A DIFFERENCE SCHEME FOR THE HAMILTONIAN EQUATION*

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In the recent DD-5 Beijing conference, Feng Kang proposed three types of difference schemes for the Hamiltonian equation from the viewpoint of symplectic geometry. In this paper, we give a further discussion on these schemes and propose another difference scheme suitable for the nonquadric Hamiltonian function of second order.

We consider the following system of canonical equations

$$\begin{cases} \frac{dp_\nu}{dt}=\frac{-\partial H}{\partial q_\nu}, \\ \frac{dq_\nu}{dt}=\frac{\partial H}{\partial p_\nu}, \end{cases} \quad \nu=1,2,\cdots,n \tag{1.1}$$

with Hamiltonian function $H(p_1, p_2, \cdots, p_n, q_1, q_2, \cdots, q_n)$. Let the space R^{2n} be equipped with a symplectic structure defined by the differential two form

$$\omega^2=dp\wedge dq, \quad z=\begin{bmatrix} z_1 \\ z_2 \\ \vdots \\ z_n \end{bmatrix}=\begin{bmatrix} p \\ q \end{bmatrix}, \quad J=\begin{bmatrix} 0 & E_n \\ -E_n & 0 \end{bmatrix},$$

$$E_n=\begin{bmatrix} 1 & & 0 \\ & \ddots & \\ 0 & & 1 \end{bmatrix}, \quad J^{-1}=J'=-J=\begin{bmatrix} 0 & -E_n \\ E_n & 0 \end{bmatrix}. \tag{1.2}$$

(1.1) can be rewritten as

$$\frac{dz}{dt}=J^{-1}H_z=-JH_z \tag{1.3}$$

with solution $z(t)$.

Assume that for each t, $z(0)\to z(t)$ defines a diffeomorphism $g(t)$. Then its Jocobian $G(t)$ is a symplectic matrix, i.e.

$$G'(t)JG(t)=J. \tag{1.4}$$

Suppose H_z can be written as $A(z)z$. Then equation (1.3) has the form

$$\frac{dz}{dt}=-JA(z)z. \tag{1.5}$$

We call the first scheme investigated in [1] (one-leg C-N difference scheme) the

* Received September 19, 1984

Euler scheme

$$\frac{z^{n+1}-z^n}{\Delta t}=-JA\frac{z^{n+1}+z^n}{2}. \tag{1.6}$$

Multiplying (1.6) by $A\frac{z^{n+1}+z^n}{2}$ and summing over all m and noting that J is antisymmetric, we have

$$\left(\frac{z^{n+1}-z^n}{\Delta t},\ A\frac{z^{n+1}+z^n}{2}\right)=0.$$

If the matrix is a symmetric constant, we have

$$(z^{n+1},\ Az^{n+1})=(z^n,\ Az^n). \tag{1.7}$$

Let $\|H\|^{n+1}=(z^{n+1},\ Az^{n+1})$. Therefore we have

$$\|H\|^{n+1}=\|H\|^n=\cdots=\|H\|^0. \tag{1.7$'$}$$

The amplification of this scheme is $\left[I+\frac{\tau}{2}JA\right]^{-1}\left[I-\frac{\tau}{2}JA\right]$, which is a symplectic operator. When (1.5) is well posed, then this scheme is absolutely stable.

Now we consider the hopscotch method for the system of equation (1.5). The method requires that we combine the simple one-step processes

$$z^{n+1}=z^n-\Delta t\,JAz^n, \tag{1.8}$$

$$z^{n+1}=z^n-\Delta t\,JAz^{n+1} \tag{1.9}$$

using them at alternate node points on the t-axis. If (1.8) is used at those points with m even and (1.9) is used at those with m odd, and if we define

$$\theta^m=\begin{cases}1, & \text{if } m \text{ is even},\\ 0, & \text{otherwise},\end{cases}$$

then the hopscotch method is

$$z^{n+1}+\Delta t\theta^{n+1}JAz^{n+1}=z^n-\Delta t\theta^n JAz^n. \tag{1.10}$$

Writing (1.10) with $(n+1)$ replacing n and eliminating z^{n+1} from this equation, we have

$$z^{n+2}=z^n-\Delta t\theta^n(JAz^{n+2}+JAz^n)-2\Delta t\theta^{n+1}JAz^{n+1}. \tag{1.11}$$

When n is odd, the above equation reduces to

$$z^{n+2}=z^n-2\Delta tJAz^{n+1} \tag{1.12}$$

which is just the leap-frog scheme. Multiplying (1.12) by Az^{n+1} on both sides and summing over all space points, we have

$$(z^{n+2},\ Az^{n+1})=(z^{n+1},\ Az^n). \tag{1.13}$$

We first use the forward time difference scheme

$$\frac{z^1-z^0}{\Delta t}=-JAz^0. \tag{1.14}$$

We obtain

$$(z^1,\ Az^0)=(z^0,\ Az^0).$$

Therefore

$$(z^{n+2},\ Az^{n+1})=(z^{n+1},\ Az^n)=\cdots=(z^1,\ Az^0)=(z^0,\ Az^0). \tag{1.15}$$

We call these schemes quasi-energy conservative. Let (1.12) be rewritten in form