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 Donald

Greenspan [Greenspan 1973, 1974]. 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. Robert Labudde [Labudde 1980] 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 [Lee 1987]. 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. Yuhua Wu has shown that such schemes admit a natural, discrete variational principle [Wu 1990]. 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 [Lee 1987]. 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 [Greenspan 1973]. 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 [Shibberu 1992]. ("DTH" is an abbreviation of "Discrete-Time Hamiltonian.") DTH dynamics 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 [Shibberu 1992].) 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 $\mathcal{I}$ given by (1) is stationary for the trajectory $q(t)$ of a dynamical system with Lagrangian function $L(q, \dot{q})$ [Goldstein 1980].

$$\mathcal{I} = \int_{t_0}^{t_f} L(q(t), \dot{q}(t))\, dt \tag{1}$$

The principle of least action is another variational principle of mechanics. The following motivation for the principle of least action is based on [Lanczos 1970]. Consider now the Legendre transformation $\dot{q} \to p$ and $L(q, \dot{q}) \to H(q, p)$ where p and $H(q, p)$ are given by

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

$$H(q, p) = p\dot{q}(q, p) - L(q, \dot{q}(q, p)) \tag{3}$$

(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, $\mathcal{I}$ can be expressed as

$$\mathcal{I} = \int_{t_0}^{t_f} (p\dot{q} - H(q, p))\, dt \tag{4}$$

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

$$\mathcal{I} = \int_{\tau_0}^{\tau_f} \left(p\frac{dq}{d\tau} - H(q, p)\frac{dt}{d\tau} \right) d\tau \tag{5}$$

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

$$\mathcal{I} = \int_{\tau_0}^{\tau_f} \left(p\frac{dq}{d\tau} + \wp\frac{dt}{d\tau} \right) d\tau \tag{6}$$

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, $\wp$ 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 τ.)

Definition 1 (Action Integral) *Assume $p(\tau), q(\tau), \wp(\tau)$ and $t(\tau)$ are differentiable functions of τ on the interval $[\tau_0, \tau_N]$. The action integral of a Hamiltonian dynamical system is defined to be*

$$A(p(\tau), q(\tau), \wp(\tau), t(\tau)) = \int_{\tau_0}^{\tau_f} \left(p(\tau)\frac{dq(\tau)}{d\tau} + \wp(\tau)\frac{dt(\tau)}{d\tau} \right) d\tau \tag{7}$$

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 $p(\tau), q(\tau), \wp(\tau)$ and $t(\tau)$ which cause the action integral to be stationary under the constraint*

$$\wp + H(q,p) = 0 \tag{8}$$

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

The constraint (8) in Definition 2 is necessary because $\wp$ is defined to be equal to $-H(q,p)$ in (6) and thus $\wp$ 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 Hamiltonian function $H(q,p)$ and initial conditions $q(\tau_0) = q_0$, $p(\tau_0) = p_0$, $t(\tau_0) =$*

0 and $\wp(\tau_0) = -H(q_0, p_0)$ is a solution of the following system of differential equations.

$$\frac{dq}{d\tau} = \lambda(\tau)\frac{\partial H(q,p)}{\partial p} \tag{9}$$

$$\frac{dp}{d\tau} = -\lambda(\tau)\frac{\partial H(q,p)}{\partial q} \tag{10}$$

$$\frac{dt}{d\tau} = \lambda(\tau) \tag{11}$$

$$\frac{d\wp}{d\tau} = 0 \tag{12}$$

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

$$g(q,p,\wp) = \wp + H(q,p) \tag{13}$$

$$f(p(\tau), q(\tau), \wp(\tau), t(\tau), \lambda(\tau)) = A(p(\tau), q(\tau), \wp(\tau), t(\tau)) - \int_{\tau_0}^{\tau_N} \lambda(\tau) g(q(\tau), p(\tau), \wp(\tau))\, d\tau \tag{14}$$

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

$$f(p(\tau), q(\tau), \wp(\tau), t(\tau), \lambda(\tau)) = \int_{\tau_0}^{\tau_N} L(q(\tau), q'(\tau), p(\tau), t'(\tau), \wp(\tau), \lambda(\tau))\, d\tau \tag{15}$$

where

$$L(q, q', p, t', \wp, \lambda) = pq' + \wp t' - \lambda(\wp + H(q,p)) \tag{16}$$

and where the notation q' and t' has been used for $dq(\tau)/d\tau$ and $dt(\tau)/d\tau$. The action integral subject to $g(q,p,\wp) = 0$ 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.

$$\frac{d}{d\tau}\left(\frac{\partial L}{\partial p'}\right) - \frac{\partial L}{\partial p} = 0 \tag{17}$$

$$\frac{d}{d\tau}\left(\frac{\partial L}{\partial q'}\right) - \frac{\partial L}{\partial q} = 0 \tag{18}$$

$$\frac{d}{d\tau}\left(\frac{\partial L}{\partial \wp'}\right) - \frac{\partial L}{\partial \wp} = 0 \tag{19}$$

$$\frac{d}{d\tau}\left(\frac{\partial L}{\partial t'}\right) - \frac{\partial L}{\partial t} = 0 \tag{20}$$

$$\frac{d}{d\tau}\left(\frac{\partial L}{\partial \lambda'}\right) - \frac{\partial L}{\partial \lambda} = 0 \tag{21}$$

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

$$\wp(\tau) + H(q(\tau), p(\tau)) \equiv 0 \tag{22}$$

Claim: Equations (9)–(12) imply equation (22) independently of equation (21).
<u>Proof of the claim</u>:

$$\frac{dH(q(\tau), p(\tau))}{d\tau} = \frac{\partial H}{\partial q}\frac{dq}{d\tau} + \frac{\partial H}{\partial p}\frac{dp}{d\tau} \tag{23}$$

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

$$\frac{dH}{d\tau} = \lambda(\tau)\left(\frac{\partial H}{\partial q}\frac{\partial H}{\partial p} - \frac{\partial H}{\partial p}\frac{\partial H}{\partial q}\right) \equiv 0 \tag{24}$$

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

$$\wp(\tau) + H(q(\tau), p(\tau)) \equiv \wp(\tau_0) + H(q(\tau_0), p(\tau_0)) = 0 \tag{25}$$

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

□

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 $\tau_k, k = 0, 1, \cdots N$, partition the interval $[\tau_0, \tau_N]$ into N equal intervals of length $\Delta\tau$.

$$\tau_k = \tau_0 + k\Delta\tau \quad k = 0, 1, \cdots N \tag{26}$$

$$\Delta\tau = \frac{\tau_N - \tau_0}{N} \tag{27}$$

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

$$x_k = \hat{x}(\tau_k) \quad k = 0, 1, \cdots N \tag{28}$$

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

$$\overline{x}_k = \overline{x}_k(x_{k+1}, x_k) = \frac{x_{k+1} + x_k}{2} \quad k = 0, 1, \cdots N-1 \tag{29}$$

$$\overline{x}'_k = \overline{x}'_k(x_{k+1}, x_k) = \frac{x_{k+1} - x_k}{\Delta\tau} \quad k = 0, 1, \cdots N-1 \tag{30}$$

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

$$\hat{x}(\tau) = \begin{cases} \overline{x}_k + \overline{x}'_k(\tau - \overline{\tau}_k) & \tau_k \le \tau < \tau_{k+1} \quad k = 0, 1, \cdots N-1 \\ x_N & \tau = \tau_N \end{cases} \tag{31}$$

where

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

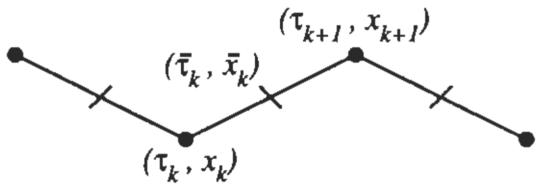


Figure 1: A piecewise-linear, continuous function.

Thus, $\hat{x}(\tau)$ is completely determined by the values of $\overline{x}_k$ and $\overline{x}'_k$ $k = 0, 1, \cdots N-1$. Since $\hat{x}(\tau)$ is continuous, $\overline{x}_k$ and $\overline{x}'_k$ must satisfy the following continuity constraint.

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

$$\frac{\overline{x}_{k+1} - \overline{x}_k}{\Delta\tau} = \frac{\overline{x}'_{k+1} + \overline{x}'_k}{2} \tag{32}$$

The proof of Lemma 1 is given in [Shibberu 1992]. The following Lemma will be used in the proof of Theorem 3.

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

$$\frac{\partial \overline{x}_k}{\partial x_k} = \frac{1}{2} \quad \frac{\partial \overline{x}'_k}{\partial x_k} = -\frac{1}{\Delta\tau}$$

$$\frac{\partial \overline{x}_k}{\partial x_{k+1}} = \frac{1}{2} \quad \frac{\partial \overline{x}'_k}{\partial x_{k+1}} = \frac{1}{\Delta\tau}$$

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

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,* $\hat{p}(\tau)$, $\hat{q}(\tau)$, $\hat{\wp}(\tau)$ *and* $\hat{t}(\tau)$ *defined on a uniform partition of* $[\tau_0, \tau_N]$, *the discrete action* A_N *of a Hamiltonian system is defined to be*

$$A_N(p_0 \cdots p_N, q_0 \cdots q_N, \wp_0 \cdots \wp_N, t_0 \cdots t_N) = \sum_{i=0}^{N-1} \left(\overline{p}_i \overline{q}'_i + \overline{\wp}_i \overline{t}'_i\right) \Delta\tau$$

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.*

$$A(\hat{p}(\tau), \hat{q}(\tau), \hat{\wp}(\tau), \hat{t}(\tau)) = A_N(p_0 \cdots p_N, q_0 \cdots q_N, \wp_0 \cdots \wp_N, t_0 \cdots t_N)$$

Proof: From Definition 1

$$A(\hat{p}(\tau), \hat{q}(\tau), \hat{\wp}(\tau), \hat{t}(\tau)) = \int_{\tau_0}^{\tau_N} \left(p(\tau)\frac{dq(\tau)}{d\tau} + \wp(\tau)\frac{dt(\tau)}{d\tau} \right) d\tau$$

Since $\hat{q}(\tau)$ and $\hat{t}(\tau)$ are piecewise-linear, it follows from (31) that $d\hat{q}(\tau)/d\tau = \overline{q}'_i$ and $d\hat{t}(\tau)/d\tau = \overline{t}'_i$ for $\tau_i < \tau < \tau_{i+1}$, $i = 0, 1, \cdots N-1$. Therefore

$$A(\hat{p}(\tau), \hat{q}(\tau), \hat{\wp}(\tau), \hat{t}(\tau)) = \sum_{i=0}^{N-1} \left(\overline{q}'_i \int_{\tau_i}^{\tau_{i+1}} \hat{p}(\tau)\, d\tau + \overline{t}'_i \int_{\tau_i}^{\tau_{i+1}} \hat{\wp}(\tau)\, d\tau \right)$$

Since

$$\int_{\tau_i}^{\tau_{i+1}} \hat{p}(\tau)\, d\tau = \overline{p}_i\, \Delta\tau$$

and

$$\int_{\tau_i}^{\tau_{i+1}} \hat{\wp}(\tau)\, d\tau = \overline{\wp}_i\, \Delta\tau$$

we have

$$\begin{aligned} A(\hat{p}(\tau), \hat{q}(\tau), \hat{\wp}(\tau), \hat{t}(\tau)) &= \sum_{i=0}^{N-1} (\overline{p}_i \overline{q}'_i + \wp_i \overline{t}'_i)\, \Delta\tau \\ &= A_N \end{aligned}$$

□

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 $\hat{p}(\tau), \hat{q}(\tau), \hat{\wp}(\tau)$ and $\hat{t}(\tau)$ which cause the discrete action to be stationary under the constraint*

$$\overline{\wp}_k + H(\overline{q}_k, \overline{p}_k) = 0 \quad k = 0, 1, \cdots N-1 \tag{33}$$

The endpoints q_0, q_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 Hamitonian systems.

Theorem 3 *The discrete-time trajectory of a Hamiltonian system with Hamiltonian function $H(q,p)$ and initial conditions $\hat{q}(\bar{t}_0) = \bar{q}_0$, $\hat{p}(\bar{t}_0) = \bar{p}_0$, $\hat{t}(\bar{t}_0) = \bar{t}_0$, $\hat{\wp}(\bar{t}_0) = -H(\bar{q}_0, \bar{p}_0)$ is a solution of the following system of equations.*

$$\frac{\bar{q}_{k+1} - \bar{q}_k}{\Delta\tau} = \frac{1}{2}\left[\lambda_{k+1}\frac{\partial H(\bar{q}_{k+1}, \bar{p}_{k+1})}{\partial \bar{p}_{k+1}} + \lambda_k \frac{\partial H(\bar{q}_k, \bar{p}_k)}{\partial \bar{p}_k}\right] \tag{34}$$

$$\frac{\bar{p}_{k+1} - \bar{p}_k}{\Delta\tau} = -\frac{1}{2}\left[\lambda_{k+1}\frac{\partial H(\bar{q}_{k+1}, \bar{p}_{k+1})}{\partial \bar{q}_{k+1}} + \lambda_k \frac{\partial H(\bar{q}_k, \bar{p}_k)}{\partial \bar{q}_k}\right] \tag{35}$$

$$\frac{\bar{t}_{k+1} - \bar{t}_k}{\Delta\tau} = \frac{1}{2}[\lambda_{k+1} + \lambda_k] \tag{36}$$

$$\frac{\bar{\wp}_{k+1} - \bar{\wp}_k}{\Delta\tau} = 0 \tag{37}$$

where $k = 0, 1, \cdots N-2$.

$$\bar{q}'_k = \lambda_k \frac{\partial H(\bar{q}_k, \bar{p}_k)}{\partial \bar{p}_k} \tag{38}$$

$$\bar{t}'_k = \lambda_k \tag{39}$$

$$0 = \bar{\wp}_k + H(\bar{q}_k, \bar{p}_k) \tag{40}$$

where $k = 0, 1, \cdots N-1$.

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

$$\bar{\wp}_k + H(\bar{q}_k, \bar{p}_k) = 0 \quad k = 0, 1, \cdots N-1$$

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

$$g(\bar{q}_k, \bar{p}_k, \bar{\wp}_k) = \bar{\wp}_k + H(\bar{q}_k, \bar{p}_k) \tag{41}$$

and let

$$f(p_0 \cdots p_N, q_0 \cdots q_N, \wp_0 \cdots \wp_N, t_0 \cdots t_N, \lambda_0 \cdots \lambda_{N-1}) = \\ A_N - \textstyle\sum_{i=0}^{N-1} \lambda_i \, g(\overline{q}_i, \overline{p}_i, \overline{\wp}_i). \tag{42}$$

where λ_i in (42) are Lagrange multipliers. We have then that A_N, subject to $g(\overline{q}_k, \overline{p}_k, \overline{\wp}_k) = 0$ for $k = 0, 1, \cdots N-1$, is stationary when the partial derivatives of f with the possible exception of $\partial f/\partial q_0$, $\partial f/\partial q_N$, $\partial f/\partial t_0$ and $\partial f/\partial t_N$ 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, parital derivatives with respect to these variables may not be zero. From (41), (42) and the definition of A_N

$$f = \sum_{i=0}^{N-1} \left[\overline{p}_i \overline{q}'_i + \overline{\wp}_i \overline{t}'_i - \lambda_i \left(\overline{\wp}_i + H(\overline{q}_i, \overline{p}_i)\right)\right] \Delta\tau \tag{43}$$

Equating to zero the partial derivatives $\partial f/\partial q_{k+1}$, $\partial f/\partial p_{k+1}$, $\partial f/\partial t_{k+1}$ and $\partial f/\partial \wp_{k+1}$ for $k = 0, 1, \cdots N-2$ implies equations (34) –(37) as follows. From (43) for $k = 0, 1, \cdots N-2$

$$\frac{\partial f}{\partial p_{k+1}} = \frac{\partial}{\partial p_{k+1}} \sum_{i=0}^{N-1} \left[\overline{p}_i \overline{q}'_i + \overline{\wp}_i \overline{t}'_i - \lambda_i \left(\overline{\wp}_i + \overline{H}_i\right)\right] \Delta\tau \tag{44}$$

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

$$\begin{aligned} \frac{\partial f}{\partial p_{k+1}} &= \frac{\partial}{\partial p_{k+1}} \left[\overline{p}_k \overline{q}'_k - \lambda_k \overline{H}_k + \overline{p}_{k+1} \overline{q}'_{k+1} - \lambda_{k+1} \overline{H}_{k+1}\right] \Delta\tau \\ &= \left[\frac{\partial \overline{p}_k}{\partial p_{k+1}} \overline{q}'_k - \lambda_k \frac{\partial \overline{H}_k}{\partial \overline{p}_k} \frac{\partial \overline{p}_k}{\partial p_{k+1}} \right. \\ &\quad \left. + \frac{\partial \overline{p}_{k+1}}{\partial p_{k+1}} \overline{q}'_{k+1} - \lambda_{k+1} \frac{\partial \overline{H}_k}{\partial \overline{p}_{k+1}} \frac{\partial \overline{p}_{k+1}}{\partial p_{k+1}} \right] \end{aligned}$$

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

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

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

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

Therefore

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

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

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

From Lemma 2 $\partial\overline{q}'_k/\partial q_{k+1}=1/\Delta\tau$ and $\partial\overline{q}'_{k+1}/\partial q_{k+1}=-1/\Delta\tau$. Therefore

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

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

$$\frac{\partial f}{\partial\lambda_k}=\frac{\partial}{\partial\lambda_k}\sum_{i=0}^{N-1}\left[\overline{p}_i\overline{q}'_i+\overline{\wp}_i\overline{t}'_i-\lambda_i\left(\overline{\wp}_i+\overline{H}_i\right)\right]\Delta\tau \tag{46}$$

$$=\left(\wp_k+\overline{H}_k\right)\Delta\tau \tag{47}$$

Equating $\partial f/\partial\lambda_k$ to zero implies equation (40). Now since p_0, p_N, $\wp_0$ and $\wp_N$ are free to vary, the function f is not stationary unless the partial derivative $\partial f/\partial p_0$, $\partial f/\partial p_N$, $\partial f/\partial\wp_0$ and $\partial f/\partial\wp_N$ are also equal to zero. Equating these partial derivatives to zero implies equations (38)–(39) as follows. From (43) we have

$$\frac{\partial f}{\partial p_0}=\frac{\partial}{\partial p_0}\sum_{i=0}^{N-1}\left[\overline{p}_i\overline{q}'_i+\overline{\wp}_i\overline{t}'_i-\lambda_i\left(\overline{\wp}_i+\overline{H}_i\right)\right]\Delta\tau$$

The terms on the right side of (4) depend on p_0 only for $i=0$. Therefore

$$\frac{\partial f}{\partial p_0}=\frac{\partial}{\partial p_0}\left[\overline{p}_0\overline{q}'_0-\lambda_0\overline{H}_0\right]\Delta\tau \tag{48}$$

$$= \left[\frac{\partial \overline{p}_0}{\partial p_0}\overline{q}'_0 - \lambda_0 \frac{\partial \overline{H}_0}{\partial \overline{p}_0}\frac{\partial \overline{p}_0}{\partial p_0}\right]\Delta\tau \quad (49)$$

$$= \left[\overline{q}'_0 - \lambda_0 \frac{\partial \overline{H}_0}{\partial \overline{p}_0}\right]\frac{\partial \overline{p}_0}{\partial p_0}\Delta\tau \quad (50)$$

From Lemma 2 $\partial\overline{p}_0/\partial p_0 = \frac{1}{2} \neq 0$. Therefore, $\partial f/\partial p_0 = 0$ implies

$$\overline{q}'_0 = \lambda_0 \frac{\partial \overline{H}_0}{\partial \overline{p}_0} \quad (51)$$

Similarly, $\partial f/\partial \wp_0 = 0$ implies

$$\overline{t}'_0 = \lambda_0 \quad (52)$$

Using the continuity constraints on $\hat{q}(\tau)$ and $\hat{t}(\tau)$ we can express equations (34) and (36) as follows.

$$\frac{\overline{q}'_{k+1} + \overline{q}'_k}{2} = \frac{1}{2}\left[\lambda_{k+1}\frac{\partial \overline{H}_{k+1}}{\partial \overline{p}_{k+1}} + \lambda_k \frac{\partial \overline{H}_k}{\partial \overline{p}_k}\right] \quad (53)$$

$$\frac{\overline{t}'_{k+1} + \overline{t}'_k}{2} = \frac{1}{2}[\lambda_{k+1} + \lambda_k] \quad (54)$$

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

$$\overline{q}'_k = \lambda_k \frac{\partial \overline{H}_k}{\partial \overline{p}_k} \quad (55)$$

$$\overline{t}'_k = \lambda_k \quad (56)$$

Substituting for $\overline{q}'_k$ and $\overline{t}'_k$ in (53) and (54) and solving for $\overline{q}'_{k+1}$ and $\overline{t}'_{k+1}$ we have

$$\overline{q}'_{k+1} = \lambda_{k+1}\frac{\partial \overline{H}_{k+1}}{\partial \overline{p}_{k+1}} \quad (57)$$

$$\overline{t}'_{k+1} = \lambda_{k+1} \quad (58)$$

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

Finally, we evaluate $\partial f/\partial p_N$ and $\partial f/\partial \wp_N$.

$$\frac{\partial f}{\partial p_N} = \frac{\partial}{\partial p_N}\left[\overline{p}_{N-1}\overline{q}'_{N-1} - \lambda_{N-1}\overline{H}_{N-1}\right]\Delta\tau \tag{59}$$

$$= \left[\overline{q}'_{N-1} - \lambda_{N-1}\frac{\partial \overline{H}_{N-1}}{\partial \overline{p}_{N-1}}\right]\frac{\partial \overline{p}_{N-1}}{\partial p_N}\Delta\tau \tag{60}$$

Thus, $\partial f/\partial p_N = 0$ implies

$$\overline{q}'_{N-1} = \lambda_{N-1}\frac{\partial \overline{H}_{N-1}}{\partial \overline{p}_{N-1}} \tag{61}$$

Similarly, $\partial f/\partial \wp_N = 0$ implies

$$\overline{t}'_{N-1} = \lambda_{N-1} \tag{62}$$

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 $\overline{p}_k$, $\overline{q}_k$, $\overline{t}_k$, $\overline{\wp}_k$ and λ_k and the values of $\overline{q}'_k$ and $\overline{t}'_k$. The values of $\overline{p}'_k$ and $\overline{\wp}'_k$ 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, $\hat{p}(\tau)$, $\hat{q}(\tau)$, $\hat{\wp}(\tau)$ and $\hat{t}(\tau)$ defined on a uniform partition of $[\tau_0, \tau_N]$, the modified discrete action $\mathcal{A}_N$ of a Hamiltonian system is defined to be*

$$\mathcal{A}_N(p_0 \cdots p_N, q_0 \cdots q_N, \wp_0 \cdots \wp_N, t_0 \cdots t_N) =$$

$$\frac{1}{2}(q_0p_0+t_0\wp_0)+\sum_{k=1}^{N-1}\left[\frac{1}{2}(\overline{q}_i\overline{p}'_i-\overline{q}'_i\overline{p}_i)+\frac{1}{2}(\overline{t}_i\overline{\wp}'_i-\overline{t}'_i\overline{\wp}_i)\right]\Delta\tau+\frac{1}{2}(q_Np_N+t_N\wp_N)$$

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 $\hat{p}(\tau)$, $\hat{q}(\tau)$, $\hat{\wp}(\tau)$ and $\hat{t}(\tau)$ which cause the modified discrete action to be stationary under the constraint*

$$\overline{\wp}_k+H(\overline{q}_k,\overline{p}_k)=0 \quad k=0,1,\cdots N-1 \tag{63}$$

The endpoints q_0, t_0 and p_N, $\wp_N$ 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 $\hat{q}(\overline{t}_0)=\overline{q}_0$, $\hat{p}(\overline{t}_0)=\overline{p}_0$, $\hat{t}(\overline{t}_0)=0$, $\hat{\wp}(\overline{t}_0)=-H(\overline{q}_0,\overline{p}_0)$ is a solution of the following system of equations.*

$$\frac{\overline{q}_{k+1}-\overline{q}_k}{\Delta\tau} = \frac{1}{2}\left[\lambda_{k+1}\frac{\partial H(\overline{q}_{k+1},\overline{p}_{k+1})}{\partial\overline{p}_{k+1}}+\lambda_k\frac{\partial H(\overline{q}_k,\overline{p}_k)}{\partial\overline{p}_k}\right] \tag{64}$$

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

$$\frac{\overline{t}_{k+1}-\overline{t}_k}{\Delta\tau} = \frac{1}{2}\left[\lambda_{k+1}+\lambda_k\right] \tag{66}$$

$$\frac{\overline{\wp}_{k+1}-\overline{\wp}_k}{\Delta\tau} = 0 \tag{67}$$

where $k=0,1,\cdots N-2$

$$\overline{q}'_k = \lambda_k\frac{\partial H(\overline{q}_k,\overline{p}_k)}{\partial\overline{p}_k} \tag{68}$$

$$\overline{p}'_k = -\lambda_k\frac{\partial H(\overline{q}_k,\overline{p}_k)}{\partial\overline{q}_k} \tag{69}$$

$$\overline{t}'_k = \lambda_k \tag{70}$$

$$\overline{\wp}'_k = 0 \tag{71}$$

$$0 = \overline{\wp}_k+H(\overline{q}_k,\overline{p}_k) \tag{72}$$

where $k=0,1,\cdots N-1$.

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

$$\overline{\wp}_k + H(\overline{q}_k, \overline{p}_k) = 0 \quad k = 0, 1, \cdots N-1$$

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

$$g(\overline{q}_k, \overline{p}_k, \overline{\wp}_k) = \overline{\wp}_k + H(\overline{q}_k, \overline{p}_k) \tag{73}$$

and now let

$$f(p_0 \cdots p_N, q_0 \cdots q_N, \wp_0 \cdots \wp_N, t_0 \cdots t_N, \lambda_0 \cdots \lambda_{N-1}) = \mathcal{A}_N + \textstyle\sum_{i=0}^{N-1} \lambda_i \, g(\overline{q}_i, \overline{p}_i, \overline{\wp}_i) \tag{74}$$

where in (74) we have used the modified discrete action $\mathcal{A}_N$. We have then that $\mathcal{A}_N$, subject to $g(\overline{q}_k, \overline{p}_k, \overline{\wp}_k) = 0$ for $k = 0, 1, \cdots N-1$, is stationary when the partial derivatives of f with the possible exception of $\partial f/\partial q_0$, $\partial f/\partial t_0$, $\partial f/\partial p_N$ and $\partial f/\partial \wp_N$ are equal to zero. From (73), (74) and the definition of $\mathcal{A}_N$

$$\begin{aligned} f \; = \; & \frac{1}{2}(q_0 p_0 + t_0 \wp_0) + \\ & \sum_{i=1}^{N-1} \left[\frac{1}{2}(\overline{q}_i \overline{p}'_i - \overline{q}'_i \overline{p}_i) + \frac{1}{2}(\overline{t}_i \overline{\wp}'_i - \overline{t}'_i \overline{\wp}_i) + \lambda_i \left(\overline{\wp}_i + \overline{H}_i \right) \right] \Delta\tau + \\ & \frac{1}{2}(q_N p_N + t_N \wp_N) \end{aligned} \tag{75}$$

where again we have used the abbreviation $\overline{H}_i$ for $H(\overline{q}_i, \overline{p}_i)$. Equating to zero the partial derivatives $\partial f/\partial p_{k+1}$, $\partial f/\partial q_{k+1}$, $\partial f/\partial \wp_{k+1}$ and $\partial f/\partial t_{k+1}$ for $k = 0, 1, \cdots N-2$ implies equations (64)–(67) as follows. From (75) for $k = 0, 1, \cdots N-2$

$$\begin{aligned} \frac{\partial f}{\partial p_{k+1}} \; = \; & \frac{\partial}{\partial p_{k+1}} \left[\frac{1}{2}(\overline{q}_k \overline{p}'_k - \overline{q}'_k \overline{p}_k) \right. \\ & \left. + \frac{1}{2}(\overline{q}_{k+1} \overline{p}'_{k+1} - \overline{q}'_{k+1} \overline{p}_{k+1}) + (\lambda_k \overline{H}_k + \lambda_{k+1} \overline{H}_{k+1}) \right] \Delta\tau \\ = \; & \left[\frac{1}{2}\overline{q}_k (\frac{1}{\Delta\tau}) - \frac{1}{2}\overline{q}'_k (\frac{1}{2}) + \frac{1}{2}\overline{q}_{k+1}(-\frac{1}{\Delta\tau}) \right. \end{aligned}$$

$$
\begin{aligned}
& - \frac{1}{2}\overline{q}'_{k+1}(\frac{1}{2}) + \lambda_k \frac{\partial \overline{H}_k}{\partial \overline{p}_k}(\frac{1}{2}) + \lambda_{k+1}\frac{\partial \overline{H}_{k+1}}{\partial \overline{p}_{k+1}}(\frac{1}{2})\Bigg] \Delta\tau \\
= & \left[-\frac{1}{2}\left(\frac{\overline{q}_{k+1} - \overline{q}_k}{\Delta\tau}\right) - \frac{1}{2}\left(\frac{\overline{q}'_{k+1} + \overline{q}'_k}{2}\right)\right. \\
& \left. + \frac{1}{2}\left(\lambda_{k+1}\frac{\partial \overline{H}_{k+1}}{\partial \overline{p}_{k+1}} + \lambda_k \frac{\partial \overline{H}_k}{\partial \overline{p}_k}\right)\right] \Delta\tau \\
= & \left[-\left(\frac{\overline{q}_{k+1} - \overline{q}_k}{\Delta\tau}\right) + \frac{1}{2}\left(\lambda_{k+1}\frac{\partial \overline{H}_{k+1}}{\partial \overline{p}_{k+1}} + \lambda_k \frac{\partial \overline{H}_k}{\partial \overline{p}_k}\right)\right] \Delta\tau
\end{aligned}
$$

where we have used Lemmas 1 and 2. Thus, $\partial f/\partial p_{k+1} = 0$ implies equation (64). Equations (65)–(67) are derived in a similar fashion.

$$
\begin{aligned}
\frac{\partial f}{\partial p_0} &= \frac{\partial}{\partial p_0}\left[\frac{1}{2}q_0 p_0 + \frac{1}{2}(\overline{q}_0 \overline{p}'_0 - \overline{q}'_0 \overline{p}_0)\Delta\tau + \lambda_0 \overline{H}_0 \Delta\tau\right] \\
&= \frac{1}{2}q_0 + \frac{1}{2}\left[\overline{q}_0(-\frac{1}{\Delta\tau}) - \overline{q}'_0(\frac{1}{2})\right]\Delta\tau + \lambda_0 \frac{\partial \overline{H}_0}{\partial \overline{p}_0}(\frac{1}{2})\Delta\tau \\
&= \frac{1}{2}\left[q_0 - (\overline{q}_0 + \overline{q}'_0 \frac{\Delta\tau}{2}) + \lambda_0 \frac{\partial \overline{H}_0}{\partial \overline{p}_0}\Delta\tau\right] \\
&= \frac{1}{2}\left[\frac{q_0 - q_1}{\Delta\tau} + \lambda_0 \frac{\partial \overline{H}_0}{\partial \overline{p}_0}\right]\Delta\tau \\
&= \frac{1}{2}\left[-\overline{q}'_0 + \lambda_0 \frac{\partial \overline{H}_0}{\partial \overline{p}_0}\right]\Delta\tau
\end{aligned}
$$

where we have used the fact that $q_1 = (\overline{q}_0 + \overline{q}'_0 \frac{\Delta\tau}{2})$. Therefore, $\partial f/\partial p_0 = 0$ implies

$$
\overline{q}'_0 = \lambda_0 \frac{\partial \overline{H}_0}{\partial \overline{p}_0} \tag{76}
$$

Assume for some $k = 0, 1, \cdots N-2$ that

$$
\overline{q}'_k = \lambda_k \frac{\partial \overline{H}_k}{\partial \overline{p}_k} \tag{77}
$$

Then equation (64) and Lemma 1 imply that

$$
\overline{q}'_{k+1} = \lambda_{k+1}\frac{\partial \overline{H}_{k+1}}{\partial \overline{p}_{k+1}} \tag{78}
$$

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

$$\begin{aligned}\frac{\partial f}{\partial q_N} &= \frac{\partial}{\partial q_N}\left[\frac{1}{2}q_N p_N + \frac{1}{2}(\overline{q}_{N-1}\overline{p}'_{N-1} - \overline{q}'_{N-1}\overline{p}_{N-1})\Delta\tau + \lambda_{N-1}\overline{H}_{N-1}\Delta\tau\right] \\ &= \frac{1}{2}p_N + \frac{1}{2}\left[(\frac{1}{2})\overline{p}'_{N-1} - (\frac{1}{\Delta\tau})\overline{p}_{N-1}\right]\Delta\tau + \lambda_{N-1}\frac{\partial\overline{H}_{N-1}}{\partial\overline{q}_{N-1}}(\frac{1}{2})\Delta\tau \\ &= \frac{1}{2}\left[p_N - (\overline{p}_{N-1} - \overline{p}'_{N-1}\frac{\Delta\tau}{2}) + \lambda_{N-1}\frac{\partial\overline{H}_{N-1}}{\partial\overline{q}_{N-1}}\Delta\tau\right] \\ &= \frac{1}{2}\left[\frac{p_N - p_{N-1}}{\Delta\tau} + \lambda_{N-1}\frac{\partial\overline{H}_{N-1}}{\partial\overline{q}_{N-1}}\right]\Delta\tau \\ &= \frac{1}{2}\left[\overline{p}'_{N-1} + \lambda_{N-1}\frac{\partial\overline{H}_{N-1}}{\partial\overline{q}_{N-1}}\right]\Delta\tau\end{aligned}$$

Thus, $\partial f/\partial q_N = 0$ implies

$$\overline{p}'_{N-1} = -\lambda_{N-1}\frac{\partial\overline{H}_{N-1}}{\partial\overline{q}_{N-1}} \tag{79}$$

Using the continuity constraint on $\hat{p}(\tau)$ and equations (65) and (79) we can, by induction, establish equation (69) in the same way equation (68) was established. Equations (70)–(71) are derived in a similar manner. Finally, equation (72) follows directly from the equation $\partial f/\partial\lambda_k = 0, \quad k = 0, 1, \cdots N-1$.

□

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*

$$S(q_0, t_0, p_N, \wp_N) = f\ |_{\hat{q},\hat{p},\hat{t},\hat{\wp}} \tag{80}$$

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

$$\frac{\partial S}{\partial q_0} = p_0, \ \frac{\partial S}{\partial t_0} = \wp_0, \ \frac{\partial S}{\partial p_N} = q_N, \ \frac{\partial S}{\partial \wp_N} = t_N \tag{81}$$

Proof:

$$\begin{aligned}
\frac{\partial S}{\partial q_0} &= \frac{\partial f}{\partial q_0}\,|_{\hat{q},\hat{p},\hat{t},\hat{\wp}} \\
&= \frac{1}{2}p_0 + \frac{\partial}{\partial q_0}\left[\frac{1}{2}(\overline{q}_0\overline{p}'_0 - \overline{q}'_0\overline{p}_0) + \lambda_0\overline{H}_0\right]\Delta\tau \\
&= \frac{1}{2}p_0 + \left[\frac{1}{2}(\frac{1}{2})\overline{p}'_0 - \frac{1}{2}(-\frac{1}{\Delta\tau})\overline{p}_0 + \lambda_0\frac{\partial\overline{H}_0}{\partial\overline{q}_0}(\frac{1}{2})\right]\Delta\tau \\
&= \frac{1}{2}p_0 + \frac{1}{2}\left[\overline{p}_0 + \overline{p}'_0\frac{\Delta\tau}{2} + \lambda_0\frac{\partial\overline{H}_0}{\partial\overline{q}_0}\Delta\tau\right]
\end{aligned} \tag{82}$$

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

$$\lambda_0\frac{\partial\overline{H}_0}{\partial\overline{q}_0} = -\overline{p}'_0 \tag{83}$$

Substituting (83) in (82) we have

$$\begin{aligned}
\frac{\partial S}{\partial q_0} &= \frac{1}{2}p_0 + \frac{1}{2}\left[\overline{p}_0 + \overline{p}'_0\frac{\Delta\tau}{2} - \overline{p}'_0\Delta\tau\right] \\
&= \frac{1}{2}p_0 + \frac{1}{2}\left[\overline{p}_0 - \overline{p}'_0\frac{\Delta\tau}{2}\right] \\
&= \frac{1}{2}p_0 + \frac{1}{2}p_0 \\
&= p_0
\end{aligned}$$

Similarly,

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

$$
\begin{aligned}
&= \frac{1}{2}\left[\overline{q}_{N-1} - \overline{q}'_{N-1}\frac{\Delta\tau}{2} + \lambda_{N-1}\frac{\partial \overline{H}_{N-1}}{\partial \overline{p}_{N-1}}\Delta\tau\right] + \frac{1}{2}q_N \\
&= \frac{1}{2}[\overline{q}_{N-1} - \overline{q}'_{N-1}\frac{\Delta\tau}{2} + \overline{q}'_{N-1}\Delta\tau] + \frac{1}{2}q_N \\
&= \frac{1}{2}\left[\overline{q}_{N-1} + \overline{q}'_{N-1}\frac{\Delta\tau}{2}\right] + \frac{1}{2}q_N \\
&= \frac{1}{2}q_N + \frac{1}{2}q_N \\
&= q_N
\end{aligned}
$$

We also have

$$
\begin{aligned}
\frac{\partial S}{\partial t_0} &= \frac{\partial f}{\partial t_0}|_{\hat{q},\hat{p},\hat{t},\hat{\wp}} \\
&= \frac{1}{2}\wp_0 + \frac{\partial}{\partial t_0}\left[\frac{1}{2}(\overline{t}_0\overline{\wp}'_0 - \overline{t}'_0\overline{\wp}_0)\right]\Delta\tau \\
&= \frac{1}{2}\wp_0 + \frac{1}{2}\left[(\frac{1}{2})\overline{\wp}'_0 - (-\frac{1}{\Delta\tau})\overline{\wp}_0\right]\Delta\tau \\
&= \frac{1}{2}\wp_0 + \frac{1}{2}\left[\overline{\wp}_0 + \overline{\wp}'_0\frac{\Delta\tau}{2}\right] \\
&= \frac{1}{2}\wp_0 + \frac{1}{2}\wp_1
\end{aligned}
$$

Equation (71) implies $\wp_1 = \wp_0$. Thus, we have

$$
\frac{\partial S}{\partial t_0} = \wp_0
$$

Finally,

$$
\begin{aligned}
\frac{\partial S}{\partial \wp_N} &= \frac{\partial f}{\partial \wp_N}|_{\hat{q},\hat{p},\hat{t},\hat{\wp}} \\
&= \frac{\partial}{\partial \wp_N}\left[\frac{1}{2}(\overline{t}_{N-1}\overline{\wp}'_{N-1} - \overline{t}'_{N-1}\overline{\wp}_{N-1}) + \lambda_{N-1}\overline{\wp}_{N-1}\right]\Delta\tau + \frac{1}{2}t_N \\
&= \left[\frac{1}{2}\overline{t}_{N-1}(\frac{1}{\Delta\tau}) - \frac{1}{2}\overline{t}'_{N-1}(\frac{1}{2}) + \lambda_{N-1}(\frac{1}{2})\right]\Delta\tau + \frac{1}{2}t_N \\
&= \frac{1}{2}\left[\overline{t}_{N-1} - \overline{t}'_{N-1}\frac{\Delta\tau}{2} + \lambda_{N-1}\Delta\tau\right] + \frac{1}{2}t_N \\
&= \frac{1}{2}\left[\overline{t}_{N-1} - \overline{t}'_{N-1}\frac{\Delta\tau}{2} + \overline{t}'_{N-1}\Delta\tau\right] + \frac{1}{2}t_N
\end{aligned}
$$

$$
\begin{aligned}
&= \frac{1}{2}\left[\bar{t}_{N-1} + \bar{t}'_{N-1}\frac{\Delta\tau}{2}\right] + \frac{1}{2}t_N \\
&= \frac{1}{2}t_N + \frac{1}{2}t_N \\
&= t_N
\end{aligned}
$$

□

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

$$\bar{q}_{k+1} - \bar{q}_k - \frac{\Delta\tau}{2}\left[\lambda_{k+1}\frac{\partial \overline{H}_{k+1}}{\partial \bar{p}_{k+1}} + \lambda_k\frac{\partial \overline{H}_k}{\partial \bar{p}_k}\right] = 0 \tag{84}$$

$$\bar{p}_{k+1} - \bar{p}_k + \frac{\Delta\tau}{2}\left[\lambda_{k+1}\frac{\partial \overline{H}_{k+1}}{\partial \bar{q}_{k+1}} + \lambda_k\frac{\partial \overline{H}_k}{\partial \bar{q}_k}\right] = 0 \tag{85}$$

$$\overline{H}_{k+1} - \overline{H}_k = 0 \tag{86}$$

Proof: Equations (84)–(85) follow directly from (64)–(65). From (72) we have $\bar{\wp}_k = -\overline{H}_k$. Substituting for $\bar{\wp}_k$ and $\bar{\wp}_{k+1}$ in (67) and multiplying by $\Delta\tau$ we obtain (86).

□

Observe that once $\bar{q}_{k+1}$, $\bar{p}_{k+1}$ and λ_{k+1} are obtained from equations (84)–(86) $\bar{t}_{k+1}$ can be obtained explicitly from equation (66) and $\bar{q}'_k$, $\bar{p}'_k$ and $\bar{t}'_k$ 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 $\bar{p}_{k+1} = \bar{p}_k$, $k = 0, 1, \cdots N-1$

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 $\bar{t}_k$ 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 $k = 0, 1, \cdots N-1$ [Shibberu 1992]. (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 λ_0, q_0 and p_0 to represent λ_k, $\bar{q}_k$ and $\bar{p}_k$ and λ, q and p to represent λ_{k+1}, $\bar{q}_{k+1}$ and $\bar{p}_{k+1}$. We will also use H_q^0 and H_p^0 to represent $\partial\overline{H}_k/\partial\bar{q}_k$ and $\partial\overline{H}_k/\partial\bar{p}_k$ and H_q and H_p to represent $\partial\overline{H}_{k+1}/\partial\bar{q}_{k+1}$ and $\partial\overline{H}_{k+1}/\partial\bar{p}_{k+1}$.

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

$$F(q,p,\lambda) = 0 \tag{87}$$

where

$$F(q,p,\lambda) = \begin{bmatrix} q - q_0 - \frac{\Delta\tau}{2}\left(\lambda H_p + \lambda_0 H_p^0\right) \\ p - p_0 + \frac{\Delta\tau}{2}\left(\lambda H_q + \lambda_0 H_q^0\right) \\ H(q,p) - H(q_0,p_0) \end{bmatrix} \tag{88}$$

Let DF represent the Jacobian matrix of F. Then

$$DF = \begin{bmatrix} 1 - (\frac{\lambda\Delta\tau}{2})H_{qp} & -(\frac{\lambda\Delta\tau}{2})H_{pp} & -(\frac{\Delta\tau}{2})H_p \\ (\frac{\lambda\Delta\tau}{2})H_{qq} & 1 + (\frac{\lambda\Delta\tau}{2})H_{qp} & (\frac{\Delta\tau}{2})H_q \\ H_q & H_p & 0 \end{bmatrix} \tag{89}$$

and

$$\det(DF) = -\frac{\lambda(\Delta\tau)^2}{4}\Psi(q,p) \tag{90}$$

where

$$\Psi(q,p) = H_{qq}(H_p)^2 - 2H_{qp}H_qH_p + H_{pp}(H_q)^2 \tag{91}$$

From (90) we see that equation (87) is singular when $\Delta\tau = 0$. Assuming λ_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 follow 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 [Shibberu 1992].

For Hamiltonian systems with positive-definite Hessian matrices, $\Psi(q_0, p_0) = 0$ if and only if (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, $\Psi(q,p) \equiv 0$ 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, $\hat{q}(t)$. 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

$$E(q,v) = \frac{1}{2}mv^2 + V(q) \tag{92}$$

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

$$\frac{dq}{dt} = v \tag{93}$$

$$\frac{dv}{dt} = -\frac{1}{m}\frac{\partial V(q)}{\partial q} \tag{94}$$

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

$$\frac{\overline{q}_{k+1} - \overline{q}_k}{\Delta t} = \frac{\overline{v}_{k+1} + \overline{v}_k}{2} \tag{95}$$

$$\frac{\overline{v}_{k+1} - \overline{v}_k}{\Delta t} = -\frac{1}{m}\frac{\partial V\left((\overline{q}_{k+1} + \overline{q}_k)/2\right)}{\partial q} \tag{96}$$

where

$$\overline{q}_k = \frac{q_{k+1} + q_k}{2}$$

$$\overline{v}_k = \frac{q_{k+1} - q_k}{\Delta t} = \overline{q}'_k$$

The trapezoidal scheme is given by

$$\frac{\overline{q}_{k+1} - \overline{q}_k}{\Delta t} = \frac{\overline{v}_{k+1} + \overline{v}_k}{2} \tag{97}$$

$$\frac{\overline{v}_{k+1} - \overline{v}_k}{\Delta t} = -\frac{1}{m}\left(\frac{\partial V(\overline{q}_{k+1})/\partial q + \partial V(\overline{q}_k)/\partial q}{2}\right) \tag{98}$$

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

A discretization scheme due to Donald Greenspan [Greenspan 1973] is given by the equations

$$\frac{\overline{q}_{k+1} - \overline{q}_k}{\Delta t} = \frac{\overline{v}_{k+1} + \overline{v}_k}{2} \tag{99}$$

$$\frac{\overline{v}_{k+1} - \overline{v}_k}{\Delta t} = -\frac{1}{m}\frac{V(\overline{q}_{k+1}) - V(\overline{q}_k)}{\overline{q}_{k+1} - \overline{q}_k} \tag{100}$$

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

$$E(\overline{q}_{k+1}, \overline{v}_{k+1}) - E(\overline{q}_k, \overline{v}_k) = \frac{m}{2}(\overline{v}_{k+1}^2 - \overline{v}_k^2) + V(\overline{q}_{k+1}) - V(\overline{q}_k) =$$

$$m\left(\frac{\overline{v}_{k+1} + \overline{v}_k}{2}\right)\left(\frac{\overline{v}_{k+1} - \overline{v}_k}{\Delta t}\right)\Delta t + \left(\frac{V(\overline{q}_{k+1}) - V(\overline{q}_k)}{\overline{q}_{k+1} - \overline{q}_k}\right)\left(\frac{\overline{q}_{k+1} - \overline{q}_k}{\Delta t}\right)\Delta t \tag{101}$$

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

$$E(\overline{q}_{k+1}, \overline{v}_{k+1}) - E(\overline{q}_k, \overline{v}_k) = 0$$

Again, equation (99) insures the continuity of $\hat{q}(t)$.

A fourth discretization scheme due to T.D. Lee [Lee 1987] can be derived in the following manner. Let A_D given by

$$A_D = \sum_{i=0}^{N-1} \left[\frac{1}{2} m\overline{v}_i^2 - \overline{V}(i)\right] (t_{i+1} - t_i) \tag{102}$$

be the "discrete action" of a Newtonian potential system where

$$\overline{v}_i = \frac{q_{i+1} - q_i}{t_{i+1} - t_i} \tag{103}$$

and where the "discrete potential" $\overline{V}(i)$ is given by

$$\overline{V}(i) = \frac{1}{q_{i+1} - q_i} \int_{q_i}^{q_{i+1}} V(q)dq \tag{104}$$

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

$$\frac{\partial A_D}{\partial q_{k+1}} = 0 \tag{105}$$

$$\frac{\partial A_D}{\partial t_{k+1}} = 0 \tag{106}$$

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

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

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

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

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

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

$$- m\left(\overline{v}_{k+1} - \overline{v}_k\right) - \left(\frac{\partial \overline{V}(k+1)}{\partial q_{k+1}}\left(t_{k+2} - t_{k+1}\right) + \frac{\partial \overline{V}(k)}{\partial q_{k+1}}\left(t_{k+1} - t_k\right)\right) \quad (107)$$

Similarly, from (102) we have

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

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

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

$$\left.\frac{1}{2} m \frac{(q_{k+2} - q_{k+1})^2}{t_{k+2} - t_{k+1}} - \overline{V}(k+1)(t_{k+2} - t_{k+1})\right] =$$

$$-\frac{1}{2} m \frac{(q_{k+1} - q_k)^2}{(t_{k+1} - t_k)^2} - \overline{V}(k) + \frac{1}{2} m \frac{(q_{k+2} - q_{k+1})^2}{(t_{k+2} - t_{k+1})^2} + \overline{V}(k+1) =$$

$$\left(\frac{1}{2} m \overline{v}_{k+1}^2 + \overline{V}(k+1)\right) - \left(\frac{1}{2} m \overline{v}_k^2 + \overline{V}(k)\right) \quad (108)$$

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

$$\overline{v}_{k+1} - \overline{v}_k = -\frac{1}{m}\left(\frac{\partial \overline{V}(k+1)}{\partial q_{k+1}}\left(t_{k+2} - t_{k+1}\right) + \frac{\partial \overline{V}(k)}{\partial q_{k+1}}\left(t_{k+1} - t_k\right)\right) \quad (109)$$

$$\left(\frac{1}{2} m \overline{v}_{k+1}^2 + \overline{V}(k+1)\right) - \left(\frac{1}{2} m \overline{v}_k^2 + \overline{V}(k)\right) = 0 \quad (110)$$

In order to resolve certain pecularities which arise in the application of (109)–(110) to the simple harmonic oscillator, D'Innocenzo et al [D'Innocenzo et al 1987] have proposed a new definition for $\overline{V}(i)$ given by (104). They propose that $\overline{V}(i)$ be defined to be

$$\overline{V}(i) = V(\overline{q}_i) \quad (111)$$

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

$$\overline{v}_{k+1} - \overline{v}_k = -\frac{1}{2m}\left(\frac{\partial V(\overline{q}_{k+1})}{\partial \overline{q}_{k+1}}\left(t_{k+2} - t_{k+1}\right) + \frac{\partial V(\overline{q}_k)}{\partial \overline{q}_k}\left(t_{k+1} - t_k\right)\right) \quad (112)$$

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

where

$$\overline{q}_k = \frac{q_{k+1} + q_k}{2} \tag{114}$$

$$\overline{v}_k = \frac{q_{k+1} - q_k}{t_{k+1} - t_k} \tag{115}$$

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 Legandre's transformation we have

$$p = \frac{\partial L}{\partial v} = mv \tag{117}$$

and

$$\begin{aligned} H(q,p) &= pv - L(q,v) \\ &= pv - \left(\frac{1}{2}mv^2 - V(q)\right) \\ &= p(\frac{1}{m}p) - \frac{1}{2}m(\frac{1}{m}p)^2 + V(q) \\ &= \frac{1}{2m}p^2 + V(q) \end{aligned} \tag{118}$$

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

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

$$\frac{\overline{p}_{k+1} - \overline{p}_k}{\Delta\tau} = -\frac{1}{2}\left[\lambda_{k+1}\frac{\partial V(\overline{q}_{k+1})}{\partial\overline{q}_{k+1}} + \lambda_k\frac{\partial V(\overline{q}_k)}{\partial\overline{q}_k}\right] \tag{120}$$

$$\left(\frac{1}{2m}\overline{p}_{k+1}^2 + V(\overline{q}_{k+1})\right) - \left(\frac{1}{2m}\overline{p}_k^2 + V(\overline{q}_k)\right) = 0 \tag{121}$$

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

$$\overline{q}'_k = \frac{1}{m}\lambda_k \overline{p}_k \tag{122}$$

$$\overline{p}'_k = -\lambda_k \frac{\partial V(\overline{q}_k)}{\partial \overline{q}_k} \tag{123}$$

$$\overline{t}'_k = \lambda_k \tag{124}$$

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 $\overline{q}_k$, $\overline{v}_k$, $\overline{p}_k$, and $\overline{t}_k$ for $k = 0, 1, \cdots N-1$. We can show this in the following way. Dividing both sides of (112) by $\Delta\tau$ and multiplying by m we have

$$\frac{m\overline{v}_{k+1} - m\overline{v}_k}{\Delta\tau} = -\frac{1}{2}\left[\frac{\partial V(\overline{q}_{k+1})}{\partial \overline{q}_{k+1}}\left(\frac{t_{k+2} - t_{k+1}}{\Delta\tau}\right) + \frac{\partial V(\overline{q}_k)}{\partial \overline{q}_k}\left(\frac{t_{k+1} - t_k}{\Delta\tau}\right)\right]$$

Equation (122) and (124) imply that

$$\begin{aligned} \overline{p}_k &= \frac{m}{\lambda_k}\overline{q}'_k \\ &= \frac{m}{\overline{t}'_k}\overline{q}'_k \\ &= m\overline{v}_k \end{aligned} \tag{125}$$

From (124) and (125) we have

$$\frac{\overline{p}_{k+1} - \overline{p}_k}{\Delta\tau} = -\frac{1}{2}\left[\lambda_{k+1}\frac{\partial V(\overline{q}_{k+1})}{\partial \overline{q}_{k+1}} + \lambda_k \frac{\partial V(\overline{q}_k)}{\partial \overline{q}_k}\right]$$

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

$$\begin{aligned} \frac{\overline{q}_{k+1} - \overline{q}_k}{\Delta\tau} &= \frac{1}{\Delta\tau}\left[\frac{q_{k+2} + q_{k+1}}{2} - \frac{q_{k+1} + q_k}{2}\right] \\ &= \frac{1}{2}\left[\left(\frac{q_{k+2} - q_{k+1}}{t_{k+2} - t_{k+1}}\right)\left(\frac{t_{k+2} - t_{k+1}}{\Delta\tau}\right) + \left(\frac{q_{k+1} - q_k}{t_{k+1} - t_k}\right)\left(\frac{t_{k+1} - t_k}{\Delta\tau}\right)\right] \\ &= \frac{1}{2}\left[\overline{v}_{k+1}\overline{t}'_{k+1} + \overline{v}_k \overline{t}'_k\right] \end{aligned} \tag{126}$$

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

$$\frac{\bar{q}_{k+1} - \bar{q}_k}{\Delta\tau} = \frac{1}{2}\left[\lambda_{k+1}\bar{v}_{k+1} + \lambda_k \bar{v}_k\right] \tag{127}$$

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

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

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.

Next we present numerical results for two Newtonian potential systems—a simple pendulum with the potential function

$$V(q) = -\cos(q) \tag{128}$$

and an inverse square law system with the potential function

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

The value $m = 1$ is used for both systems. (Numerical results for the Kepler problem in Cartesian coordinates are given in [Shibberu 1992].)

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 λ_{k+1} fixed. Then, equation (86) is used to solve for λ_{k+1}, again using Newton's method. The details of the algorithm are given in [Shibberu 1992].

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

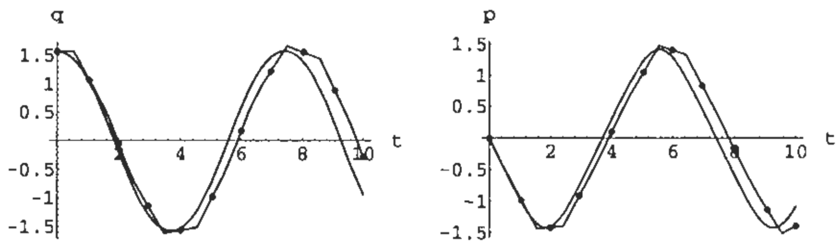
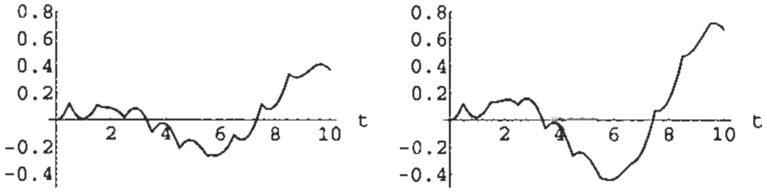
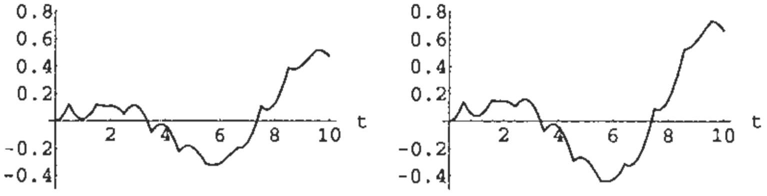


Figure 2: A trajectory of a simple pendulum and the corresponding DTH trajectory for $\Delta\tau = 1.07145$.



(a) midpoint scheme (b) trapezoidal scheme



(c) discrete mechanics (d) DTH dynamics

Figure 3: Errors in q for the trajectory of Figure 2. For (a)–(c) $\Delta t = 1$. For (d) $\Delta\tau = 1.07145$.

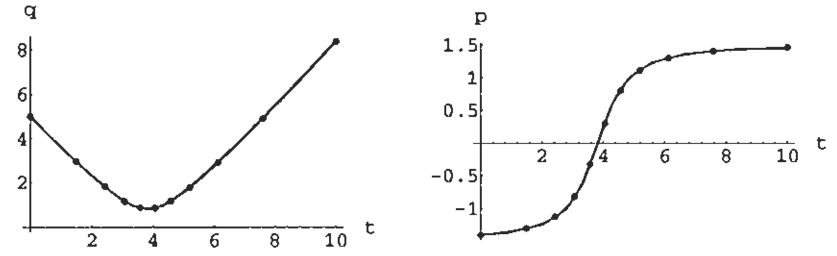


Figure 4: The trajectory for an inverse square law potential and the corresponding DTH trajectory for $\Delta\tau = 1.843271$.

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 schemes have. For the inverse square law system, however, DTH dynamics has roughly an order of magnitute 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 uniquenss of DTH trajectories is the condition $\Psi(q_0, p_0) \neq 0$ where

$$\Psi(q,p) = H_{qq}(H_p)^2 - 2H_{qp}H_qH_p + H_{pp}(H_q)^2$$

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.

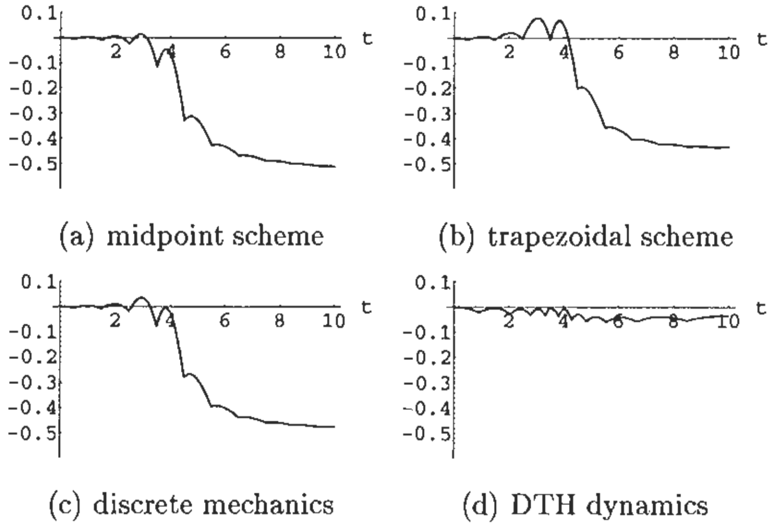
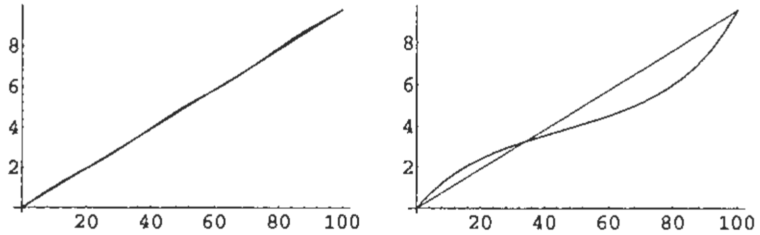


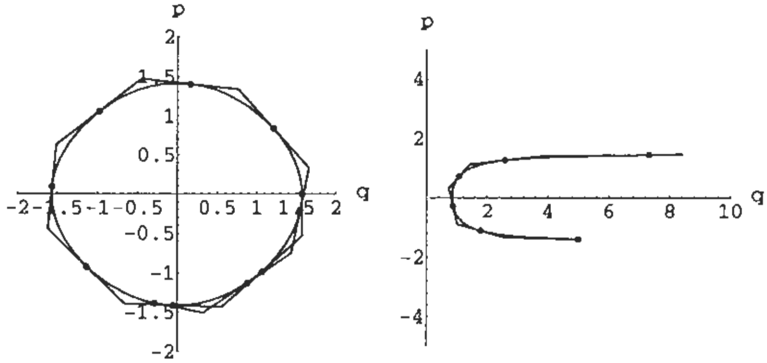
Figure 5: q for the trajectory of Figure 4. For (a)–(c) $\Delta t = 1$. For (d) $\Delta \tau = 1.843271$.



(a) simple pendulum ($\Delta \tau = 0.107145$)

(b) inverse square law ($\Delta \tau = 0.1843271$)

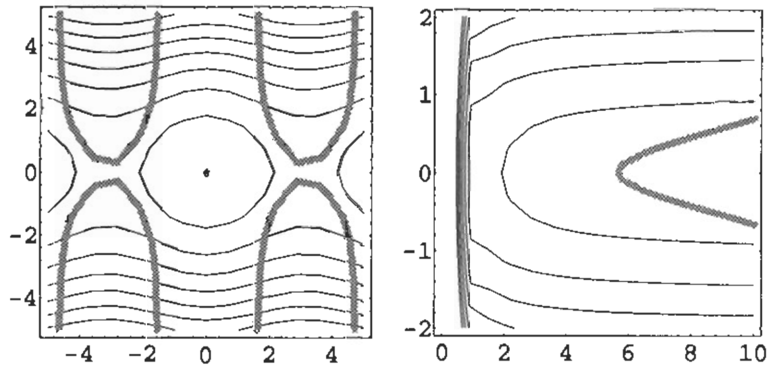
Figure 6: Time parametrization of DTH trajectories.



(a) simple pendulum
($\Delta\tau = 1.07145$)

(b) inverse square law
($\Delta\tau = 3.5$)

Figure 7: DTH trajectories and energy conserving manifolds.



(a) simple pendulum

(b) inverse square law

Figure 8: Phase portraits. Shaded regions indicate where $\Psi(q,p) = 0$.

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 τ_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 where $\mathbf{z}^{(k)} = \hat{\mathbf{z}}(\tau_k)$ are the vertices of $\hat{\mathbf{z}}(\cdot)$. Define $\overline{\mathbf{z}}^{(k)} = (\mathbf{z}^{(k+1)} + \mathbf{z}^{(k)})/2$ and $\overline{\mathbf{z}}'^{(k)} = (\mathbf{z}^{(k+1)} - \mathbf{z}^{(k)})/\Delta\tau$, for $k = 0, 1, \cdots N-1$. The $N-1$ values of $\overline{\mathbf{z}}^{(k)}$ and $\overline{\mathbf{z}}'^{(k)}$ completely determine $\hat{\mathbf{z}}(\cdot)$.

Consider a Hamiltonian system with Hamiltonian function $H(\mathbf{z})$ where $\mathbf{z} = (\mathbf{q}, \mathbf{p})^T$ and where $\mathbf{q}, \mathbf{p} \in \Re^{n+1}$ 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 $\mathbf{J}$ is defined to be the skew-symmetric matrix

$$\mathbf{J} = \begin{bmatrix} 0 & I_{n+1} \\ -I_{n+1} & 0 \end{bmatrix}$$

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 $\hat{\mathbf{z}} : [\tau_0, \tau_N] \longrightarrow \Re^{2n+2}$ for which the sum:*

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

is stationary. The endpoints $\overline{\mathbf{q}}^{(0)}$ and $\overline{\mathbf{p}}^{(N)}$ are assumed fixed. For a Hamiltonian system with a Hamiltonian function $H(\mathbf{z})$, the function $\mathcal{H}(\mathbf{z})$ is defined to be:

$$\mathcal{H}(\mathbf{z}) = z_{2n+2} + H(\mathbf{z})$$

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

Theorem 6 (DTH Equations of Motion) *A piecewise-linear, continuous function* $\hat{\mathbf{z}} : [\tau_0, \tau_N] \longrightarrow \Re^{2n+2}$ *is a DTH trajectory if and only if* $\overline{\mathbf{z}}^{(k)}$ *and* $\overline{\mathbf{z}}'^{(k)}$ *satisfy the following equations:*

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

$$\overline{\mathbf{z}}'^{(k)} = \lambda_k\mathbf{J}\frac{\partial\mathcal{H}(\overline{\mathbf{z}}^{(k)})}{\partial\overline{\mathbf{z}}^{(k)}} \quad k = 0, 1, \cdots N-1 \tag{131}$$

$$\mathcal{H}(\overline{\mathbf{z}}^{(k)}) = 0 \quad k = 0, 1, \cdots N-1 \tag{132}$$

Theorem 1 is proved by equating the partial derivatives of $\mathcal{A}\left[\Delta\tau, \lambda_0, \cdots \lambda_{N-1}, \hat{\mathbf{z}}(\cdot)\right]$ to zero and simplifying the resulting equations. The details of the proof are given in [Shibberu 1992].

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* $U \subset \Re^{2n+2}$ *is open. Assume also that* $\lambda_0 > 0$ *and that there exists a* $\overline{\mathbf{z}}^{(0)} \in U$ *such that* $\mathcal{H}(\overline{\mathbf{z}}^{(0)}) = 0$ *and* $\Psi(\overline{\mathbf{z}}^{(0)}) \neq 0$ *where:*

$$\Psi(\mathbf{z}) = \left[\mathbf{J}\mathcal{H}_z(\mathbf{z})\right]^T \mathcal{H}_{zz}(\mathbf{z}) \left[\mathbf{J}\mathcal{H}_z(\mathbf{z})\right]$$

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

The proof is based on the Newton-Kantorovich Theorem and is given in [Shibberu 1992].

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 [Shibberu 1992].

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 [Shibberu 1992].

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