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Hamiltonian-Conserving Discrete Canonical Equations Based on Variational Difference Quotients

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New discrete mechanics based on the assumption of the discrete time is proposed. The discrete mechanics does not contain any continuous differentiation, but contains only difference quotients Resulting discrete Hamiltonian's canonical equations are single time-step difference equations and exactly conserve the Hamiltonian The canonical equations give the numerical results more accurately than the Heun scheme and the 4th-order Runge–Kutta scheme

1 INTRODUCTION

In the classical mechanics, the motion of a particle is predicted by Lagrange's equations, or the canonical equations based on the Hamiltonian. These theories are constructed on the assumption that the coordinates and momentums of particles are functions of continuous time. We may call the mechanics continuous mechanics.

Electronic digital computers stimulate the development of discrete mechanics where the time is regarded as discrete. Discrete mechanics have been proposed by Maeda [1], Holm *et al.* [2], and Gotusso [3]. All of the discrete mechanics use the functional $G[\xi(t), ...]$, where G is, for example, the Lagrangian, and the argument function $\xi(t)$ is the generalized coordinate of a particle, depending on time t. The methods proposed by Maeda [1] and Holm *et al.* [2] allow the variational derivative of G with respect to ξ; that is to say, the methods include the expression $\partial G/\partial \xi$. Thus we may call these as quasi-discrete mechanics or semi-discrete mechanics. The methods succeed in retaining without special difficulty

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many features inherent to continuous mechanics. The methods, however, sometimes fail to preserve invariants, such as the total energy of the system with sufficient accuracy. In view of the numerical solution of the equations of mechanics, conservation of the invariants over a long time with sufficient accuracy is indispensable. The method proposed by Gotusso [3] does not use the variational derivative $\partial G/\partial \xi$, but replaces $\partial G/\partial \xi$ by a finite difference quotient. The method can easily produce a scheme which preserves invariants but fails to retain features inherent to continuous mechanics. In this paper, we propose a new discrete mechanics which satisfies exact conservation of the Hamiltonian and retains features inherent to continuous mechanics. The present discrete mechanics does not allow any variational derivative $\partial G/\partial \xi$, but uses a variational difference quotient $\Delta_\xi G$ in place of $\partial G/\partial \xi$.

2. Variational Difference Quotient and Discrete Lagrangian

We consider the functional $G(\xi^1, \xi^2, ..., \xi^\mu)$, where ξ^i is the argument function depending on time t, and μ denotes the number of degrees of freedom. In continuous mechanics, the variation δG of G is given by

$$\delta G(\boldsymbol{\xi}) = G(\boldsymbol{\eta}) - G(\boldsymbol{\xi}) = \sum_{i=1}^{\mu} \delta\xi^i \frac{\partial G}{\partial \xi^i}, \tag{2.1}$$

where $\boldsymbol{\xi} = (\xi^1, ..., \xi^\mu)$, $\boldsymbol{\eta} = (\eta^1, ..., \eta^\mu)$, and $\delta\boldsymbol{\xi} = (\delta\xi^1, ..., \delta\xi^\mu) = \boldsymbol{\eta} - \boldsymbol{\xi}$. In obtaining Eq. (2.1), we have assumed that $|\delta\xi^i| \ll 1$.

In order to construct the discrete mechanics, we do not allow the variational derivative $\partial G/\partial \xi$, so that we need a substitute for the variational derivative. The method of constructing discrete mechanics is based on the following algebraic identity proposed by Gotusso [3].

$$\begin{aligned}
\delta G(\boldsymbol{\xi}) &= G(\boldsymbol{\eta}) - G(\boldsymbol{\xi}) \\
&= G(\eta^1, ..., \eta^{\mu-1}, \eta^\mu) - G(\eta^1, .., \eta^{\mu-2}, \eta^{\mu-1}, \xi^\mu) \\
&\quad + G(\eta^1, ..., \eta^{\mu-2}, \eta^{\mu-1}, \xi^\mu) - G(\eta^1, ..., \eta^{\mu-2}, \xi^{\mu-1}, \xi^\mu) \\
&\quad + G(\eta^1, ..., \eta^{\mu-3}, \eta^{\mu-2}, \xi^{\mu-1}, \xi^\mu) - G(\eta^1, ..., \eta^{\mu-3}, \xi^{\mu-2}, \xi^{\mu-1}, \xi^\mu) \\
&\quad \cdots\cdots \\
&\quad + G(\eta^1, ..., \eta^{i-1}, \eta^i, \xi^{i+1}, ..., \xi^\mu) - G(\eta^1, ..., \eta^{i-1}, \xi^i, \xi^{i+1}, ..., \xi^\mu) \\
&\quad \cdots\cdots \\
&= G(\eta^1, \eta^2, ..., \eta^\mu) - G(\xi^1, ..., \xi^\mu),
\end{aligned} \tag{2.2}$$

where the second term of the right-hand side is canceled with the third term, and so on. We define the variational difference quotient $\Delta_{\xi^i} G$ by

$$\Delta_{\xi^i} G(\xi)|_{\eta} = \frac{1}{\eta^i - \xi^i} [G(\eta^1, ..., \eta^{i-1}, \eta^i, \xi^{i+1}, ..., \xi^{\mu}) - G(\eta^1, ..., \eta^{i-1}, \xi^i, \xi^{i+1}, ..., \xi^{\mu})]. \tag{2.3}$$

The subscript η means that the variational difference quotient $\Delta_{\xi} G(\xi)|_{\eta}$ is evaluated by using values of G at ξ and η. Then Eq. (2.2) becomes

$$\delta G(\xi) = \sum_{i=1}^{\mu} (\eta^i - \xi^i)\, \Delta_{\xi^i} G(\xi)|_{\eta} = \sum_{i=1}^{\mu} \delta\xi^i\, \Delta_{\xi^i} G(\xi)|_{\eta}. \tag{2.4}$$

Equation (2.4) corresponds to Eq. (2.1) in the continuous version. In Eq. (2.4) we do not require the condition $|\delta\xi^i| \ll 1$. This is an interesting feature that is different from the continuous mechanics based on Eq. (2.1).

Figure 1 illustrates the variational difference quotient $\Delta_{\xi^i} G|_{\eta}$ when $\mu = 3$. Vectors 1, 2, and 3 denote $\delta\xi^1 \Delta_{\xi^1} G|_{\eta}$, $\delta\xi^2 \Delta_{\xi^2} G|_{\eta}$, and $\delta\xi^3 \Delta_{\xi^3} G|_{\eta}$, respectively. In Fig. 1 there exist 3! (= 6) possible different pathes from (ξ^1, ξ^2, ξ^3) to (η^1, η^2, η^3).

We consider the Lagrangian $L(\boldsymbol{x}, \boldsymbol{p})$ which contains the generalized coordinate $\boldsymbol{x} = (x_1, x_2, .., x_f)$ and momentum $\boldsymbol{p} = (p_1, p_2, ..., p_f)$ as the argument functions. The action $J(N)$ is given by

$$J(N) = \sum_{n=0}^{N-1} \tau^n L(\boldsymbol{x}^n, \boldsymbol{p}^n), \tag{2.5}$$

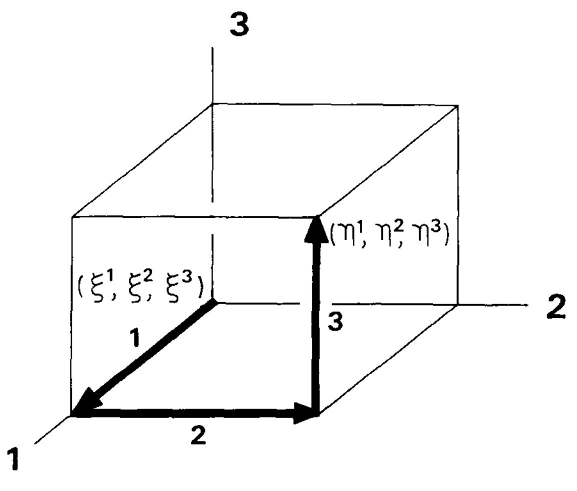

FIG 1. Illustration of $\Delta_{\xi^i} G(\xi)|_{\eta}$ when $\mu = 3$

where n and N are integers representing time and τ^n is the time interval given by

$$\tau^n = t^{n+1} - t^n \qquad \text{or} \qquad t^n = \sum_{m=1}^{n} \tau^{m-1} + t^0.$$

$L(\boldsymbol{x}, \boldsymbol{p})$ in Eq. (2.5) is reduced to $G(\xi)$ noted above, if we put $\mu = 2f$ and $(\xi) = (\boldsymbol{x}, \boldsymbol{p})$. In order to simplify notation, we introduce the operator $\Theta(n)$ by

$$\Theta(n)\, G(\xi) = G(\xi^n),$$

so that Eq. (2.5) becomes

$$J(N) = \sum_{n=0}^{N-1} \Theta(n)\, \tau L(\boldsymbol{x}, \boldsymbol{p}). \tag{2.6}$$

If we put $\boldsymbol{x} \to \boldsymbol{x} + \delta \boldsymbol{x} = \boldsymbol{y}$ and $\boldsymbol{p} \to \boldsymbol{p} + \delta \boldsymbol{p} = \boldsymbol{q}$, then $J(N) \to J(N) + \delta J(N)$. Some books use $\boldsymbol{q}$ to represent the generalized coordinate [4]. We should note that in this paper $\boldsymbol{q}$ denotes the generalized momentum. We obtain

$$\begin{aligned} \delta J(N) &= \sum_{n=0}^{N-1} \Theta(n)\, \tau [L(\boldsymbol{y}, \boldsymbol{q}) - L(\boldsymbol{x}, \boldsymbol{p})] \\ &= \sum_{n=0}^{N-1} \Theta(n)\, \tau \sum (\delta x_i \Delta_{x_i} + \delta p_i \Delta_{p_i})\, L(\boldsymbol{x}, \boldsymbol{p})|_{\boldsymbol{y} = \boldsymbol{x} + \delta \boldsymbol{x}, \boldsymbol{q} = \boldsymbol{p} + \delta \boldsymbol{p}}, \end{aligned}$$

where $\Delta_{x_i} L$ and $\Delta_{p_i} L$ are defined in the way similar to. (2.3). $\delta \boldsymbol{x}$ and $\delta \boldsymbol{p}$ are arbitrary, so that we obtain

$$\Delta_{x_i} L(\boldsymbol{x}, \boldsymbol{p})|_{\boldsymbol{y}, \boldsymbol{q}} = 0 \qquad (i = 1 \sim f,\ \boldsymbol{y} = \boldsymbol{x} + \delta \boldsymbol{x},\ \boldsymbol{q} = \boldsymbol{p} + \delta \boldsymbol{p}), \tag{2.7}$$

$$\Delta_{p_i} L(\boldsymbol{x}, \boldsymbol{p})|_{\boldsymbol{y}, \boldsymbol{q}} = 0 \qquad (i = 1 \sim f,\ \boldsymbol{y} = \boldsymbol{x} + \delta \boldsymbol{x},\ \boldsymbol{q} = \boldsymbol{p} + \delta \boldsymbol{p}), \tag{2.8}$$

which may be called as the discrete Lagrange equations.

We should note here that the order of argument functions $(\boldsymbol{x}, \boldsymbol{p})$ in Eqs. (2.7) and (2.8) are arbitrary. In other words, we can put $(\boldsymbol{x}, \boldsymbol{p}) = (x_1, p_1, x_2, p_2, \ldots)$, $(\boldsymbol{x}, \boldsymbol{p}) = (p_2, x_2, p_1, x_1, \ldots)$, and so on. Gotusso [3] also derived the discrete Lagrange equations using the Lagrangian $L(\boldsymbol{x}, \dot{\boldsymbol{x}})$, where $\dot{\boldsymbol{x}}$ denotes the generalized velocity, while our discrete Lagrangian contains the generalized momentum $\boldsymbol{p}$ as the argument function. Our final goal is not to obtain the discrete Lagrange equation, but to obtain the discrete canonical equations from Eqs. (2.7) and (2.8).

3. Discrete Canonical Equations Based on Backward Time-Difference Velocity

We use the lag operator l defined by $l(\boldsymbol{x}^n, \boldsymbol{p}^n) = (\boldsymbol{x}^{n-1}, \boldsymbol{p}^{n-1})$, and relate the Lagrangian $L(\boldsymbol{x}, \boldsymbol{p})$ with the discrete Hamiltonian $H(\boldsymbol{x}, \boldsymbol{p})$ by

$$L(\boldsymbol{x}, \boldsymbol{p}) = \sum_{i=1}^{f} p_i \frac{(I-l)x_i}{\tau} - H(\boldsymbol{x}, \boldsymbol{p}), \tag{3.1}$$

where I denotes the identity operator, i.e., $I(\boldsymbol{x}^n, \boldsymbol{p}^n) = (\boldsymbol{x}^n, \boldsymbol{p}^n)$. $(I-l)x_i/\tau$ in Eq. (3.1) is the backward time-difference velocity. We line up $(\boldsymbol{x}, \boldsymbol{p})$ in Eq. (3.1) in the order

$$(\boldsymbol{x}, \boldsymbol{p}) = (x_{i_1}, p_{i_1}, x_{i_2}, p_{i_2}, \ldots, x_{i_f}, p_{i_f}), \tag{3.2}$$

where $i_1, i_2, \ldots$ or i_f is equal to one value among $1 \sim f$. In Eq. (3.2) we put x_i to the left of p_i

Let us substitute Eq. (3.1) into Eq (2.8), where $\boldsymbol{y}$ and $\boldsymbol{q}$ are arbitrary. We put $(\boldsymbol{y}, \boldsymbol{q}) = l^{-1}(\boldsymbol{x}, \boldsymbol{p}) = (\boldsymbol{x}^{n+1}, \boldsymbol{p}^{n+1})$ when $(\boldsymbol{x}, \boldsymbol{p}) = (\boldsymbol{x}^n, \boldsymbol{p}^n)$ in Eq. (2.8) to obtain from the definition of Eq. (2.3)

$$\begin{aligned}
&\Delta_{p_i} L(\boldsymbol{x}, \boldsymbol{p})|_{(\boldsymbol{y}, \boldsymbol{q}) = l^{-1}(\boldsymbol{x}, \boldsymbol{p})} \\
&= \frac{l}{l^{-1}p_i - p_i} [L(\ldots, l^{-1}x_i, l^{-1}p_i, \ldots) - L(\ldots, l^{-1}x_i, p_i, \ldots)], \\
&= \frac{l}{l^{-1}p_i - p_i} \left[(l^{-1}p_i - p_i) \frac{(I-l)\, l^{-1}x_i}{\tau} - H(\ldots, l^{-1}p_i, \ldots) + H(\ldots, p_i, \ldots) \right], \\
&= 0.
\end{aligned}$$

This equation gives

$$\frac{\Delta_t x_i}{\tau} = \Delta_{p_i} H(\boldsymbol{x}, \boldsymbol{p})|_{(\boldsymbol{y}, \boldsymbol{q}) = l^{-1}(\boldsymbol{x}, \boldsymbol{p})} \qquad (i = 1 \sim f), \tag{3.3}$$

where Δ_t is defined by

$$\Delta_t = l^{-1} - I,$$

and $\Delta_{p_i} H(\boldsymbol{x}, \boldsymbol{p})$ is defined by the same way as in Eq. (2.3). Explicit expressions of Eq. (3.3) for $f = 2$ will be given by Eqs. (5.1) and (5.2), where we put $(\boldsymbol{x}, \boldsymbol{p}) = (\boldsymbol{x}^n, \boldsymbol{p}^n)$.

Substitution of Eq. (3.1) into Eq. (2.6) gives

$$J(N)=\sum_{n=0}^{N-1}\Theta(n)\left[\sum_{i=1}^{f}p_i(I-l)x_i-\tau H(\boldsymbol{x},\boldsymbol{p})\right]. \tag{3.4}$$

If we use the identity $I=l^{-1}+(I-l^{-1})$, the contribution of the term containing $p_i l x_i$ in Eq. (3.4) becomes

$$\begin{aligned}&\sum_{n=0}^{N-1}\Theta(n)\sum_{i=1}^{f}[l^{-1}+(I-l^{-1})](p_i l x_i)\\&\quad=\sum_{n=0}^{N-1}\Theta(n)\sum_{i=1}^{f}(l^{-1}p_i)x_i+\sum_{n=0}^{N-1}\Theta(n)\sum_{i=1}^{f}(I-l^{-1})(p_i l x_i),\end{aligned}$$

where we have used the relation $l^{-1}(p_i l x_i)=(l^{-1}p_i)x_i$. The last term in the above equation plays no role, because

$$\sum_{n=0}^{N-1}\Theta(n)\sum_{i=1}^{f}(I-l^{-1})(p_i l x_i)=[\Theta(0)-\Theta(N)]\sum_{i=1}^{f}(p_i l x_i)$$

and the variations of the right-hand side are assumed zero in the classical mechanics. Thus Eq. (3.4) becomes

$$J(N)=\sum_{n=0}^{N-1}\Theta(n)\left(\sum_{i=1}^{f}[(I-l^{-1})p_i]x_i-\tau H(\boldsymbol{x},\boldsymbol{p})\right). \tag{3.5}$$

The reduction of Eq. (3.5) from Eq. (3.4) corresponds to the integration by parts in the continuous version.

Comparing Eq. (2.6) and Eq. (3 5), we put

$$L(\boldsymbol{x},\boldsymbol{p})=\sum_{i=1}^{f}\frac{(I-l^{-1})p_i}{\tau}x_i-H(\boldsymbol{x},\boldsymbol{p}). \tag{3.6}$$

We substitute Eq. (3.6) into (2.7), and put $(\boldsymbol{y},\boldsymbol{q})=l^{-1}(\boldsymbol{x},\boldsymbol{p})$ in Eq. (2.7). Equation (3.2) leads to

$$-\frac{\Delta_t p_i}{\tau}=\Delta_{x_i}H(\boldsymbol{x},\boldsymbol{p})|_{(\boldsymbol{y},\boldsymbol{q})=l^{-1}(\boldsymbol{x},\boldsymbol{p})}\qquad(i=1\sim f). \tag{3.7}$$

Equations (3 3) and (3.7) constitute the discrete canonical equations. Equations (3.3) and (3.7) contain only $(\boldsymbol{x},\boldsymbol{p})$ and $l^{-1}(\boldsymbol{x},\boldsymbol{p})$ and contain no quantities such as $l(\boldsymbol{x},\boldsymbol{p})$, $l^{-2}(\boldsymbol{x},\boldsymbol{p})$, etc., so that Eqs. (3.3) and (3.7) are single-step difference equations for $\boldsymbol{x}$ and $\boldsymbol{p}$. Since the right-hand sides of Eqs. (3.3) and (3.7) contain $l^{-1}(\boldsymbol{x},\boldsymbol{p})$ as well as $(\boldsymbol{x},\boldsymbol{p})$, eqs. (3.3) and (3.7) are implicit schemes.

We show that the conservation of Hamiltonian $H(\boldsymbol{x}, \boldsymbol{p})$ is assured automatically by Eqs. (3.3) and (3.7) as

$$\begin{aligned}\Delta_t H(\boldsymbol{x}, \boldsymbol{p}) &= (l^{-1} - I)\, H(\boldsymbol{x}, \boldsymbol{p}) = H(l^{-1}\boldsymbol{x}, l^{-1}\boldsymbol{p}) - H(\boldsymbol{x}, \boldsymbol{p}) \\ &= \sum_{i=1}^{f} \{[(l^{-1} - I)x_i]\, \Delta_{x_i} + [(l^{-1} - I)\, p_i]\, \Delta_{p_i}\}\, H(\boldsymbol{x}, \boldsymbol{p})|_{(\boldsymbol{y},\boldsymbol{q}) = l^{-1}(\boldsymbol{x},\boldsymbol{p})} \\ &= \sum_{i=1}^{f} [(\Delta_t x_i)\, \Delta_{x_i} + (\Delta_t p_i)\, \Delta_{p_i}]\, H(\boldsymbol{x}, \boldsymbol{p})|_{(\boldsymbol{y},\boldsymbol{q}) = l^{-1}(\boldsymbol{x},\boldsymbol{p})}. \end{aligned} \tag{3.8}$$

Substitutions of Eqs. (3.3) and (3.7) into $\Delta_t x_i$ and $\Delta_t p_i$ in the right-hand side leads to $\Delta_t H(\boldsymbol{x},\boldsymbol{p}) = 0$ which means the conservation of the Hamiltonian.

4. Discrete Canonical Equations Based on Forward Time-Difference Velocity

In this section we start from the Lagrangian based on the forward time-difference velocity as

$$L(\boldsymbol{x}, \boldsymbol{p}) = \sum_{i=1}^{f} p_i \frac{(l^{-1} - I)x_i}{\tau} - H(\boldsymbol{x}, \boldsymbol{p}). \tag{4.1}$$

The order of $(\boldsymbol{x}, \boldsymbol{p})$ is given by

$$(\boldsymbol{x}, \boldsymbol{p}) = (p_{i_1}, x_{i_1}, p_{i_2}, x_{i_2}, \ldots, p_{i_f}, x_{i_f}). \tag{4.2}$$

Substituting Eq. (4.1) into Eq. (2.8) and putting $(\boldsymbol{y}, \boldsymbol{q}) = l^{-1}(\boldsymbol{x}, \boldsymbol{p})$, we obtain

$$\frac{\Delta_t x_i}{\tau} = \Delta_{p_i} H(\boldsymbol{x}, \boldsymbol{p})|_{(\boldsymbol{y},\boldsymbol{q}) = l^{-1}(\boldsymbol{x},\boldsymbol{p})} \qquad (i = l \sim f). \tag{4.3}$$

From Eq. (4.1) we can obtain

$$L(\boldsymbol{x}, \boldsymbol{p}) = \sum_{i=1}^{f} \frac{(l - I)\, p_i}{\tau} x_i - H(\boldsymbol{x}, \boldsymbol{p}), \tag{4.4}$$

in a similar way to the reduction of Eq. (3.6) from Eq. (3.1). Substituting Eq. (4.4) into Eq. (2.7) and putting $(\boldsymbol{y}, \boldsymbol{q}) = l^{-1}(\boldsymbol{x}, \boldsymbol{p})$, we obtain

$$-\frac{\Delta_t p_i}{\tau} = \Delta_{x_i} H(\boldsymbol{x}, \boldsymbol{p})|_{(\boldsymbol{y},\boldsymbol{q}) = l^{-1}(\boldsymbol{x},\boldsymbol{p})} \qquad (i = l \sim f). \tag{4.5}$$

Equations (4.3) and (4.5) constitute the discrete canonical equations, which are implicit single-step difference equations for $\boldsymbol{x}$ and $\boldsymbol{p}$. Only the difference between

Eqs. (3.3) and (4.3) and the difference between Eqs. (3.7) and (4.5) lie in the order of $(\boldsymbol{x}, \boldsymbol{p})$. That is to say, Eqs. (4.3)and (4.5) are based on the order of Eq. (4.2), while Eqs. (3.3) and (3.7) are based on the order of Eq. (3.2). In the quite same way as Eq. (3.8) we can prove from Eqs. (4.3) and (4.5) that $\Delta_t H(\boldsymbol{x}, \boldsymbol{p}) = 0$ which means the conservation of the Hamiltonian.

5. Applications of Discrete Canonical Equations to Two-Body Problem

If we put $(\boldsymbol{x}, \boldsymbol{p}) = (x_1^n, p_1^n, x_2^n, p_2^n)$ and $I^{-1}(\boldsymbol{x}, \boldsymbol{p}) = (x_1^{n+1}, p_1^{n+1}, x_2^{n+1}, p_2^{n+1})$, Eq. (3.3) gives

$$\frac{x_1^{n+1} - x_1^n}{\tau} = \frac{1}{p_1^{n+1} - p_1^n} [H(x_1^{n+1}, p_1^{n+1}, x_2^n, p_2^n) - H(x_1^{n+1}, p_1^n, x_2^n, p_2^n)], \tag{5.1}$$

$$\frac{x_2^{n+1} - x_2^n}{\tau} = \frac{1}{p_2^{n+1} - p_2^n} [H(x_1^{n+1}, p_1^{n+1}, x_2^{n+1}, p_2^{n+1}) - H(x_1^{n+1}, p_1^{n+1}, x_2^{n+1}, p_2^n)], \tag{5.2}$$

and Eq. (3.7) gives

$$-\frac{p_1^{n+1} - p_1^n}{\tau} = \frac{1}{x_1^{n+1} - x_1^n} [H(x_1^{n+1}, p_1^n, x_2^n, p_2^n) - H(x_1^n, p_1^n, x_2^n, p_2^n)], \tag{5.3}$$

$$-\frac{p_2^{n+1} - p_2^n}{\tau} = \frac{1}{x_2^{n+1} - x_2^n} [H(x_1^{n+1}, p_1^{n+1}, x_2^{n+1}, p_2^n) - H(x_1^{n+1}, p_1^{n+1}, x_2^n, p_2^n)]. \tag{5.4}$$

It is easy to show that Eqs. (5.1)–(5.4) are accurate to the order of τ. In order to improve the accuracy, we use the following equations in addition to Eqs. (5.1)–(5.4).

If we put $(\boldsymbol{x}, \boldsymbol{p}) = (x_2^n, p_2^n, x_1^n, p_1^n)$, Eqs. (3.3) and (3.7) gives

$$\frac{x_1^{n+1} - x_1^n}{\tau} = \frac{1}{p_1^{n+1} - p_1^n} [H(x_2^{n+1}, p_2^{n+1}, x_1^{n+1}, p_1^{n+1}) - H(x_2^{n+1}, p_2^{n+1}, x_1^{n+1}, p_1^n)], \tag{5.5}$$

$$\frac{x_2^{n+1} - x_2^n}{\tau} = \frac{1}{p_2^{n+1} - p_2^n} [H(x_2^{n+1}, p_2^{n+1}, x_1^n, p_1^n) - H(x_2^{n+1}, p_2^n, x_1^n, p_1^n)], \tag{5.6}$$

$$-\frac{p_1^{n+1} - p_1^1}{\tau} = \frac{1}{x_1^{n+1} - x_1^n} [H(x_2^{n+1}, p_2^{n+1}, x_1^{n+1}, p_1^n) - H(x_2^{n+1}, p_2^{n+1}, x_1^n, p_1^n)], \tag{5.7}$$

$$-\frac{p_2^{n+1} - p_2^n}{\tau} = \frac{1}{x_2^{n+1} - x_2^n} [H(x_2^{n+1}, p_2^n, x_1^n, p_1^n) - H(x_2^n, p_2^n, x_1^n, p_1^n)]. \tag{5.8}$$

If we put $(\boldsymbol{x}, \boldsymbol{p}) = (p_1^n, x_1^n, p_2^n, x_2^n)$, Eqs. (4.3) and (4.5) give

$$\frac{x_1^{n+1} - x_1^n}{\tau} = \frac{1}{p_1^{n+1} - p_1^n} [H(p_1^{n+1}, x_1^n, p_2^n, x_2^n) - H(p_1^n, x_1^n, p_2^n, x_2^n)], \tag{5.9}$$

$$\frac{x_2^{n+1} - x_2^n}{\tau} = \frac{1}{p_2^{n+1} - p_2^n} [H(p_1^{n+1}, x_1^{n+1}, p_2^{n+1}, x_2^n) - H(p_1^{n+1}, x_1^{n+1}, p_2^n, x_2^n)], \tag{5.10}$$

$$-\frac{p_1^{n+1} - p_1^n}{\tau} = \frac{1}{x_1^{n+1} - x_1^n} [H(p_1^{n+1}, x_1^{n+1}, p_2^n, x_2^n) - H(p_1^{n+1}, x_1^n, p_2^n, x_2^n)], \tag{5.11}$$

$$-\frac{p_2^{n+1} - p_2^n}{\tau} = \frac{1}{x_2^{n+1} - x_2^n} [H(p_1^{n+1}, x_1^{n+1}, p_2^{n+1}, x_2^{n+1}) - H(p_1^{n+1}, x_1^{n+1}, p_2^{n+1}, x_2^n)]. \tag{5.12}$$

If we put $(\boldsymbol{x}, \boldsymbol{p}) = (p_2^n, x_2^n, p_1^n, x_1^n)$ Eqs. (4.3) and (4.5) give

$$\frac{x_1^{n+1} - x_1^n}{\tau} = \frac{1}{p_1^{n+1} - p_1^n} [H(p_2^{n+1}, x_2^{n+1}, p_1^{n+1}, x_1^n) - H(p_2^{n+1}, x_2^{n+1}, p_1^n, x_1^n)], \tag{5.13}$$

$$\frac{x_2^{n+1} - x_2^n}{\tau} = \frac{1}{p_2^{n+1} - p_2^n} [H(p_2^{n+1}, x_2^n, p_1^n, x_1^n) - H(p_2^n, x_2^n, p_1^n, x_1^n)], \tag{5.14}$$

$$-\frac{p_1^{n+1} - p_1^n}{\tau} = \frac{1}{x_1^{n+1} - x_1^n} [H(p_2^{n+1}, x_2^{n+1}, p_1^{n+1}, x_1^{n+1}) - H(p_2^{n+1}, x_2^{n+1}, p_1^{n+1}, x_1^n)], \tag{5.15}$$

$$-\frac{p_2^{n+1} - p_2^n}{\tau} = \frac{1}{x_2^{n+1} - x_2^n} [H(p_2^{n+1}, x_2^{n+1}, p_1^n, x_1^n) - H(p_2^{n+1}, x_2^n, p_1^n, x_1^n)] \tag{5.16}$$

We calcululate

[Eq. (5.1) + Eq. (5.5) + Eq. (5.9) + Eq. (5.13)]/4,

[Eq. (5 2) + Eq. (5.6) + Eq. (5.10) + Eq (5.14)]/4,

[Eq. (5 3) + Eq. (5.7) + Eq. (5.11) + Eq. (5.15)]/4,

[Eq. (5 4) + Eq. (5.8) + Eq. (5.12) + Eq (5.16)]/4,

and rearrange the order of $(\boldsymbol{x}, \boldsymbol{p})$ to (x_1, p_1, x_2, p_2) to obtain

$$\frac{x_1^{n+1} - x_1^n}{\tau} = \frac{1}{4(p_1^{n+1} - p_1^n)} \sum_{k,m=n}^{n+1} [H(x_1^k, p_1^{n+1}, x_2^m, p_2^m) - H(x_1^k, p_1^n, x_2^m, p_2^m)], \tag{5.17}$$

$$\frac{x_2^{n+1} - x_2^n}{\tau} = \frac{1}{4(p_2^{n+1} - p_2^n)} \sum_{k,m=n}^{n+1} [H(x_1^m, p_1^m, x_2^k, p_2^{n+1}) - H(x_1^m, p_1^m, x_2^k, p_2^n)], \tag{5.18}$$

$$-\frac{p_1^{n+1}-p_1^n}{\tau}=\frac{1}{4(x_1^{n+1}-x_1^n)}\sum_{k,m=n}^{n+1}\left[H(x_1^{n+1}, p_1^k, x_2^m, p_2^m)-H(x_1^n, p_1^k, x_2^m, p_2^m)\right], \tag{5.19}$$

$$-\frac{p_2^{n+1}-p_2^n}{\tau}=\frac{1}{4(x_2^{n+1}-x_2^n)}\sum_{k,m=n}^{n+1}\left[H(x_1^m, p_1^m, x_2^{n+1}, p_2^k)-H(x_1^m, p_1^m, x_2^n, p_2^k)\right], \tag{5.20}$$

which are symmetrical with respect to $(x_1, p_1, x_2, p_2)^n$ and $(x_1, p_1, x_2, p_2)^{n+1}$ and are accurate to the order of τ^2.

Let us define the Hamiltonian $H(\boldsymbol{x}, \boldsymbol{p})$ by

$$H(x_1, p_1, x_2, p_2)=\frac{1}{2}(p_1^2+p_2^2)+\cos x_1-1+\frac{\varepsilon}{2}p_1^2\cos x_2, \tag{5.21}$$

where ε is constant. If $\varepsilon=0$, the analytic solution of Eq. (5.21) exists. That is to say, $p_2=$const and (x_1, p_1) in the phase space are given by Fig. 2. If $\varepsilon\neq 0$, the orbits of particles become chaotic, and there exists no analytic solution. In the study of chaotic topology, we should eliminate carefully the error arising from the numerical computation. Otherwise the numerical error leads to false chaos. For example, if we put $\varepsilon=0$ and $(x_1, p_1, x_2, p_2)_{t=0}=(\pi, 2, 0, 0)$, then $H=0$ and the exact trajectory of particle "1" lies on the separatrix in Fig. 2. The wrong numerical computation,

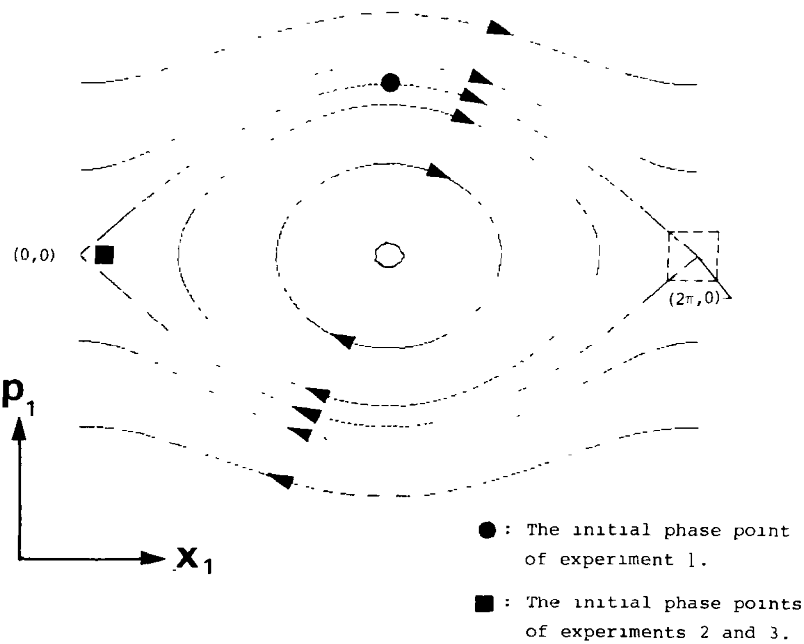

FIG 2 Analytical trajectories of phase point in (x_1, p_1) space, when $H=p_1^2/2+\cos x_1-1$

TABLE I

Examples of Heun Scheme and Hamiltonian-Conserving Scheme

Scheme	Predictor	Corrector	Accuracy
Hamiltonian-conserving scheme	(Euler Scheme)	(Hamiltonian-conserving scheme)	
	$x_1^{n+1} - x_1^n = \tau p_1^n[1 + \varepsilon \cos(x_2^n)]$	$x_1^{n+1} - x_1^n = \frac{1}{2}\tau \left\{1 + \frac{\varepsilon}{2}[\cos(x_2^{n+1}) + \cos(x_2^n)]\right\}(p_1^{n+1} + p_1^n)$	
	$x_2^{n+1} - x_2^n = \tau p_2^n$	$x_2^{n+1} - x_2^n = \frac{1}{2}\tau(p_2^{n+1} + p_2^n)$	$O(\tau^2)$
	$p_1^{n+1} - p_1^n = \tau \sin(x_1^n)$	$p_1^{n+1} - p_1^n = -\tau \frac{\cos(x_1^{n+1}) - \cos(x_1^n)}{x_1^{n+1} - x_1^n}$	
	$p_2^{n+1} - p_2^n = \frac{\varepsilon}{2}\tau(p_1^n)^2 \sin(x_2^n)$	$p_2^{n+1} - p_2^n = -\tau \frac{\varepsilon}{4} \frac{\cos(x_2^{n+1}) - \cos(x_2^n)}{x_2^{n+1} - x_2^n}[(p_1^{n+1})^2 + (p_1^n)^2]$	
Heun scheme	(Euler scheme)	(Trapezoidal scheme)	
		$x_1^{n+1} - x_1^n = \frac{1}{2}\tau \{p_1^{n+1}[l + \varepsilon \cos(x_2^{n+1})] + p_1^n[1 + \varepsilon \cos(x_2^n)]\}$	
		$x_2^{n+1} - x_2^n = \frac{1}{2}\tau(p_2^{n+1} + p_2^n)$	$O(\tau^2)$
		$p_1^{n+1} - p_1^n = \frac{1}{2}\tau [\sin(x_1^{n+1}) + \sin(x_1^n)]$	
		$p_2^{n+1} - p_2^n = \frac{\varepsilon}{4}\tau [(p_1^{n+1})^2 \sin(x_2^{n+1}) + (p_1^n)^2 \sin(x_2^n)]$	

however, gives no exact trajectory and may lead to chaotic behavior of the particle. The present Hamiltonian-conserving scheme leads to no such false chaos, as shown below.

Substitution of Eq. (5.21) into Eqs. (5.17)–(5.20) gives the Hamiltonian-conserving scheme as seen in Table I, which contains $(x, p)^{n+1}$ in the right-hand side as an implicit scheme. We use the Euler scheme as the predictor; that is to say, we obtain $(x, p)^{n+1}$ from $(x, p)^n$ using the Euler scheme. The $(x, p)^{n+1}$ obtained thus are substituted into the right-hand side of the Hamiltonian-conserving scheme. The $(x, p)^{n+1}$ reevaluated are again substituted into $(x, p)^{n+1}$ in the right-hand side. The iteration is repeated until convergent $(x, p)^{n+1}$ are obtained.

We compare the present Hamiltonian-conversing scheme to the Heun scheme [5], the 4th-order Runge–Kutta scheme, and the 4th-order Runge–Kutta scheme with the Hamiltonian corrector. The Hamiltonian corrector in the last scheme will be explained in the Appendix. The Heun scheme given in Table I consists of the Euler scheme and the trapezoidal scheme. As in the case of the Hamiltonian-conserving scheme, the Euler scheme works as the predictor giving $(x, p)^{n+1}$ from $(x, p)^n$. The $(x, p)^{n+1}$ obtained thus are substituted into the right-hand side of the trapezoidal scheme.

EXPERIMENT 1. We put $\varepsilon = 0$ in Eq. (5.21) and give the initial condition by

$$(x_1, p_1, x_2, p_2)_{t=0} = (\pi, 2, 0, 0),$$

which leads to $H = 0$ and lies on the separatix, as shown in Fig. 2. Figure 3 shows numerical trajetories in the rectangle surrounded by the broken line in Fig. 2.

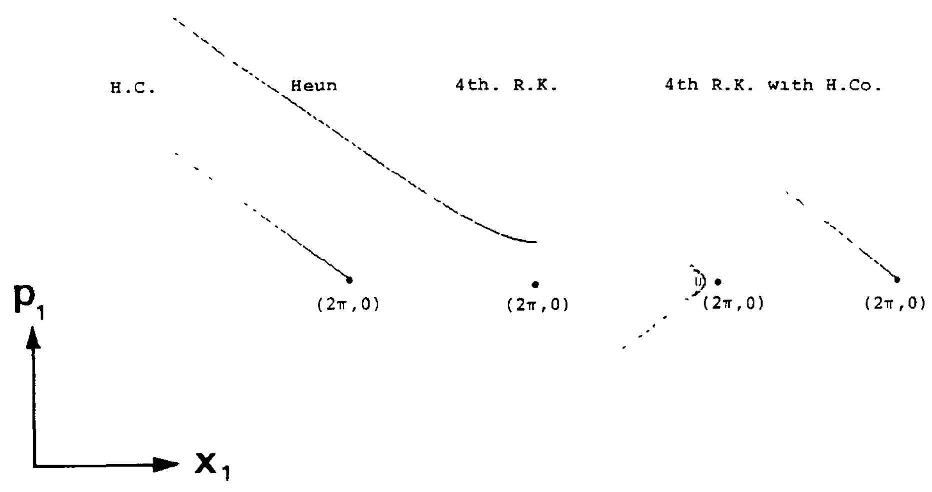

FIG 3 Experiment 1 Trajectories near $(2\pi, 0)$ $H = p_1^2/2 + \cos x_1 - 1$, $(x_1, p_1)_{t=0} = (\pi, 2)$

In Fig. 3, H.C. means the Hamiltonian-conserving scheme, 4th R.K. means the 4th-order Runge–Kutta scheme, and 4th R.K. with H.Co. means the 4th-order Runge–Kutta scheme with the Hamiltonian corrector. The time intervals τ in the time integration are listed in Table II. The time integration is made from $t=0$ to $t=t_{\max}$. The number of iteration refers to the usage of correctors in the H.C. and Heun schemes, and to the usage of the Hamiltonian corrector in the 4th R.K. with H.Co. scheme.The max $|\Delta H|$ in Table II denotes the maximum error of the Hamiltonian.

The Hamiltonian-conserving and Heun schemes give the solutions accurate to $O(\tau^2)$, while the 4th-order Runge–Kutta with and without Hamiltonian corrector give the solutions accurate to $O(\tau^4)$. The time intervals τ in Table II make the error of the four schemes about the same order.

If we disregard the rounding-off error, the Hamiltonian-conserving scheme gives exactly max $|\Delta H|=0$, so that max $|\Delta H|=1.2\times 10^{-15}$ in Table II comes from the rounding-off error. Experiment 1 was made by using numbers of double precision (16 figures). From Table II, we see that the Hamiltonian-conserving scheme gives the best trajectory in the phase space.

EXPERIMENT 2. We put $\varepsilon=0$ in Eq. (5 21) and give the initial condition by

$$(x_1, p_1, x_2, p_2)_{t=0}=(0\,01, 0, 0, 0),$$

which, as shown in Fig. 2, lies inside and near the separatix. In this case the analytic trajectory in the phase space (x_1, p_1) is closed and the period of one cycle is about 23.9. The numerical trajectories in the rectangle surrounded by the broken line in Fig. 2 are shown in Fig. 4. The time interval τ etc. are listed in Table III. We calculated the trajectories for $t<t_{\max}=1000$, so that the phase point (x_1, p_1) turns round about 41 times. When the phase point obtained by the Heun scheme goes to the right beyond $x_1>2\pi$, we use the periodic condition, i.e., when $x_1>2\pi$, we put $x_1\to x_1-2\pi$ and $p_1\to p_1$. When $\tau>0.1$, we fail to obtain a stable numerical solution based on the 4th-order Runge–Kutta schemes without Hamiltonian corrector. This comes from the fact that the 4th-order Runge–Kutta scheme is an

TABLE II

Experiment 1 $(x_1, p_1, x_2, p_2)_{t=0}=(\pi, 2, 0, 0)$

Scheme	τ	$t_{\max}$	Number of iteration	max $\lvert\Delta H\rvert$	Behavior of trajectory near separatrix $(x_1, p_1)=(2\pi, 0)$
H C	10^{-2}	100	10	$1\,2\times 10^{-15}$	Approach $(2\pi, 0)$
Heun	10^{-2}	100	10	$3\,3\times 10^{-5}$	Go to right
4th R K	10^{-1}	100	/	$6\,1\times 10^{-6}$	Return to left
4th R K with H Co	10^{-1}	100	10	$1\,0\times 10^{-5}$	Approach $(2\pi, 0)$

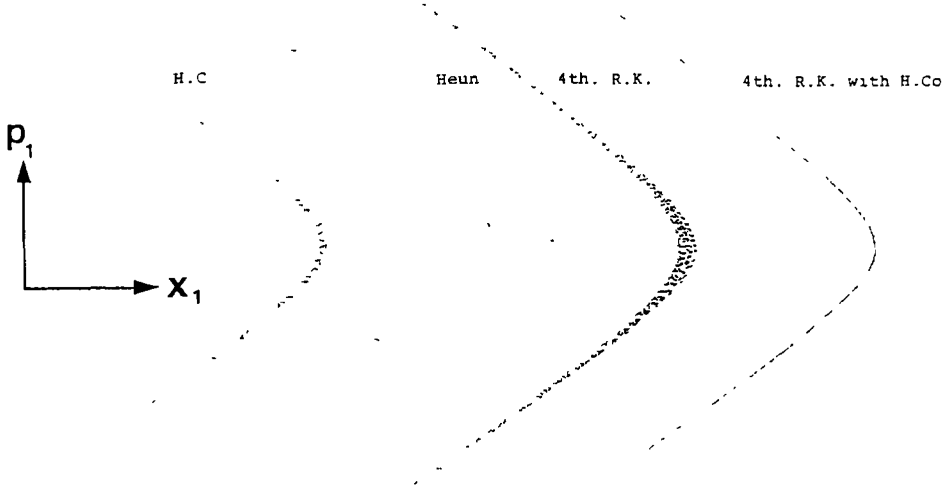

FIG 4 Experiment 2 Trajectories near $(2\pi, 0)$ $H = p_1^2/2 + \cos x_1 - 1$, $(x_1, p_1)_{t=0} = (0.01, 0)$

explicit scheme in contrast to the Hamiltonian-conserving and Heun schemes. From Fig. 4 and Table III, we may see that the best scheme is the Hamiltonian-conserving scheme. Experiment 2 and the following Experiment 3 were made by using numbers of single precision (8 figures).

EXPERIMENT 3. We put $\varepsilon = 0.01$ in Eq. (5.21) and give the initial condition by

$$(x_1, p_1, x_2, p_2)_{t=0} = (0.01, 0, 0, \sqrt{2}),$$

The time interval τ etc. are listed in Table IV. We use the periodic condition, i.e., when $x_{1,2} > 2\pi$, we put $x_{1,2} \to x_{1,2} - 2\pi$. Figure 5 gives the Poincaré maps indicating value of (x_1, p_1) when $x_2 = 0$ or 2π. From Fig. 5 we see that the Hamiltonian-conserving and Heun schemes give similar Poincaré maps. The comparison of max $|\Delta H|$ in Table IV, however, means that the Hamiltonian-conserving scheme gives the trajectory more accurate than the Heun scheme.

TABLE III

Experiment 2 $(x_1, p_1, x_2, p_2)_{t=0} = (0.01, 0, 0, 0)$

Scheme	τ	t_{max}	Number of iteration	max $\|\Delta H\|$	Behavior of trajectory near separatrix
H.C	0 7	1000	10	$1\ 7 \times 10^{-5}$	Almost closed
Heun	0 7	1000	10	7.6×10^{-4}	Chaotic
4th R K	0 1	1000	/	$3\ 2 \times 10^{-5}$	Nearly closed
4th R K with H Co	0 1	1000	10	$4\ 7 \times 10^{-7}$	Closed

TABLE IV

Experiment 3 $(x_1, p_1, x_2, p_2)_{t=0} = (0.01, 0, 0, \sqrt{2})$

Scheme	τ	t_{max}	Number of iteration	max $\lvert\Delta H\rvert$	Behavior of trajectory
H.C.	0.5	2000	10	2.3×10^{-5}	Chaotic
Heun	0.5	2000	10	2.3×10^{-3}	Chaotic

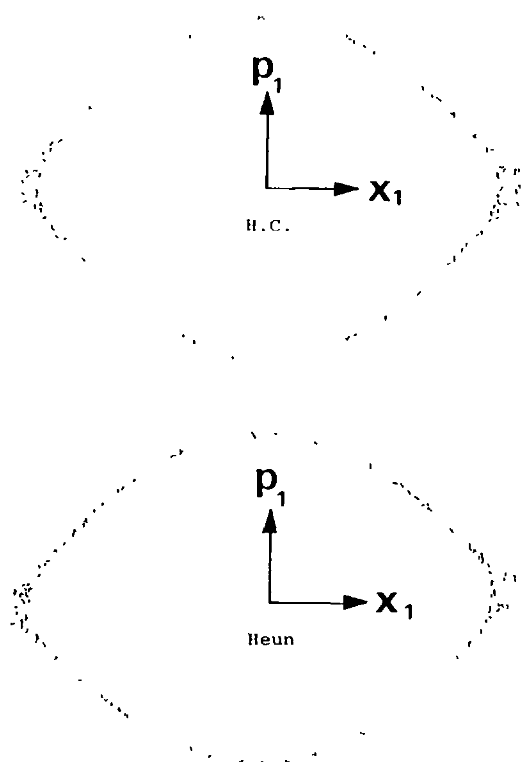

FIG. 5. Experiment 3. Poincaré maps $H = (p_1^2 + p_2^2)/2 + \cos x_1 - 1 + 0.005 \cdot p_1^2 \cos x_2$, $(x_1, p_1, x_2, p_2)_{t=0} = (0.01, 0, 0, \sqrt{2})$.

6. Discussions

Our method of constructing the discrete mechanics uses no continuous differentiation and is based on the variational difference quotient $\Delta_\xi G(\xi)$ defined by Eq. (2.3). The order of $(\xi^1, \xi^2, ..., \xi^\mu)$ or $(x_1, p_1, x_2, p_2, .., x_f, p_f)$ is arbitrary, as shown by Eqs. (3.2) and (3.4). Equations (3.2) and (4.2) means that there exist $f!$ different possible ways of setting the order of $(x_1, p_1, x_2, p_2, ..., x_f, p_f)$. This lack of symmetry may be the shortcoming of our method. We, however, can change the order of $(x_1, p_1, ..., x_f, p_f)$ at each time-step. One of the ways of recovering the symmetry is to change the order at each time-step or, for example, at every ten time-steps. As shown by Eqs. (5.17)–(5.20), or the Hamiltonian-conserving scheme in Table I, the recovery of symmetry increases the accuracy of the Hamiltonian-conserving scheme.

The Hamiltonian-conserving and Heun schemes have the error of $O(\tau^3)$, and the 4th-order Runge–Kutta scheme have the error of $O(\tau^5)$. We should note that, as shown in Fig. 6, the error of the Hamiltonian-conserving scheme has a different feature from the other schemes. That is to say, if we disregard the rounding-off error, the phase point $\xi = (x, p)$ given by the Hamiltonian-conserving scheme always lies on the equi-Hamiltonian plane, so that the phase point only has a phase error in the equi-Hamiltonian plane. Another scheme, such as the Heun scheme or the 4th-order Runge–Kutta scheme, has the isotropic error as shown in Fig. 6. The Hamiltonian-corrector which will be explained in the Appendix reduces the isotropic error to only a phase error.

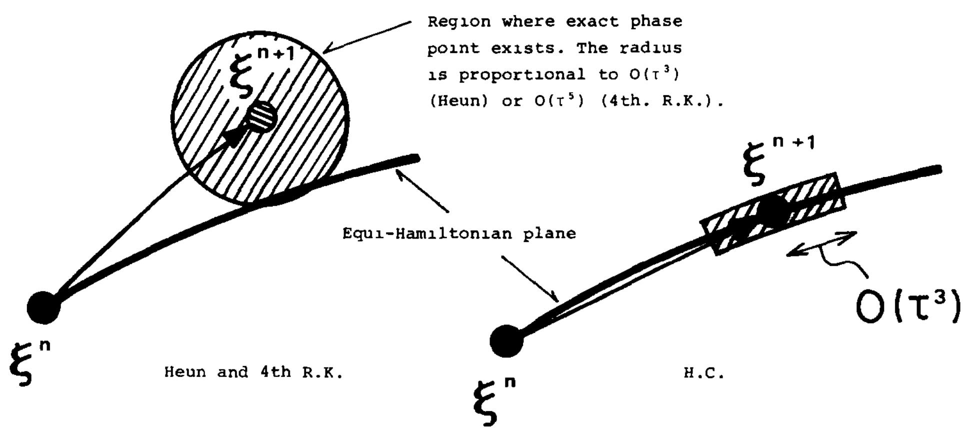

Fig. 6 Error regions of the Heun, 4th-order Runge–Kutta, and Hamiltonian-conserving schemes $(\xi) = (x, p)$.

APPENDIX: HAMILTONIAN CORRECTOR

The conservation of the Hamiltonian is not necessary assured in the Heun and 4th-order Runge–Kutta schemes. The trajectory given by the schemes may be given by line between $\bar{\xi}^{n+1}$ and ξ^n in Fig. 7, where $\xi = (\boldsymbol{x}, \boldsymbol{p})$. If we denote the accurate phase point by ξ^{n+1}, then in order to obtain ξ^{n+1} from $\bar{\xi}^{n+1}$, we need $\delta\xi = \xi^{n+1} - \bar{\xi}^{n+1}$. The geometrical consideration in the continuous version gives

$$\frac{\partial H}{\partial \xi} \cdot \delta\xi = \delta H, \tag{A.1}$$

where $\delta H = H(\xi^{n+1}) - H(\bar{\xi}^{n+1}) = H(\xi^n) - H(\bar{\xi}^{n+1}) = H(\xi^0) - H(\bar{\xi}^{n+1})$. If the time interval is sufficiently small, the approximate trajectory between $\bar{\xi}^{n+1}$ and ξ^n is almost parallel to the equi-Hamiltonian plane, so that $\delta\xi$ is almost parallel to $\partial H/\partial\xi$. Therefore, from Eq. (A.1) we may put

$$\delta\xi = \frac{\delta H}{|\partial H/\partial\xi|^2} \frac{\partial H}{\partial \xi}.$$

We replace $\partial H/\partial\xi$ by the difference quotient $\Delta_\xi H(\xi)|_\eta$ defined as in Eq. (2.3) as

$$\delta\xi = \frac{\delta H}{|\Delta_\xi H(\xi)|_\eta|^2} \Delta_\xi H(\xi)|_\eta. \tag{A.2}$$

Equation (2.3) means that in order to evaluate $\Delta_\xi H(\xi)|_\eta$, values of H at the two

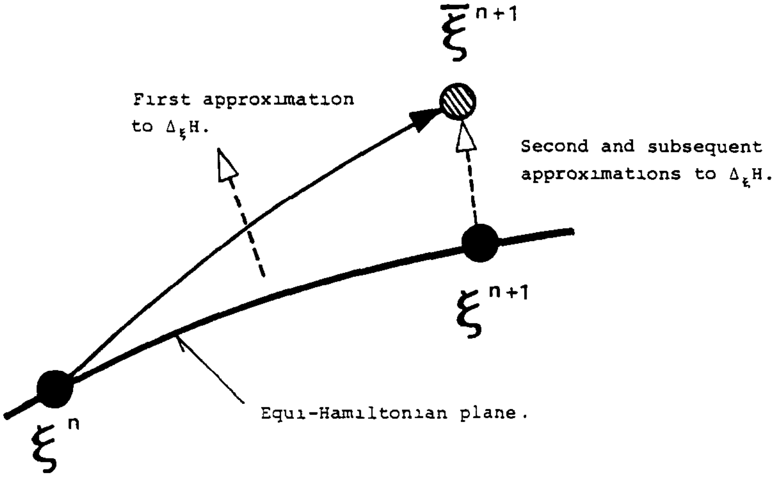

FIG 7 Illustration of the Hamiltonian corrector $(\xi) = (\boldsymbol{x}, \boldsymbol{p})$

points ξ and η are required. We put $\xi = \xi^n$ and $\eta = \bar{\xi}^{n+1}$ as a first approximation and obtain

$$\Delta_{\xi_i} H(\xi^n)|_{\eta = \bar{\xi}^{n+1}} = \frac{1}{\bar{\xi}_i^{n+1} - \xi_i^n} [H(\bar{\xi}_1^{n+1}, \bar{\xi}_2^{n+1}, ..., \bar{\xi}_{i-1}^{n+1}, \bar{\xi}_i^{n+1}, ..., \xi_\mu^n) - H(\bar{\xi}_1^{n+1}, \bar{\xi}_2^{n+1}, ..., \bar{\xi}_{i-1}^{n+1}, \xi_i^n, \xi_{i+1}^n, ..., \xi_\mu^n)]. \tag{A.3}$$

Using $\delta\xi$ obtained from Eq. (A.2) we evaluate $\xi^{n+1} = \bar{\xi}^{n+1} + \delta\xi$. In order to obtain more accurate $\Delta_\xi H|_\eta$, we replace ξ^n in Eq. (A.3) by ξ^{n+1} obtained above, reevaluate $\delta\xi$ from Eq. (A.2), and reevaluate ξ^{n+1} from $\xi^{n+1} = \xi^{n+1} + \delta\xi$. We repeat the iteration until we obtain the convergent ξ^{n+1}. In all the stages of iteration we fix the values of $\bar{\xi}^{n+1}$, so that δH $(= H(\xi^n) - H(\bar{\xi}^{n+1}))$ in Eq. (A.2) does not vary. In other words, the Hamiltonian-corrector is the implicit scheme determining ξ^{n+1} from $\bar{\xi}^{n+1}$.

Let us give examples when the Hamiltonian is given by Eq. (5.21). In Eq. (A.3) we put $\xi^n = (x_1, p_1, x_2, p_2)^n$ and $\bar{\xi}^{n+1} = (\bar{x}_1, \bar{p}_1, \bar{x}_1, \bar{p}_1)^{n+1}$. Then Eq. (A.2) gives

$$\delta x_1 = \alpha\, \Delta_{x_1} H = \alpha \frac{\cos x_1^n - \cos \bar{x}_1^{n+1}}{x_1^n - \bar{x}_1^{n+1}},$$

$$\delta x_2 = \alpha\, \Delta_{x_2} H = \alpha \frac{\varepsilon}{2} (\bar{p}_1^{n+1})^2 \frac{\cos x_2^n - \cos \bar{x}_2^{n+1}}{x_2^n - \bar{x}_2^{n+1}},$$

$$\delta p_1 = \alpha\, \Delta_{p_1} H = \alpha \frac{p_1^n + p_1^{n+1}}{2} (1 + \varepsilon \cos x_2^n),$$

$$\delta p_2 = \alpha\, \Delta_{p_2} H = \alpha \frac{p_2^n + \bar{p}_2^{n+1}}{2},$$

where

$$\alpha = \frac{\delta H}{|\Delta_\xi H(\xi)|^2} = \frac{H(x_1^n, p_1^n, x_2^n, p_2^n) - H(\bar{x}_1^{n+1}, \bar{p}_1^{n+1}, \bar{x}_2^{n+1}, \bar{p}_2^{n+1})}{(\Delta_{x_1} H)^2 + (\Delta_{x_2} H)^2 + (\Delta_{p_1} H)^2 + (\Delta_{p_2} H)^2}.$$

If we replace $(p_1^{n+1})^2$ in the second equation for δx_2 by $[(p_1^n)^2 + (\bar{p}_1^{n+1})^2]/2$, and replace $\cos x_2^n$ in the third equation for δp_1 by $(\cos x_2^n + \cos \bar{x}_2^{n+1})/2$, the four equations for δx_1, δp_1, δx_2, and δp_2 become symmetric about ξ^n and $\bar{\xi}^{n+1}$. In obtaining the numerical results in the text, we have used the symmetric equations for δx_1, etc.

References

1. S Maeda, *Math Japon* **25**, 405 (1980)
2. D Holm and B A Kupershmidt, *Av Appl Math* **6**, 52 (1985)
3 L Gotusso, *Appl Math Comput* **17**, 129 (1985)
4 H. Goldstein, *Classical Mechanics* (Addison–Wesley, Reading, 1950), L D Landau and E M Lifshitz, *Mechanics* (Pergamon, Oxford, 1976)
5 P Henrici, *Discrete Variable Methods in Ordinary Differential Equations* (Wiley, New York, 1962)