t'(\tau), \varphi(\tau), \lambda(\tau)) d\tau,
\]

where

\[
L(q, q', p, t', \varphi, \lambda) = pq' + \varphi t' - \lambda(\varphi + H(q, p)),
\]

and where the notation \( q' \) and \( t' \) has been used for \( \frac{dq(\tau)}{d\tau} \) and \( \frac{dt(\tau)}{d\tau} \). The action integral subject to \( g(q, p, \varphi) = 0 \) is stationary when the functional \( f \) given by (15) is stationary. But the functional \( f \)
is stationary when the following Euler-Lagrange equations are satisfied.

\[
\frac{d}{d\tau} \left( \frac{\partial L}{\partial p'} \right) - \frac{\partial L}{\partial p} = 0, \tag{17}
\]
\[
\frac{d}{d\tau} \left( \frac{\partial L}{\partial q'} \right) - \frac{\partial L}{\partial q} = 0, \tag{18}
\]
\[
\frac{d}{d\tau} \left( \frac{\partial L}{\partial \lambda'} \right) - \frac{\partial L}{\partial \lambda} = 0. \tag{21}
\]

By substituting the Lagrangian (16) in equations (17)-(20), we obtain equations (9)-(12). Substituting (16) in (21) results in the identity

\[
\text{CLAIM:} \text{ Equations (9)-(12) imply equation (22) independently of equation (21).}
\]

\[
\text{PROOF OF THE CLAIM:} \quad \frac{dH(q(\tau),p(\tau))}{d\tau} = \lambda \left( \frac{\partial H}{\partial q} \frac{dq}{d\tau} + \frac{\partial H}{\partial p} \frac{dp}{d\tau} \right) = 0. \tag{23}
\]

Substituting (9) and (10) in (23), we have that

\[
\frac{dH(q(\tau),p(\tau))}{d\tau} = \lambda \left( \frac{\partial H}{\partial q} \frac{dq}{d\tau} + \frac{\partial H}{\partial p} \frac{dp}{d\tau} \right) = 0. \tag{24}
\]

Therefore, (9) and (10) imply that \( H(q(\tau),p(\tau)) \) is constant. Equation (12) implies \( \varphi(\tau) \) is constant also. We have then that

\[
\varphi(\tau) + H(q(\tau),p(\tau)) \equiv \varphi(\tau_0) + H(q(\tau_0),p(\tau_0)) = 0 \tag{25}
\]

as claimed, since from the initial conditions, \( q(\tau_0) = 0, p(\tau_0) = 0, \) and \( \varphi(\tau_0) = H(q_0,p_0). \)

The claim in the proof of Theorem 1 implies that for the Lagrangian (16), equation (21) is not independent from equation (17)-(20). The situation is very different for the discrete-time theory to be discussed shortly.

3. PIECEWISE-LINEAR CONTINUOUS FUNCTIONS

Assume the points \( \tau_k, \) \( k = 0,1,\ldots N, \) partition the interval \([\tau_0, \tau_N]\) into \( N \) equal intervals of length \( \Delta \tau. \)

\[
\tau_k = \tau_0 + k\Delta \tau, \quad k = 0,1,\ldots N, \tag{26}
\]
\[
\Delta \tau = \frac{\tau_N - \tau_0}{N}. \tag{27}
\]

Assume \( \hat{x}(\tau) \) is a piecewise-linear, continuous function of \( \tau \) as shown in Figure 1. Define

\[
x_k = \hat{x}(\tau_k), \quad k = 0,1,\ldots N. \tag{28}
\]

These \( x_k \)'s will be called vertices of \( \hat{x}(\tau). \) Clearly, \( \hat{x}(\tau) \) is completely determined by its vertices. Define

\[
x_k = x_k(x_{k+1},x_k) = \frac{x_{k+1} + x_k}{2}, \quad k = 0,1,\ldots N - 1, \tag{29}
\]
\[
x_k = x_k(x_{k+1},x_k) = \frac{x_{k+1} - x_k}{\Delta \tau}, \quad k = 0,1,\ldots N - 1. \tag{30}
\]
Figure 1. A piecewise-linear, continuous function.

(Note that $\xi_k$ in (30) is not the derivative of $\xi_k$ and that both $\xi_k$ and $\xi'_k$ are defined at the midpoints of the partition of $[\tau_0, \tau_N]$.) Since $\dot{\chi}(\tau)$ is piecewise-linear, it can be expressed in terms of the values of $\xi_k$ and $\xi'_k$ in the following way.

$$\dot{\chi}(\tau) = \begin{cases} \xi_k + \xi'_k(\tau - \tau_k), & \tau_k \leq \tau < \tau_{k+1}, \quad k = 0, 1, \ldots, N - 1, \\ \xi_N, & \tau = \tau_N, \end{cases}$$

where

$$\xi_k = \frac{\tau_{k+1} - \tau_k}{2}.$$  

Thus, $\dot{\chi}(\tau)$ is completely determined by the values of $\xi_k$ and $\xi'_k$, $k = 0, 1, \ldots N - 1$. Since $\dot{\chi}(\tau)$ is continuous, $\xi_k$ and $\xi'_k$ must satisfy the following continuity constraint.

**Lemma 1. (Continuity Constraint)** A piecewise-linear function is continuous if and only if

$$\frac{\xi_{k+1} - \xi_k}{\Delta \tau} = \frac{\xi'_{k+1} + \xi'_k}{2}.$$  

The proof of Lemma 1 is given in [6]. The following lemma will be used in the proof of Theorem 3.

**Lemma 2.** From (29) and (30) it follows that

$$\frac{\partial \xi_k}{\partial x_k} = \frac{1}{2}, \quad \frac{\partial \xi'_k}{\partial x_k} = -\frac{1}{\Delta \tau}, \quad \frac{\partial \xi_k}{\partial x_{k+1}} = \frac{1}{2}, \quad \frac{\partial \xi'_k}{\partial x_{k+1}} = \frac{1}{\Delta \tau},$$

for $k = 0, 1, \ldots N - 1$.

### 4. DTH PRINCIPLE OF STATIONARY ACTION

We now motivate the discrete variational principle on which DTH dynamics is based. (Recall "DTH" is an abbreviation for discrete-time Hamiltonian.) First, we define the discrete action of a Hamiltonian system as follows.

**Definition 3. (Discrete Action)** For piecewise-linear, continuous functions, $\dot{p}(\tau)$, $\dot{q}(\tau)$, $\dot{\phi}(\tau)$, and $\dot{\chi}(\tau)$ defined on a uniform partition of $[\tau_0, \tau_N]$, the discrete action $A_N$ of a Hamiltonian system is defined to be

$$A_N(p_0 \cdots p_N, q_0 \cdots q_N, p_0 \cdots p_N, t_0 \cdots t_N) = \sum_{i=0}^{N-1} (\overline{p}_i \overline{q}'_i + \overline{p}'_i \overline{q}_i) \Delta \tau.$$  

The above definition is motivated by the following theorem which states that for piecewise-linear, continuous functions, the action integral given by Definition 1 is exactly equal to the discrete action in Definition 3.

**Theorem 2.** For piecewise-linear, continuous functions, the action integral and the discrete action are equal.

$$A(\dot{p}(\tau), \dot{q}(\tau), \dot{\phi}(\tau), \dot{\chi}(\tau)) = A_N(p_0 \cdots p_N, q_0 \cdots q_N, p_0 \cdots p_N, t_0 \cdots t_N).$$
PROOF. From Definition 1,
\[
A(\dot{p}(\tau),\dot{q}(\tau),\dot{\varphi}(\tau),\dot{t}(\tau)) = \int_{\tau_0}^{\tau_N} \left( p(\tau) \frac{dq(\tau)}{d\tau} + q(\tau) \frac{dp(\tau)}{d\tau} \right) d\tau.
\]
Since $\dot{q}(\tau)$ and $\dot{t}(\tau)$ are piecewise-linear, it follows from (31) that $\frac{dq(\tau)}{d\tau} = \overline{q}_i'$ and $\frac{dt(\tau)}{d\tau} = \overline{t}_i'$, for $\tau_i < \tau < \tau_{i+1}$, $i = 0, 1, \ldots N - 1$. Therefore,
\[
A(\dot{p}(\tau),\dot{q}(\tau),\dot{\varphi}(\tau),\dot{t}(\tau)) = \sum_{i=0}^{N-1} \left( \overline{q}_i' \int_{\tau_i}^{\tau_{i+1}} \dot{p}(\tau) d\tau + \overline{t}_i' \int_{\tau_i}^{\tau_{i+1}} \dot{\varphi}(\tau) d\tau \right).
\]
Since
\[
\int_{\tau_i}^{\tau_{i+1}} \dot{p}(\tau) d\tau = \overline{p}_i \Delta \tau,
\]
and
\[
\int_{\tau_i}^{\tau_{i+1}} \dot{\varphi}(\tau) d\tau = \overline{\varphi}_i \Delta \tau,
\]
we have
\[
A(\dot{p}(\tau),\dot{q}(\tau),\dot{\varphi}(\tau),\dot{t}(\tau)) = \sum_{i=0}^{N-1} \left( \overline{q}_i' \overline{p}_i \Delta \tau + \overline{t}_i' \overline{\varphi}_i \Delta \tau \right) = A_N.
\]
We are now in a position to present a discrete version of the principle of least action.
DEFINITION 4. (Discrete Principle of Least Action) The discrete-time trajectory of a Hamiltonian system with Hamiltonian function $H(q,p)$ is given by piecewise-linear, continuous functions $\ddot{q}(\tau), \ddot{q}(\tau), \ddot{\varphi}(\tau)$, and $\ddot{t}(\tau)$ which cause the discrete action to be stationary under the constraint
\[
\overline{p}_k + H(\overline{q}_k,\overline{p}_k) = 0, \quad k = 0, 1, \ldots N - 1.
\]
The endpoints $q_0, q_N, \varphi_0, \varphi_N, t_0$, and $t_N$ are assumed to be fixed.

Observe that in the discrete version of the principle of least action, constraint (8) is enforced only at the midpoints of a piecewise-linear, continuous trajectory.

We now use the discrete principle of least action to derive difference equations for Hamiltonian systems.

THEOREM 3. The discrete-time trajectory of a Hamiltonian system with the Hamiltonian function $H(q,p)$ and initial conditions $\ddot{q}(t_0) = \ddot{q}_0, \ddot{q}(t_0) = \ddot{p}_0, \ddot{\varphi}(t_0) = \ddot{\varphi}_0, \ddot{t}(t_0) = \ddot{t}_0, \ddot{\varphi}(t_0) = \ddot{\varphi}_0 = -H(\overline{q}_0,\overline{p}_0)$ is a solution of the following system of equations.
\[
\begin{align*}
\frac{\overline{q}_{k+1} - \overline{q}_k}{\Delta \tau} &= \frac{1}{2} \left[ \lambda_{k+1} \frac{\partial H(\overline{q}_{k+1},\overline{p}_{k+1})}{\partial \overline{p}_{k+1}} + \lambda_k \frac{\partial H(\overline{q}_k,\overline{p}_k)}{\partial \overline{p}_k} \right], \\
\frac{\overline{p}_{k+1} - \overline{p}_k}{\Delta \tau} &= -\frac{1}{2} \left[ \lambda_{k+1} \frac{\partial H(\overline{q}_{k+1},\overline{p}_{k+1})}{\partial \overline{q}_{k+1}} + \lambda_k \frac{\partial H(\overline{q}_k,\overline{p}_k)}{\partial \overline{q}_k} \right], \\
\frac{\ddot{t}_{k+1} - \ddot{t}_k}{\Delta \tau} &= \frac{1}{2} \left[ \lambda_{k+1} + \lambda_k \right], \\
\frac{\ddot{\varphi}_{k+1} - \ddot{\varphi}_k}{\Delta \tau} &= 0,
\end{align*}
\]
where $k = 0, 1, \ldots N - 2$.
\[
\begin{align*}
\ddot{q}_k &= \lambda_k \frac{\partial H(\overline{q}_k,\overline{p}_k)}{\partial \overline{p}_k}, \\
\ddot{\varphi}_k &= \lambda_k, \\
0 &= \ddot{t}_k + H(\overline{q}_k,\overline{p}_k),
\end{align*}
\]
where $k = 0, 1, \ldots N - 1$.  

\[
\]
PROOF. By the discrete principle of least action, a discrete-time trajectory of a Hamiltonian system is given by piecewise-linear, continuous functions which cause the discrete action $A_N$ to be stationary under the constraint

$$\varphi_k + H(q_k, p_k) = 0, \quad k = 0, 1, \ldots, N - 1,$$

where the endpoints $q_0, q_N, t_0$ and $t_N$ are fixed. Let

$$g(q_k, \bar{p}_k, \overline{p}_k) = \bar{p}_k + H(q_k, \bar{p}_k),$$

and let

$$f(p_0 \cdots p_N, q_0 \cdots q_N, \varphi_0 \cdots \varphi_N, t_0 \cdots t_N, \lambda_0 \cdots \lambda_{N-1}) = A_N - \sum_{i=0}^{N-1} \lambda_i g(q_i, \bar{p}_i, \overline{p}_i),$$

where $\lambda_i$ in (42) are Lagrange multipliers. We have then that $A_N$, subject to $g(q_k, \bar{p}_k, \overline{p}_k) = 0$ for $k = 0, 1, \ldots, N - 1$, is stationary when the partial derivatives of $f$ with the possible exception of $\frac{\partial f}{\partial p_0}, \frac{\partial f}{\partial q_0}, \frac{\partial f}{\partial t_0}$, and $\frac{\partial f}{\partial t_N}$ are equal to zero. The exception is necessary because the endpoints $q_0, q_N, t_0$, and $t_N$ are assumed to be fixed, and therefore, partial derivatives with respect to these variables may not be zero. From (41), (42), and the definition of $A_N$,

$$f = \sum_{i=0}^{N-1} \left[ \bar{p}_i \bar{q}_i' + \overline{p}_i \overline{q}_i' - \lambda_i (\bar{p}_i + H(q_i, \bar{p}_i)) \right] \Delta \tau.$$  (43)

Equating to zero the partial derivatives $\frac{\partial f}{\partial p_k}$, $\frac{\partial f}{\partial q_k}$, $\frac{\partial f}{\partial t_k}$, and $\frac{\partial f}{\partial t_{k+1}}$, for $k = 0, 1, \ldots, N - 2$, implies equations (34)–(37) as follows. From (43), for $k = 0, 1, \ldots, N - 2,$

$$\frac{\partial f}{\partial p_{k+1}} = \sum_{i=0}^{N-1} \left[ \bar{p}_i \bar{q}_i' + \overline{p}_i \overline{q}_i' - \lambda_i (\bar{p}_i + H(q_i, \bar{p}_i)) \right] \Delta \tau.$$  (44)

where we have used the abbreviation $\bar{H}_i$ for $H(q_i, \bar{p}_i)$. The terms on the right hand side of (44) depend on $p_{k+1}$ only for $i = k$ and $i = k + 1$. Therefore,

$$\frac{\partial f}{\partial p_{k+1}} = \frac{\partial}{\partial p_{k+1}} \left[ p_k q_k' - \lambda_k \bar{H}_k + \bar{p}_{k+1} \bar{q}_{k+1}' - \lambda_{k+1} \bar{H}_{k+1} \right] \Delta \tau$$

$$= \left[ \frac{\partial p_k}{\partial p_{k+1}} \bar{q}_k' - \lambda_k \frac{\partial \bar{H}_k}{\partial p_k} + \frac{\partial \bar{p}_{k+1}}{\partial p_{k+1}} \bar{q}_{k+1}' - \lambda_{k+1} \frac{\partial \bar{H}_{k+1}}{\partial p_{k+1}} \right].$$

From Lemma 2, $\frac{\partial p_k}{\partial p_{k+1}} = 1/2$ and $\frac{\partial \bar{p}_{k+1}}{\partial p_{k+1}} = 1/2$. Therefore,

$$\frac{\partial f}{\partial p_{k+1}} = \left[ \bar{q}_{k+1}' + \bar{q}_k' \frac{1}{2} - \frac{1}{2} \left( \lambda_{k+1} \frac{\partial \bar{H}_{k+1}}{\partial p_{k+1}} + \lambda_k \frac{\partial \bar{H}_k}{\partial p_k} \right) \right] \Delta \tau.$$  (45)

From the continuity constraint on $\dot{q}(\tau)$ (Lemma 1)

$$\frac{\bar{q}_{k+1}' + \bar{q}_k'}{2} = \frac{\bar{q}_{k+1} - \bar{q}_k}{\Delta \tau}.$$  

Therefore,

$$\frac{\partial f}{\partial p_{k+1}} = \left[ \frac{\bar{q}_{k+1} - \bar{q}_k}{\Delta \tau} \frac{1}{2} \left( \lambda_{k+1} \frac{\partial \bar{H}_{k+1}}{\partial p_{k+1}} + \lambda_k \frac{\partial \bar{H}_k}{\partial p_k} \right) \right] \Delta \tau.$$  

from which it follows that $\frac{\partial f}{\partial p_{k+1}} = 0$ implies equation (34). Similarly,

$$\frac{\partial f}{\partial q_{k+1}} = \left[ \frac{\partial q_{k+1}'}{\partial q_{k+1}} - \lambda_k \frac{\partial \bar{H}_k}{\partial q_k} + \bar{p}_{k+1} \frac{\partial q_{k+1}'}{\partial q_{k+1}} - \lambda_{k+1} \frac{\partial \bar{H}_{k+1}}{\partial q_{k+1}} \right] \Delta \tau.$$
From Lemma 2, \( \frac{\partial q_{k+1}}{\partial q_{k+1}} = 1/\Delta \tau \) and \( \frac{\partial q_{k+1}}{\partial q_{k+1}} = -1/\Delta \tau \). Therefore,

\[
\frac{\partial f}{\partial q_k} = \left[ \frac{-\bar{q}_{k+1} - \bar{q}_k}{\Delta \tau} - \frac{1}{2} \left( \lambda_{k+1} \frac{\partial \bar{H}_{k+1}}{\partial q_{k+1}} + \lambda_k \frac{\partial \bar{H}_k}{\partial q_k} \right) \right] \Delta \tau.
\]

Thus, \( \frac{\partial f}{\partial q_{k+1}} = 0 \) implies equation (35). By equating \( \frac{\partial f}{\partial q_{k+1}} \) and \( \frac{\partial f}{\partial q_{k+1}} \) to zero, we can obtain equations (36) and (37) in a similar fashion. For \( k = 0, 1, \ldots, N - 1 \),

\[
\frac{\partial f}{\partial \lambda_k} = \frac{\partial}{\partial \lambda_k} \sum_{i=0}^{N-1} \left[ \bar{p}_i q_i' + \bar{p}_i H_i' - \lambda_i (\bar{q}_i + \bar{H}_i) \right] \Delta \tau
\]

(46)

Thus, \( \frac{\partial f}{\partial \lambda_k} \) to zero implies equation (40). Now since \( p_0, p_N, \varphi_0, \) and \( \varphi_N \) are free to vary, the function \( f \) is not stationary unless the partial derivative \( \frac{\partial f}{\partial p_0}, \frac{\partial f}{\partial p_N}, \frac{\partial f}{\partial q_0} \) and \( \frac{\partial f}{\partial q_N} \) are also equal to zero. Equating these partial derivatives to zero implies equations (38)-(39) as follows. From (43), we have

\[
\frac{\partial f}{\partial p_0} = \frac{\partial}{\partial p_0} \sum_{i=0}^{N-1} \left[ \bar{p}_i q_i' + \bar{p}_i H_i' - \lambda_i (\bar{q}_i + \bar{H}_i) \right] \Delta \tau.
\]

(48a)

The terms on the right side of (48a) depend on \( p_0 \) only for \( i = 0 \). Therefore,

\[
\frac{\partial f}{\partial p_0} = \frac{\partial}{\partial p_0} \left[ p_0 q_0' - \lambda_0 H_0 \right] \Delta \tau,
\]

(48b)

\[
- \frac{\partial p_0}{p_0} q_0' + \lambda_0 \frac{\partial H_0}{p_0} \frac{\partial p_0}{p_0} \Delta \tau,
\]

(49)

\[
q_0' - \lambda_0 \frac{\partial H_0}{p_0} \frac{\partial p_0}{p_0} \Delta \tau.
\]

(50)

From Lemma 2, \( \frac{\partial q_k}{\partial q_k} = 1/2 \neq 0 \). Therefore, \( \frac{\partial f}{\partial p_0} = 0 \) implies

\[
q_0' = \lambda_0 \frac{\partial H_0}{p_0}.
\]

(51)

Similarly, \( \frac{\partial f}{\partial p_N} = 0 \) implies

\[
q_N' = \lambda_N.
\]

(52)

Using the continuity constraints on \( q'(\tau) \) and \( \bar{q}'(\tau) \), we can express equations (34) and (36) as follows.

\[
\frac{q_{k+1}'}{2} + \frac{q_k'}{2} = \frac{1}{2} \left[ \lambda_{k+1} \frac{\partial \bar{H}_{k+1}}{\partial p_{k+1}} + \lambda_k \frac{\partial \bar{H}_k}{\partial p_k} \right],
\]

(53)

\[
\frac{\bar{q}_{k+1}'}{2} + \frac{\bar{q}_k'}{2} = \frac{1}{2} \left[ \lambda_{k+1} + \lambda_k \right].
\]

(54)

We now show by induction that equations (51) and (52) hold true for \( k = 1, 2, \ldots, N - 1 \). Assume for some \( k, 0 \leq k \leq N - 2 \), that

\[
q_k' = \lambda_k \frac{\partial \bar{H}_k}{\partial p_k},
\]

(55)

\[
\bar{q}_k' = \lambda_k.
\]

(56)

Substituting for \( q_k' \) and \( \bar{q}_k' \) in (53) and (54) and solving for \( q_{k+1}' \) and \( \bar{q}_{k+1}' \), we have

\[
q_{k+1}' = \lambda_{k+1} \frac{\partial \bar{H}_{k+1}}{\partial p_{k+1}},
\]

(57)

\[
\bar{q}_{k+1}' = \lambda_{k+1}.
\]

(58)
From (51) and (52), we see that (55) and (56) hold true for \( k = 0 \). Therefore, by induction, equations (55) and (56) must hold true for all \( k = 0, 1, \ldots N - 1 \).

Finally, we evaluate \( \frac{\partial f}{\partial p_N} \) and \( \frac{\partial f}{\partial p_N} \).

\[
\frac{\partial f}{\partial p_N} = \frac{\partial}{\partial p_N} \left[ \tilde{p}_{N-1} \lambda - \lambda N^{-1} \tilde{p}_{N-1} \right] \frac{\partial ^2 H}{\partial p_{N-1}^2} \Delta \tau,
\]

\[
= \left[ \lambda N^{-1} - \lambda N^{-1} \frac{\partial ^2 H}{\partial p_{N-1}^2} \right] \frac{\partial p_{N-1} \Delta \tau}{}.
\]

Thus, \( \frac{\partial f}{\partial p_N} = 0 \) implies

\[
\lambda N^{-1} = \frac{\partial H}{\partial p_{N-1}}.
\]

Similarly, \( \frac{\partial f}{\partial p_N} = 0 \) implies

\[
\lambda N^{-1} = \frac{\partial H}{\partial p_{N-1}}.
\]

Observe that both (61) and (62) are in agreement with equations (38) and (39) for \( k = N - 1 \).

The discrete principle of least action described above does not completely determine piecewise-linear, continuous trajectories. As we can see from the equations of Theorem 3, the discrete principle of least action only determines the values of \( \bar{p}_k, \bar{q}_k, \bar{t}_k, \bar{\omega}_k \), and \( \lambda_k \) and the values of \( \bar{q}_k \) and \( \bar{t}_k \). The values of \( \bar{p}_k \) and \( \bar{\omega}_k \) remain indeterminate. Clearly, equations (61) and (62) imply (38) and (39) independently of equations (51) and (52). Thus, allowing free variations in the momentum coordinates at \( k = 0 \) yields the same equations as the equations obtained by allowing free variations in the momentum coordinates at \( k = N \). We now present a new variational principle which completely determines piecewise-linear, continuous trajectories for both position and momentum coordinates. The new principle is based on a new definition for the discrete action and it permits variations in the momentum coordinates at \( k = 0 \) and variations in the position coordinates at \( k = N \).

**Definition 5.** (Modified Discrete Action) For piecewise-linear, continuous functions \( \bar{p}(\tau), \bar{q}(\tau), \bar{\dot{q}}(\tau), \) and \( \bar{t}(\tau) \) defined on a uniform partition of \([\tau_0, \tau_N]\), the modified discrete action \( A_N \) of a Hamiltonian system is defined to be

\[
A_N(p_0 \cdots p_N, q_0 \cdots q_N, \bar{p}_0 \cdots \bar{p}_N, t_0 \cdots t_N) = \frac{1}{2} \left[ q_0 \bar{p}_0 + t_0 \bar{q}_0 + \sum_{k=1}^{N-1} \left( \frac{1}{2} (q_k \bar{p}_k - q_k \bar{p}_k) + \frac{1}{2} (\bar{t}_k \bar{p}_k - \bar{t}_k \bar{p}_k) \right) \Delta \tau + \frac{1}{2} (q_N \bar{p}_N + t_N \bar{q}_N). \right.
\]

**Definition 6.** (DTH Principle of Stationary Action) The DTH trajectory of a Hamiltonian system with Hamiltonian function \( H(q, p) \) is given by piecewise-linear, continuous functions \( \bar{p}(\tau), \bar{q}(\tau), \bar{\dot{q}}(\tau), \) and \( \bar{t}(\tau) \) which cause the modified discrete action to be stationary under the constraint

\[
\bar{p}_k + H(\bar{q}_k, \bar{p}_k) = 0, \quad k = 0, 1, \ldots N - 1.
\]

The endpoints \( q_0, t_0, \) and \( p_N, \bar{p}_N \) are assumed to be fixed.

In the following theorem, the DTH principle of stationary action is used to derive the difference equations of DTH dynamics.

**Theorem 4.** (DTH Equations of Dynamics) The DTH trajectory of a Hamiltonian system with Hamiltonian function \( H(q, p) \) and initial conditions \( \bar{q}(t_0) = \bar{q}_0, \bar{p}(t_0) = \bar{p}_0, \bar{t}(t_0) = 0, \bar{\dot{q}}(t_0) = -H(\bar{q}_0, \bar{p}_0) \) is a solution of the following system of equations.

\[
\frac{\bar{q}_{k+1} - \bar{q}_k}{\Delta \tau} = \frac{1}{2} \left[ \lambda_{k+1} \frac{\partial H(\bar{q}_{k+1}, \bar{p}_{k+1})}{\partial \bar{p}_{k+1}} + \lambda_k \frac{\partial H(\bar{q}_k, \bar{p}_k)}{\partial \bar{p}_k} \right],
\]
\[ \frac{\bar{p}_{k+1} - \bar{p}_k}{\Delta \tau} = -\frac{1}{2} \left[ \lambda_{k+1} \frac{\partial H(\bar{q}_{k+1}, \bar{p}_{k+1})}{\partial \bar{q}_{k+1}} + \lambda_k \frac{\partial H(\bar{q}_k, \bar{p}_k)}{\partial \bar{q}_k} \right], \quad (65) \]

\[ \frac{\bar{t}_{k+1} - \bar{t}_k}{\Delta \tau} = \frac{1}{2} [\lambda_{k+1} + \lambda_k], \quad (66) \]

\[ \frac{\bar{p}_{k+1} - \bar{p}_k}{\Delta \tau} = 0, \quad (67) \]

where \( k = 0, 1, \ldots N - 2, \)

\[ \bar{q}_k' = \lambda_k \frac{\partial H(\bar{q}_k, \bar{p}_k)}{\partial \bar{p}_k}, \quad (68) \]

\[ \bar{p}_k' = -\lambda_k \frac{\partial H(\bar{q}_k, \bar{p}_k)}{\partial \bar{q}_k}, \quad (69) \]

\[ \bar{t}_k' = \lambda_k, \quad (70) \]

\[ \bar{p}_k' = 0, \quad (71) \]

\[ 0 = \bar{p}_k + H(\bar{q}_k, \bar{p}_k), \quad (72) \]

where \( k = 0, 1, \ldots N - 1. \)

**Proof.** The DTH principle of stationary action states that the discrete-time trajectory of a Hamiltonian system is given by piecewise-linear, continuous functions which cause the modified discrete action \( \mathcal{A}_N \) to be stationary under the constraint

\[ \bar{p}_k + H(\bar{q}_k, \bar{p}_k) = 0, \quad k = 0, 1, \ldots N - 1, \]

where the endpoints \( q_0, t_0, p_N, \) and \( p_N \) are fixed. As in the proof of Theorem 3, let

\[ g(\bar{q}_k, \bar{p}_k, \bar{p}_k) = \bar{p}_k + H(\bar{q}_k, \bar{p}_k), \quad (73) \]

and now let

\[ f(p_0 \cdots p_N, q_0 \cdots q_N, \bar{q}_0 \cdots \bar{q}_N, \bar{p}_0 \cdots \bar{p}_N, \lambda_0 \cdots \lambda_{N-1}) = \mathcal{A}_N + \sum_{i=0}^{N-1} \lambda_i g(\bar{q}_i, \bar{p}_i, \bar{p}_i), \quad (74) \]

where in (74) we have used the modified discrete action \( \mathcal{A}_N \). We have then that \( \mathcal{A}_N \), subject to \( g(\bar{q}_k, \bar{p}_k, \bar{p}_k) = 0 \) for \( k = 0, 1, \ldots N - 1, \) is stationary when the partial derivatives of \( f \) with the possible exception of \( \frac{\partial f}{\partial \bar{q}_0}, \frac{\partial f}{\partial \bar{p}_0}, \frac{\partial f}{\partial \bar{p}_N} \) and \( \frac{\partial f}{\partial \bar{q}_N} \) are equal to zero. From (73), (74) and the definition of \( \mathcal{A}_N \)

\[ f = \frac{1}{2} (q_0 p_0 + t_0 \bar{p}_0) \]

\[ + \sum_{i=1}^{N-1} \left[ \frac{1}{2} (\bar{q}_i \bar{p}_i' - q_i' p_i) + \frac{1}{2} (\bar{t}_i \bar{p}_i' - t_i' \bar{p}_i) + \lambda_i (\bar{p}_i + \bar{H}_i) \right] \Delta \tau + \frac{1}{2} (q_N p_N + t_N \bar{p}_N). \quad (75) \]

where again we have used the abbreviation \( \bar{H}_i \) for \( H(\bar{q}_i, \bar{p}_i) \). Equating to zero the partial derivatives \( \frac{\partial f}{\partial \bar{q}_k}, \frac{\partial f}{\partial \bar{p}_k}, \frac{\partial f}{\partial \bar{p}_k} \) and \( \frac{\partial f}{\partial \bar{q}_k} \) for \( k = 0, 1, \ldots N - 2 \) implies equations (64)-(67) as follows. From (75) for \( k = 0, 1, \ldots N - 2 \)

\[ \frac{\partial f}{\partial \bar{p}_{k+1}} = \frac{\partial}{\partial \bar{p}_{k+1}} \left[ \frac{1}{2} (\bar{q}_k \bar{p}_k' - q_k' \bar{p}_k) + \frac{1}{2} (\bar{q}_{k+1} \bar{p}_{k+1} - q_{k+1}' \bar{p}_{k+1}) + (\lambda_k \bar{H}_k + \lambda_{k+1} \bar{H}_{k+1}) \right] \Delta \tau \]

\[ = \left[ \frac{1}{2} \bar{q}_k \left( \frac{1}{\Delta \tau} \right) - \frac{1}{2} \bar{q}_k' \left( \frac{1}{\Delta \tau} \right) + \frac{1}{2} \bar{q}_{k+1} \left( -\frac{1}{\Delta \tau} \right) \right. \]

\[ - \left. \frac{1}{2} \bar{q}_{k+1}' \left( \frac{1}{\Delta \tau} \right) + \lambda_k \frac{\partial \bar{H}_k}{\partial \bar{p}_k} \left( \frac{1}{\Delta \tau} \right) + \lambda_{k+1} \frac{\partial \bar{H}_{k+1}}{\partial \bar{p}_{k+1}} \left( \frac{1}{\Delta \tau} \right) \right] \Delta \tau \]
Time-Discretization

\[ \frac{\partial f}{\partial p_0} = \frac{\partial}{\partial p_0} \left[ \frac{1}{2} q_0 p_0 + \frac{1}{2} \left( q_0 p_0' - q_0 p_0 \right) \Delta \tau + \lambda_0 \frac{\partial H_0}{\partial p_0} \Delta \tau \right] \]

\[ = \frac{1}{2} q_0 + \frac{1}{2} \left[ q_0 \left( -\frac{1}{\Delta \tau} \right) - \frac{q_0'}{2} \right] \Delta \tau + \lambda_0 \frac{\partial H_0}{\partial p_0} \left( \frac{1}{2} \right) \Delta \tau \]

\[ = \frac{1}{2} \left[ \frac{q_0 - q_1}{\Delta \tau} + \lambda_0 \frac{\partial H_0}{\partial p_0} \right] \Delta \tau \]

\[ = \frac{1}{2} \left[ -\frac{q_0 + \lambda_0 \frac{\partial H_0}{\partial p_0}}{2} \right] \Delta \tau, \]

where we have used the fact that \( q_1 = \left( q_0 + \frac{q_0'}{2} \right) \). Therefore, \( \frac{\partial f}{\partial p_0} = 0 \) implies

\[ q_0' - \lambda_0 \frac{\partial H_0}{\partial p_0}. \]

Assume for some \( k = 0, 1, \ldots N - 2 \), that

\[ \bar{q}_k = \lambda_k \frac{\partial H_k}{\partial p_k}. \]

Then equation (64) and Lemma 1 imply that

\[ \bar{q}_{k+1} = \lambda_{k+1} \frac{\partial H_{k+1}}{\partial p_{k+1}}. \]

Since equation (77) holds true for \( k = 0 \), by induction we have established (68). Similarly,

\[ \frac{\partial f}{\partial q_N} = \frac{\partial}{\partial q_N} \left[ \frac{1}{2} q_N p_N + \frac{1}{2} \left( q_{N-1} p_{N-1} - q_{N-1}' \bar{p}_{N-1} \right) \Delta \tau + \lambda_{N-1} \frac{\partial H_{N-1}}{\partial q_{N-1}} \Delta \tau \right] \]

\[ = \frac{1}{2} q_N + \frac{1}{2} \left[ \left( \frac{1}{2} \right) p_{N-1}' - p_{N-1} - \frac{1}{2} \right] \Delta \tau + \lambda_{N-1} \frac{\partial H_{N-1}}{\partial q_{N-1}} \left( \frac{1}{2} \right) \Delta \tau \]

\[ = \frac{1}{2} \left[ p_{N-1} - \left( p_{N-1}' - \frac{\Delta \tau}{2} \right) + \lambda_{N-1} \frac{\partial H_{N-1}}{\partial q_{N-1}} \right] \Delta \tau \]

\[ = \frac{1}{2} \left[ p_{N-1} + \lambda_{N-1} \frac{\partial H_{N-1}}{\partial q_{N-1}} \right] \Delta \tau. \]

Thus, \( \frac{\partial f}{\partial q_N} = 0 \) implies

\[ p_{N-1}' = -\lambda_{N-1} \frac{\partial H_{N-1}}{\partial q_{N-1}}. \]

Using the continuity constraint on \( \dot{p}(\tau) \) and equations (65) and (79) we can, by induction, establish equation (69) in the same way equation (68) was established. Equations (70) and (71) are derived in a similar manner. Finally, equation (72) follows directly from the equation \( \frac{\partial f}{\partial \lambda_k} = 0 \), \( k = 0, 1, \ldots N - 1 \).
5. PROPERTIES OF DTH DYNAMICS

DTH dynamics has several interesting properties which we now describe. The function \( f \) given by equation (75) can be used to define a generating function for transformations between the vertices of a DTH trajectory.

**Theorem 5. (Generating Function for DTH Trajectories)** Assume

\[
S(q_0, t_0, p_N, \varphi_N) = f_{\phi, \dot{\phi}, \dot{\varphi}} \tag{80}
\]

where \( f \) on the right hand side of (80) is evaluated along DTH trajectories satisfying the boundary conditions \( \dot{q}(\tau_0) = q_0, \dot{t}(\tau_0) = t_0, \dot{p}(\tau_N) = p_N \) and \( \dot{\varphi}(\tau_N) = \varphi_N \). Then

\[
\frac{\partial S}{\partial q_0} = p_0, \quad \frac{\partial S}{\partial t_0} = \varphi_0, \quad \frac{\partial S}{\partial p_N} = q_N, \quad \frac{\partial S}{\partial \varphi_N} = t_N. \tag{81}
\]

**Proof.**

\[
\frac{\partial S}{\partial q_0} = \frac{\partial f}{\partial q_0} \bigg|_{\phi, \dot{\phi}, \dot{\varphi}} = \frac{1}{2} p_0 + \frac{\partial}{\partial q_0} \left[ \frac{1}{2} (\ddot{q}_0 - \ddot{q}_0 \dot{p}_0) + \lambda_0 \dot{H}_0 \right] \Delta \tau = \frac{1}{2} p_0 + \frac{1}{2} \left( \ddot{p}_0 - \frac{1}{2} \left( \frac{1}{\Delta \tau} \right) \right) \Delta \tau = \frac{1}{2} p_0 + \frac{1}{2} \left[ \ddot{p}_0 + \ddot{p}_0 \Delta \tau + \lambda_0 \frac{\partial \dot{H}_0}{\partial q_0} \Delta \tau \right]. \tag{82}
\]

Since, by assumption, \( f \) is evaluated along a DTH trajectory, from equation (69) of Theorem 4

\[
\lambda_0 \frac{\partial \dot{H}_0}{\partial q_0} = \ddot{p}_0. \tag{83}
\]

Substituting (83) in (82), we have

\[
\frac{\partial S}{\partial q_0} = \frac{1}{2} p_0 + \frac{1}{2} \left[ \ddot{p}_0 + \ddot{p}_0 \Delta \tau - \ddot{p}_0 \Delta \tau \right] = \frac{1}{2} p_0 + \frac{1}{2} \left[ \ddot{p}_0 - \ddot{p}_0 \Delta \tau \right] = \frac{1}{2} p_0 + \frac{1}{2} \ddot{p}_0 = p_0.
\]

Similarly,

\[
\frac{\partial S}{\partial p_N} = \frac{\partial}{\partial p_N} \left[ \frac{1}{2} (\ddot{q}_{N-1} \ddot{p}_{N-1} - \ddot{q}_{N-1} \ddot{p}_{N-1}) + \lambda_{N-1} \dot{H}_{N-1} \right] \Delta \tau + \frac{1}{2} q_N
\]

\[
= \left[ \frac{1}{2} \ddot{q}_{N-1} \left( \frac{1}{\Delta \tau} \right) - \frac{1}{2} \ddot{q}_{N-1} \left( \frac{1}{2} \right) + \lambda_{N-1} \frac{\partial \dot{H}_{N-1}}{\partial p_{N-1}} \left( \frac{1}{2} \right) \right] \Delta \tau + \frac{1}{2} q_N
\]

\[
= \frac{1}{2} \left[ \ddot{q}_{N-1} - \ddot{q}_{N-1} \frac{\Delta \tau}{2} + \lambda_{N-1} \frac{\partial \dot{H}_{N-1}}{\partial p_{N-1}} \Delta \tau \right] + \frac{1}{2} q_N
\]

\[
= \frac{1}{2} \left[ \ddot{q}_{N-1} - \ddot{q}_{N-1} \frac{\Delta \tau}{2} + \ddot{q}_{N-1} \Delta \tau \right] + \frac{1}{2} q_N
\]

\[
= \frac{1}{2} q_N + \frac{1}{2} q_N = q_N.
\]
We also have
\[
\frac{\partial S}{\partial t_0} = \frac{\partial f}{\partial t_0} \bigg|_{q,\phi,i,\phi} = \frac{1}{2} \varphi_0 + \frac{\partial}{\partial t_0} \left[ \frac{1}{2} \left( t_0 \varphi_0' - t_0 \varphi_0 \right) \right] \Delta \tau = \frac{1}{2} \varphi_0 + \frac{1}{2} \left( \frac{1}{2} \right) \varphi_0 - \left( -\frac{1}{\Delta \tau} \right) \varphi_0 \Delta \tau = \frac{1}{2} \varphi_0 + \frac{1}{2} \left( \varphi_0 + \varphi_0' \frac{\Delta \tau}{2} \right) = \frac{1}{2} \varphi_0 + \frac{1}{2} \varphi_1.
\]

Equation (71) implies \( \varphi_1 = \varphi_0 \). Thus, we have
\[
\frac{\partial S}{\partial t_0} = \varphi_0.
\]

Finally,
\[
\frac{\partial S}{\partial \varphi_N} = \frac{\partial f}{\partial \varphi} \bigg|_{q,\phi,i,\phi} = \frac{\partial}{\partial \varphi} \left[ \frac{1}{2} \left( t_{N-1} \varphi_{N-1} - t_{N-1} \varphi_{N-1} \right) + \lambda_{N-1} \varphi_{N-1} \right] \Delta \tau + \frac{1}{2} t_N
\]
\[
= \frac{1}{2} \left( \frac{1}{\Delta \tau} \right) - \frac{1}{2} \left( \frac{1}{\Delta \tau} \right) + \lambda_{N-1} \left( \frac{1}{\Delta \tau} \right) \Delta \tau + \frac{1}{2} t_N
\]
\[
= \frac{1}{2} \left[ t_{N-1} \varphi_{N-1} - \frac{\Delta \tau}{2} + \lambda_{N-1} \Delta \tau \right] + \frac{1}{2} t_N
\]
\[
= \frac{1}{2} \left[ t_{N-1} \varphi_{N-1} - \frac{\Delta \tau}{2} + \varphi_{N-1} \Delta \tau \right] \Delta \tau + \frac{1}{2} t_N
\]
\[
= \frac{1}{2} \left[ t_{N-1} \varphi_{N-1} + \frac{\Delta \tau}{2} \right] + \frac{1}{2} t_N
\]
\[
= \frac{1}{2} t_N + \frac{1}{2} t_N = t_N.
\]

Another property that DTH trajectories possess is that of exactly conserving the Hamiltonian function at the midpoints of each linear segment. This property is evident once the DTH equations are written in a more compact form.

**Corollary 1.** (The Reduction of the DTH Equations) The DTH trajectory of an autonomous Hamiltonian system must satisfy the following system of equations for \( k = 0, 1, \ldots, N - 1 \).

\[
\tilde{q}_{k+1} - \tilde{q}_k = \frac{\Delta \tau}{2} \left[ \lambda_{k+1} \frac{\partial H_{k+1}}{\partial p_{k+1}} + \lambda_k \frac{\partial H_k}{\partial p_k} \right] = 0, \tag{84}
\]
\[
\tilde{p}_{k+1} - \tilde{p}_k = \frac{\Delta \tau}{2} \left[ \lambda_{k+1} \frac{\partial H_{k+1}}{\partial q_{k+1}} + \lambda_k \frac{\partial H_k}{\partial q_k} \right] = 0, \tag{85}
\]
\[
H_{k+1} - H_k = 0. \tag{86}
\]

**Proof.** Equations (84),(85) follow directly from (64),(65). From (72), we have \( \tilde{p}_k = -\tilde{H}_k \). Substituting for \( \tilde{p}_k \) and \( \tilde{p}_{k+1} \) in (67) and multiplying by \( \Delta \tau \), we obtain (86).

Observe that once \( \tilde{q}_{k+1}, \tilde{p}_{k+1} \) and \( \lambda_{k+1} \) are obtained from equations (84)–(86), \( \tilde{t}_{k+1} \) can be obtained explicitly from equation (66) and \( \tilde{q}_k', \tilde{p}_k' \), and \( \tilde{t}_k' \) can be obtained explicitly from equations (68)–(70).
From equation (86) it is clear that DTH trajectories exactly conserve the Hamiltonian function at the midpoints of each linear segment. (For time dependent Hamiltonians, the right hand side of equation (67) is not zero, and therefore, the reduction implied by Corollary 1 no longer holds true.)

We turn now to the question of the existence and uniqueness of DTH trajectories. It follows from Corollary 1 and the observations which follow it that the values $\lambda_{k+1} = -\lambda_k$, $\bar{q}_{k+1} = \bar{q}_k$, and $\bar{p}_{k+1} = \bar{p}_k$, $k = 0, 1, \ldots N - 1$ determine a DTH trajectory. However, if $\lambda_{k+1} = -\lambda_k$, equation (66) implies that $\bar{t}_{k+1} = \bar{t}_k$. Clearly, we are interested in trajectories for which the time $t_k$ increases with $k$. Do such trajectories exist? For autonomous, positive-definite, linear Hamiltonian systems, such as the simple harmonic oscillator, it is possible to show that for sufficiently small $\Delta \tau$, there exists only one other DTH trajectory and this trajectory must satisfy the condition $\lambda_{k+1} = \lambda_k$ for $k = 0, 1, \ldots N - 1$ (see [6]). (Note that if this condition is satisfied, the DTH equations (64),(65) reduce to the trapezoidal scheme and equations (68),(69) reduce to the midpoint scheme, two schemes commonly used to integrate differential equations.) We will simplify the discussion for the case of nonlinear Hamiltonian systems by focusing on only one step of equations (84)-(86). We will use the notation $\lambda_0$, $q_0$, and $p_0$ to represent $\lambda_k$, $\bar{q}_k$, and $\bar{p}_k$ and $\lambda$, $q$, and $p$ to represent $\lambda_{k+1}$, $\bar{q}_{k+1}$, and $\bar{p}_{k+1}$. We will also use $H_q^0$ and $H_p^0$ to represent $\frac{\partial H}{\partial q}$ and $\frac{\partial H}{\partial p}$ to represent $\frac{\partial H_{k+1}}{\partial q_{k+1}}$ and $\frac{\partial H_{k+1}}{\partial p_{k+1}}$.

Using the above notation, one step of equations (84)-(86) can be represented by the equation

$$F(q, p, \lambda) = 0,$$

where

$$F(q, p, \lambda) = \begin{bmatrix}
q - q_0 - \frac{\Delta \tau}{2} (\lambda H_p + \lambda q H_p^0) \\
p - p_0 + \frac{\Delta \tau}{2} (\lambda H_q + \lambda \lambda H_q^0) \\
H(q, p) - H(q_0, p_0)
\end{bmatrix}.$$  

Let $DF$ represent the Jacobian matrix of $F$. Then

$$DF = \begin{bmatrix}
1 - \frac{\lambda \Delta \tau}{2} H_{q p} & -\frac{\lambda \Delta \tau}{2} H_{p p} & -\frac{\Delta \tau}{2} H_p \\
\frac{\lambda \Delta \tau}{2} H_{q q} & 1 + \frac{\lambda \Delta \tau}{2} H_{q p} & \frac{\Delta \tau}{2} H_q \\
H_q & H_p & 0
\end{bmatrix}.$$  

and

$$\det(DF) = -\frac{\lambda (\Delta \tau)^2}{4} \Psi(q, p),$$

where

$$\Psi(q, p) = H_{q q} (H_p)^2 - 2H_{q p} H_q H_p + H_{p p} (H_q)^2.$$  

From (90), we see that equation (87) is singular when $\Delta \tau = 0$. Assuming $\lambda_0$, $q_0$ and $p_0$ are given, it is possible to show that for sufficiently small nonzero values of $\Delta \tau$, a sufficient condition for the existence and local uniqueness of solutions to (87) is the condition $\Psi(q_0, p_0) \neq 0$. Corollary 1 and the observation which follows it imply that $\Psi(q_0, p_0) \neq 0$ is also a sufficient condition for the existence and local uniqueness of DTH trajectories. The details of the proof are given in [6].

For Hamiltonian systems with positive-definite Hessian matrices, $\Psi(q_0, p_0) = 0$ iff $(q_0, p_0)$ is a stationary point of the Hamiltonian vector field of $H(q, p)$. The condition $\Psi(q_0, p_0) \equiv 0$ on an open set is much more restrictive. Systems with linear Hamiltonian functions, for example, have $\Psi(q, p) \equiv 0$. For one degree of freedom systems, $\Psi(q, p) = 0$ if one of the coordinates is cyclic.
6. NEWTONIAN POTENTIAL SYSTEMS

In this section, we will compare DTH dynamics to four discretization schemes for Newtonian potential systems. Each scheme determines a piecewise-linear, continuous trajectory, \( \dot{q}(t) \). We will adhere to the notation set forth in the previous sections.

Consider a Newtonian potential system consisting of a particle with mass \( m \) acted upon by a one-dimensional field having the potential function \( V(q) \) where \( q \) is the position of the particle. The energy of this system is

\[
E(q, v) = \frac{1}{2} mv^2 + V(q),
\]

where \( v \) is the velocity of the particle. The equations of motion for the system are

\[
\frac{dq}{dt} = v,
\]

\[
\frac{dv}{dt} = -\frac{1}{m} \frac{\partial V(q)}{\partial q}.
\]

Two schemes commonly used to discretize differential equations are the midpoint and trapezoidal schemes. The midpoint scheme for equations (93),(94) is given by the equations

\[
\frac{\bar{q}_{k+1} - \bar{q}_k}{\Delta t} = \frac{\bar{v}_{k+1} + \bar{v}_k}{2},
\]

\[
\frac{\bar{v}_{k+1} - \bar{v}_k}{\Delta t} = -\frac{1}{m} \frac{\partial V((\bar{q}_{k+1} + \bar{q}_k)/2)}{\partial q},
\]

where

\[
\bar{q}_k = \frac{q_{k+1} + q_k}{2}, \quad \bar{v}_k = \frac{q_{k+1} - q_k}{\Delta t} = \bar{q}_k'.
\]

The trapezoidal scheme is given by

\[
\frac{\bar{q}_{k+1} - \bar{q}_k}{\Delta t} = \frac{\bar{v}_{k+1} + \bar{v}_k}{2},
\]

\[
\frac{\bar{v}_{k+1} - \bar{v}_k}{\Delta t} = -\frac{1}{m} \left( \frac{1}{2} \left( \frac{\partial V(q_{k+1})}{\partial q} + \frac{\partial V(q_k)}{\partial q} \right) \right).
\]

From Lemma 1, it follows that equations (95) and (97) insure the continuity of the trajectories, \( \dot{q}(t) \) determined by these two schemes.

A discretization scheme due to D. Greenspan [1] is given by the equations

\[
\frac{\bar{q}_{k+1} - \bar{q}_k}{\Delta t} = \frac{\bar{v}_{k+1} + \bar{v}_k}{2},
\]

\[
\frac{\bar{v}_{k+1} - \bar{v}_k}{\Delta t} = -\frac{1}{m} \frac{V(q_{k+1}) - V(q_k)}{\bar{q}_{k+1} - \bar{q}_k}.
\]

This scheme exactly conserves the energy given by (92) at the midpoint values \( \bar{q}_k \) and \( \bar{v}_k \) of the trajectory \( \dot{q}(t) \). That this is the case can be seen from the following.

\[
E(\bar{q}_{k+1}, \bar{v}_{k+1}) - E(\bar{q}_k, \bar{v}_k) = \frac{m}{2} \left( \frac{\bar{v}_{k+1}^2 - \bar{v}_k^2}{2} \right) + V(\bar{q}_{k+1}) - V(\bar{q}_k)
\]

\[
= m \left( \frac{\bar{v}_{k+1} + \bar{v}_k}{2} \right) \left( \frac{\bar{q}_{k+1} - \bar{q}_k}{\Delta t} \right) \Delta t
\]

\[
+ \left( \frac{V(\bar{q}_{k+1}) - V(\bar{q}_k)}{\bar{q}_{k+1} - \bar{q}_k} \right) \left( \frac{\bar{q}_{k+1} - \bar{q}_k}{\Delta t} \right) \Delta t.
\]

Substituting (99),(100) in (101), we have

\[
E(\bar{q}_{k+1}, \bar{v}_{k+1}) - E(\bar{q}_k, \bar{v}_k) = 0.
\]

Again, equation (99) insures the continuity of \( \dot{q}(t) \).
A fourth discretization scheme due to T. D. Lee [4] can be derived in the following manner. Let $A_D$ given by

$$A_D = \sum_{i=0}^{N-1} \left[ \frac{1}{2} m \bar{v}_i^2 - \bar{V}(i) \right] (t_{i+1} - t_i)$$

(102)

be the “discrete action” of a Newtonian potential system where

$$\bar{v}_i = \frac{q_{i+1} - q_i}{t_{i+1} - t_i}$$

(103)

and where the “discrete potential” $\bar{V}(i)$ is given by

$$\bar{V}(i) = \frac{1}{q_{i+1} - q_i} \int_{q_i}^{q_{i+1}} V(q) dq.$$  

(104)

The values of $q_k$ and $t_k$, $k = 1, 2, \ldots, N - 1$, are determined by the requirement that $A_D$ be stationary, namely

$$\frac{\partial A_D}{\partial q_{k+1}} = 0,$$

$$\frac{\partial A_D}{\partial t_{k+1}} = 0,$$

(105)  

(106)

for $k = 0, 1, \ldots, N - 2$. From (102) and (103), we have

$$\frac{\partial A_D}{\partial q_{k+1}} = \frac{\partial}{\partial q_{k+1}} \sum_{i=0}^{N-1} \left[ \frac{1}{2} m \bar{v}_i^2 - \bar{V}(i) \right] (t_{i+1} - t_i)$$

$$= \frac{\partial}{\partial q_{k+1}} \left[ \left( \frac{1}{2} m \bar{v}_k^2 - \bar{V}(k) \right) (t_{k+1} - t_k) + \left( \frac{1}{2} m \bar{v}_{k+1}^2 - \bar{V}(k + 1) \right) (t_{k+2} - t_{k+1}) \right]$$

$$= \left( m \bar{v}_k \frac{\partial \bar{v}_k}{\partial q_{k+1}} - \frac{\partial \bar{V}}{\partial q_{k+1}} \right) (t_{k+1} - t_k)$$

$$+ \left( m \bar{v}_{k+1} \frac{\partial \bar{v}_{k+1}}{\partial q_{k+1}} - \frac{\partial \bar{V}(k + 1)}{\partial q_{k+1}} \right) (t_{k+2} - t_{k+1})$$

$$= \left[ m \bar{v}_k \left( \frac{1}{t_{k+1} - t_k} \right) - \frac{\partial \bar{V}}{\partial q_{k+1}} \right] (t_{k+1} - t_k)$$

$$+ \left[ m \bar{v}_{k+1} \left( \frac{1}{t_{k+2} - t_{k+1}} - \frac{1}{t_{k+1} - t_{k+1}} \right) - \frac{\partial \bar{V}(k + 1)}{\partial q_{k+1}} \right] (t_{k+2} - t_{k+1})$$

$$= -m (\bar{v}_{k+1} - \bar{v}_k) - \left( \frac{\partial \bar{V}(k + 1)}{\partial q_{k+1}} \right) (t_{k+2} - t_{k+1}) + \frac{\partial \bar{V}(k)}{\partial q_{k+1}} (t_{k+1} - t_k).$$

(107)

Similarly, from (102) we have

$$\frac{\partial A_D}{\partial t_{k+1}} = \frac{\partial}{\partial t_{k+1}} \sum_{i=0}^{N-1} \left[ \frac{1}{2} m \bar{v}_i^2 - \bar{V}(i) \right] (t_{i+1} - t_i)$$

$$- \frac{\partial}{\partial t_{k+1}} \left[ \left( \frac{1}{2} m \bar{v}_k^2 - \bar{V}(k) \right) (t_{k+1} - t_k) + \left( \frac{1}{2} m \bar{v}_{k+1}^2 - \bar{V}(k + 1) \right) (t_{k+2} - t_{k+1}) \right]$$

$$= \frac{\partial}{\partial t_{k+1}} \left[ \frac{1}{2} m \frac{(q_{k+1} - q_k)^2}{t_{k+1} - t_k} - \bar{V}(k)(t_{k+1} - t_k) \right.$$

$$+ \frac{1}{2} m \frac{(q_{k+2} - q_{k+1})^2}{t_{k+2} - t_{k+1}} - \bar{V}(k + 1)(t_{k+2} - t_{k+1}) \right].$$
\[ -\frac{1}{2} m \left( \frac{q_{k+1} - q_k}{(t_{k+1} - t_k)^2} \right)^2 - \tilde{V}(k) + \frac{1}{2} m \left( \frac{q_{k+2} - q_{k+1}}{(t_{k+2} - t_{k+1})^2} \right)^2 + \tilde{V}(k+1) \]

\[ = \left( \frac{1}{2} m \tilde{v}_{k+1}^2 + \tilde{V}(k+1) \right) - \left( \frac{1}{2} m \tilde{v}_k^2 + \tilde{V}(k) \right). \tag{108} \]

From (107) and (108), we see that equations (105) and (106) imply

\[ \bar{v}_{k+1} - \bar{v}_k = -\frac{1}{m} \left( \frac{\partial \tilde{V}(k+1)}{\partial q_{k+1}} (t_{k+2} - t_{k+1}) + \frac{\partial \tilde{V}(k)}{\partial q_{k+1}} (t_{k+1} - t_k) \right), \tag{109} \]

\[ \left( \frac{1}{2} m \tilde{v}_{k+1}^2 + \tilde{V}(k+1) \right) - \left( \frac{1}{2} m \tilde{v}_k^2 + \tilde{V}(k) \right) = 0. \tag{110} \]

In order to resolve certain peculiarities which arise in the application of (109),(110) to the simple harmonic oscillator, D’Innocenzo et al. [9] have proposed a new definition for \( \tilde{V}(i) \) given by (104). They propose that \( \tilde{V}(i) \) be defined to be

\[ \tilde{V}(i) = \tilde{V}(q_i). \tag{111} \]

With the modification due to D’Innocenzo et al., the discrete mechanics equations of T. D. Lee become

\[ \bar{v}_{k+1} - \bar{v}_k = -\frac{1}{2m} \left( \frac{\partial \tilde{V}(\bar{q}_{k+1})}{\partial \bar{q}_{k+1}} (t_{k+2} - t_{k+1}) + \frac{\partial \tilde{V}(\bar{q}_k)}{\partial \bar{q}_k} (t_{k+1} - t_k) \right), \tag{112} \]

\[ \left( \frac{1}{2} m \bar{v}_{k+1}^2 + V(\bar{q}_{k+1}) \right) - \left( \frac{1}{2} m \bar{v}_k^2 + V(\bar{q}_k) \right) = 0. \tag{113} \]

where

\[ \bar{q}_k = \frac{q_{k+1} + q_k}{2}, \tag{114} \]

\[ \bar{v}_k = \frac{q_{k+1} - q_k}{t_{k+1} - t_k}. \tag{115} \]

We now derive the DTH equations for Newtonian potential systems. The Lagrangian function corresponding to the energy given by (92) is

\[ L(q,v) = \frac{1}{2} mv^2 - V(q). \tag{116} \]

Using Legrendre’s transformation, we have

\[ p = \frac{\partial L}{\partial v} = mv, \tag{117} \]

and

\[ H(q,p) = pv - L(q,v) \]

\[ = pv - \left( \frac{1}{2} mv^2 - V(q) \right) \]

\[ = p \left( \frac{1}{m} p \right) - \frac{1}{2} m \left( \frac{1}{m} p \right)^2 + V(q) \]

\[ = \frac{1}{2m} p^2 + V(q). \tag{118} \]

Substituting (118) in equations (84)–(86), we obtain

\[ \frac{\bar{q}_{k+1} - \bar{q}_k}{\Delta \tau} = \frac{1}{2m} \left[ \lambda_{k+1} \bar{p}_{k+1} + \lambda_k \bar{p}_k \right], \tag{119} \]

\[ \frac{\bar{p}_{k+1} - \bar{p}_k}{\Delta \tau} = -\frac{1}{2} \left[ \lambda_{k+1} \frac{\partial V(\bar{q}_{k+1})}{\partial q_{k+1}} + \lambda_k \frac{\partial V(\bar{q}_k)}{\partial q_k} \right]. \tag{120} \]
The equations of T. D. Lee with the modification due to D’Innocenzo et al., that is, equations (112)–(115) and the DTH equations, equations (119)–(124) determine identical values for $q_k$, $v_k$, $p_k$, and $\tilde{r}_k$ for $k = 0, 1, \ldots N - 1$. We can show this in the following way. Dividing both sides of (112) by $\Delta \tau$ and multiplying by $m$, we have

$$m \bar{q}_{k+1} - m \bar{q}_k = \frac{1}{\Delta \tau} \left[ \lambda_{k+1} \frac{\partial V(q_{k+1})}{\partial q_{k+1}} \left( \frac{t_{k+2} - t_{k+1}}{\Delta \tau} \right) + \lambda_k \frac{\partial V(q_k)}{\partial q_k} \left( \frac{t_{k+1} - t_k}{\Delta \tau} \right) \right].$$

Equation (122) and (124) imply that

$$\bar{v}_k = \frac{m}{\lambda_k} q_k,$$

$$\bar{v}_k = \frac{m}{\lambda_k} \bar{q}_k,$$

From (124) and (125), we have

$$\bar{v}_{k+1} - \bar{v}_k = \frac{1}{\Delta \tau} \left[ \lambda_{k+1} \frac{\partial V(q_{k+1})}{\partial q_{k+1}} + \lambda_k \frac{\partial V(q_k)}{\partial q_k} \right].$$

which is identical to equation (120). Using (125) to substitute for $\bar{v}_k$ and $\bar{v}_{k+1}$ in (113) results in equation (121). Finally, from equations (114) and (115)

$$\frac{\bar{q}_{k+1} - \bar{q}_k}{\Delta \tau} = \frac{1}{\Delta \tau} \left[ \frac{q_{k+2} + q_{k+1}}{2} - \frac{q_{k+1} + q_k}{2} \right]$$

$$- \frac{1}{\Delta \tau} \left[ \frac{q_{k+2} - q_{k+1}}{t_{k+2} - t_{k+1}} \left( \frac{t_{k+2} - t_{k+1}}{\Delta \tau} \right) + \frac{q_{k+1} - q_k}{t_{k+1} - t_k} \left( \frac{t_{k+1} - t_k}{\Delta \tau} \right) \right]$$

$$= \frac{1}{\Delta \tau} \left[ \bar{v}_{k+1} t'_{k+1} + \bar{v}_k t'_k \right].$$

Using equation (124) to substitute for $\bar{t}'_k$ and $\bar{t}'_{k+1}$ in (126), we have

$$\frac{\bar{q}_{k+1} - \bar{q}_k}{\Delta \tau} = \frac{1}{\Delta \tau} \left[ \lambda_{k+1} \bar{v}_{k+1} + \lambda_k \bar{v}_k \right].$$

From (125) it follows that (127) can be expressed as

$$\frac{\bar{q}_{k+1} - \bar{q}_k}{\Delta \tau} = \frac{1}{\Delta \tau} \left[ \lambda_{k+1} \bar{v}_{k+1} + \lambda_k \bar{v}_k \right].$$

which is identical to equation (119). Thus, for Newtonian potential systems, DTH dynamics and the discrete mechanics equations of T. D. Lee with the modification of D’Innocenzo et al., determine identical piecewise-linear, continuous trajectories for the position coordinate $q$. However, only DTH dynamics determines piecewise-linear, continuous trajectories for the momentum coordinate $p$. 

Equations (119)–(121) are the reduced form of the DTH equations given by Corollary 1. Substituting (118) in equations (68)–(70), we obtain the additional equations

$$\bar{q}'_k = \frac{1}{m} \lambda_k \bar{q}_k,$$

$$\bar{p}'_k = -\lambda_k \frac{\partial V(q_k)}{\partial q_k},$$

$$\bar{t}'_k = \lambda_k.$$
Next, we present numerical results for two Newtonian potential systems—a simple pendulum with the potential function

$$V(q) = -\cos(q), \quad (128)$$

and an inverse square law system with the potential function

$$V(q) = \frac{1}{q}. \quad (129)$$

The value $m = 1$ is used for both systems. (Numerical results for the Kepler problem in Cartesian coordinates are given in [6].)

The DTH equations, equations (84)–(86) are singular when $\Delta \tau = 0$. A straight-forward application of Newton’s method to these equations is likely to result in poor convergence when $\Delta \tau$ is small. Instead, a two-step iteration procedure is used. First, equations (84), (85) are solved using Newton’s method with $\lambda_{k+1}$ fixed. Then, equation (86) is used to solve for $\lambda_{k+1}$, again using Newton’s method. The details of the algorithm are given in [6].

Shown in Figure 2 are the exact trajectories and the corresponding DTH trajectories for the position and momentum coordinates of a simple pendulum. The DTH trajectories are piecewise-linear and continuous. The errors in the position coordinate, $q$, for four different schemes for the pendulum are shown in Figure 3. (Discrete Mechanics in Figure 3c refers to the discrete mechanics of Greenspan.) Because of the varying time-step of DTH dynamics, a slightly larger initial time-step was used for DTH dynamics so as to keep the total number of steps the same for all the schemes. Figures 4 and 5 show results for the inverse square law system. From Figure 3, we see that for the pendulum, DTH dynamics has roughly the same level of error as the other
Figure 4. The trajectory for an inverse square law potential and the corresponding DTH trajectory for $\Delta \tau = 1.843271$.

Figure 5. Errors in $q$ for the trajectory of Figure 4. For (a)-(c), $\Delta t = 1$. For (d), $\Delta \tau = 1.843271$.

Figure 6. Time parametrization of DTH trajectories.

schemes have. For the inverse square law system, however, DTH dynamics has roughly an order of magnitude less error than the other schemes. The explanation for this difference in error can be seen in Figure 6. For the initial conditions chosen for the pendulum, the time in DTH dynamics behaves in a nearly linear fashion resulting in a nearly uniform time-step. Time behaves in a nonlinear fashion for the inverse square law system. The effect is a nonuniform time-step which reduces the error of DTH dynamics. Figure 7 shows the exact and the DTH phase-plane trajectories for the simple pendulum and the inverse square law system. The linear segments of the DTH trajectories are tangent to the energy conserving manifolds of each system.
As was described in Section 5, a sufficient condition for the existence and local uniqueness of DTH trajectories is the condition $B(q_0, p_0) \neq 0$ where

$$
Q'(q, p) = G_{42} - W_{42} + H_{42}.
$$

The shaded regions in Figure 8 show where in the phase plane this condition does not hold for the simple pendulum and for the inverse square law system. Convergence of the two-step iteration procedure described above degrades near the shaded regions shown in Figure 8.

### 7. HAMILTONIAN SYSTEMS WITH n-DEGREES OF FREEDOM

In this section we summarize results for nonautonomous Hamiltonian systems with n-degrees of freedom. Assume the points $\tau_k$, $k = 0, 1, \ldots, N$ partition the interval $[\tau_0, \tau_N]$ into $N$ equal intervals of length $\Delta \tau = (\tau_N - \tau_0)/N$. Assume $\mathbb{R}^2 \times [\tau_0, \tau_N] \rightarrow \mathbb{R}^{n+2}$ is a piecewise-linear, continuous function of $\tau$ where $z^{(k)} = \hat{z}(\tau_k)$ are the vertices of $\mathbb{R}$. Define $\overline{Z}^{(k)} = (z^{(k+1)} + z^{(k)})/2$ and $\overline{Z}'^{(k)} = (z^{(k+1)} - z^{(k)})/\Delta \tau$, for $k = 0, 1, \ldots, N - 1$. The $N - 1$ values of $\overline{Z}^{(k)}$ and $\overline{Z}'^{(k)}$ completely determine $\hat{z}(\cdot)$.

Consider a Hamiltonian system with Hamiltonian function $H(z)$ where $z = (q, p)^T$ and where $q, p \in \mathbb{R}^{n+1}$ are the position and momentum coordinates. (In this notation, $z_{n+1}$ is the time coordinate and $z_{2n+2}$ is the momentum coordinate conjugate to time.) The matrix $J$ is defined
to be the skew-symmetric matrix

\[ J = \begin{bmatrix} 0 & I_{n+1} \\ -I_{n+1} & 0 \end{bmatrix}, \]

where \( I_{n+1} \) is the \( n+1 \) by \( n+1 \) identity matrix. The following discrete variational principle is used as the definition of DTH dynamics.

**DEFINITION 7. (DTH Principle of Stationary Action)** A DTH trajectory is a piecewise-linear, continuous function \( \tilde{x} : [\tau_0, \tau_N] \rightarrow \mathbb{R}^{2n+2} \) for which the sum:

\[
A[\Delta \tau, \lambda_0, \ldots, \lambda_{N-1}, \tilde{z}(\cdot)] = \frac{1}{2} (q_0) \Delta p_0 + \sum_{j=0}^{N-1} \left[ \frac{1}{2} (\tilde{z}(j))^T J (\tilde{z}(j)) + \lambda_j H (\tilde{z}(j)) \right] \Delta \tau + \frac{1}{2} (p_N)^T p_N
\]

is stationary. The endpoints \( q_0 \) and \( p_N \) are assumed fixed. For a Hamiltonian system with a Hamiltonian function \( H(z) \), the function \( \mathcal{H}(z) \) is defined to be:

\[ \mathcal{H}(z) = z_{2n+2} - H(z). \]

The equations of motion for DTH dynamics are given by the following theorem.

**THEOREM 6. (DTH Equations of Motion)** A piecewise-linear, continuous function \( \tilde{x} : [\tau_0, \tau_N] \rightarrow \mathbb{R}^{2n+2} \) is a DTH trajectory if and only if \( \tilde{z}^{(k)} \) and \( \tilde{z}'^{(k)} \) satisfy the following equations:

\[
\frac{\tilde{z}^{(k+1)} - \tilde{z}^{(k)}}{\Delta \tau} = \frac{1}{2} J \left[ \lambda_{k+1} \frac{\partial H (\tilde{z}^{(k+1)})}{\partial \tilde{z}^{(k+1)}} + \lambda_k \frac{\partial H (\tilde{z}^{(k)})}{\partial \tilde{z}^{(k)}} \right], \quad k = 0, 1, \ldots, N - 2, \tag{130}
\]

\[
\tilde{z}'^{(k)} = \lambda_k J \frac{\partial H (\tilde{z}^{(k)})}{\partial \tilde{z}^{(k)}}, \quad k = 0, 1, \ldots, N - 1, \tag{131}
\]

\[
\mathcal{H} (\tilde{z}^{(k)}) = 0, \quad k = 0, 1, \ldots, N - 1. \tag{132}
\]

Theorem 1 is proved by equating the partial derivatives of \( A[\Delta \tau, \lambda_0, \ldots, \lambda_{N-1}, \tilde{z}(\cdot)] \) to zero and simplifying the resulting equations. The details of the proof are given in [6].

The following theorem gives sufficient conditions for the existence and local uniqueness of DTH trajectories.

**THEOREM 7. (Existence and Uniqueness of DTH Trajectories)** Assume \( \mathcal{H} \in C^3(U) \) where \( U \subset \mathbb{R}^{2n+2} \) is open. Assume also that \( \lambda_0 > 0 \) and that there exists a \( \tilde{z}^{(0)} \in U \) such that \( \mathcal{H}(\tilde{z}^{(0)}) = 0 \) and \( \Psi(\tilde{z}^{(0)}) \neq 0 \) where:

\[ \Psi(z) = [J \mathcal{H}_z(z)]^T H_{zz}(z) [J \mathcal{H}_z(z)]. \]

Then, for any positive integer \( N \), there exists a time step \( \Delta \tau \) and a locally unique piecewise linear, continuous trajectory determined by \( \tilde{z}^{(k)} \) and \( \tilde{z}'^{(k)} \), where \( \tilde{z}^{(k)} \) and \( \tilde{z}'^{(k)} \) satisfy the DTH equations of dynamics.

The proof is based on the Newton-Kantorovich Theorem and is given in [6].

**8. CONCLUSIONS**

The DTH principle of stationary action is the bases for the discrete-time theory of Hamiltonian systems presented in this article. Unlike the discrete principle of least action (Definition 4), the DTH principle of stationary action completely determines piecewise-linear, continuous trajectories in the extended phase space of a Hamiltonian system. These trajectories exactly conserve...
the Hamiltonian function at the midpoints of each linear segment and exactly conserve at the vertices all conserved quadratic functions. The DTH equations of motion are also equivariant with respect to a collection of piecewise-linear, continuous symplectic coordinate transformations which are consistent with a special triangulation of phase space [6].

As we have shown in Theorem 5, the modified discrete action used in the DTH principle of stationary action can be used to define a generating function for transformations between the vertices of DTH trajectories. More work needs to be done in this direction, possibly by deriving a Hamilton-Jacobi equation for DTH dynamics.

The existence and uniqueness results given in Theorem 7 show that DTH dynamics can be used to simulate a very broad class of Hamiltonian systems. For Newtonian potential systems, a subclass of Hamiltonian systems, we have shown that the discrete mechanics of T. D. Lee, with the modification due to D'Innocenzo et al., and DTH dynamics, both determine identical piecewise-linear, continuous configuration space trajectories. However, only DTH dynamics determines piecewise-linear, continuous phase plane trajectories. In DTH dynamics, as in the discrete mechanics of T. D. Lee, time is a dependent dynamic variable. For linear systems, such as the simple harmonic oscillator, time behaves linearly resulting in DTH trajectories with vertices that are uniformly spaced in time.

DTH dynamics could prove to be useful in studying the long-time behavior of Hamiltonian systems. DTH dynamics could also prove to be useful as part of new algorithms for solving problems in optimal control theory. An error analysis of DTH dynamics has yet to be completed, but simulation results are encouraging [6].

REFERENCES