Journal of Computational Mathematics, Vol.17, No.6, 1999, 561–568.

A NOTE ON CONSTRUCTION OF HIGHER-ORDER SYMPLECTIC SCHEMES FROM LOWER-ORDER ONE VIA FORMAL ENERGIES*[1)]

Yi-fa Tang

State Key Laboratory of Scientific and Engineering Computing, Institute of Computational Mathematics and Scientific/Engineering Computing, Academy of Mathematics and Systems Sciences, Academia Sinica, P.O. Box 2719, Beijing 100080, P.R. China

Abstract

In this paper, we will prove by the help of formal energies only that one can improve the order of any symplectic scheme by modifying the Hamiltonian symbol H, and show through examples that this action exactly and directly simplifies Feng's way of construction of higher-order symplectic schemes by using higher-order terms of generating functions.

Key words: Hamiltonian system, Symplectic scheme, Revertible scheme, Generating function, Formal energy.

1. Introduction

First of all, let's recall the definitions of symplectic schemes, revertible schemes, and Feng's way of construction of symplectic methods via generating functions.

As well-known, the phase flow $\{g^t, t \in R\}$ of any Hamiltonian system

$$\frac{dZ}{dt} = J\nabla H(Z), \quad Z \in R^{2n} \tag{1}$$

(where $J = \begin{bmatrix} 0_n & -I_n \\ I_n & 0_n \end{bmatrix}$, $H : R^{2n} \to R^1$ is a smooth function, and ∇ is the gradient operator) is a one-parameter group of canonical (symplectic) diffeomorphisms, i.e., the Jacobian of g^t with respect to Z satisfies

$$[\frac{\partial g^t(Z)}{\partial Z}]^T J [\frac{\partial g^t(Z)}{\partial Z}] = J, \tag{2}$$

* Received September 16, 1997.

[1)] This research is supported by *China State Major Key Project for Basic Researches*, also by a grant (No. **19801034**) from *National Natural Science Foundation of China* and a grant (No. **1997-60**) from the *Bureau of Education, Chinese Academy of Sciences.*

for any H and any t (see [1]).

Equation (2) is also called *symplectic* condition.

Definition 1. *A difference scheme compatible with (1) is said to be symplectic iff its step-transition operator* $G^\tau : R^{2n} \to R^{2n}$ *is symplectic, i.e.,*

$$\left[\frac{\partial G^\tau(Z)}{\partial Z}\right]^T J \left[\frac{\partial G^\tau(Z)}{\partial Z}\right] = J \tag{3}$$

for any Hamitonian H and any sufficiently small step-size τ (see [2]).

One kind of most important symplectic schemes are the *time-revertible* (or simply, *revertible*) one.

Definition 2. *A difference scheme compatible with (1) is said to be revertible (or reversible or time-revertible or time-reversible) iff its step-transition operator* $G^\tau : R^{2n} \to R^{2n}$ *satisfies*

$$G^{-\tau} \circ G^\tau = id. \tag{4}$$

for any Hamitonian H and any sufficiently small step-size τ (see [3-5]).

The following is the technique (due to Feng *et al*) of construction of symplectic methods via generating functions (see [6]).

Suppose $4n \times 4n$ matrix $M = \begin{bmatrix} A & B \\ C & D \end{bmatrix}$ (where A, B, C, D are $2n \times 2n$ matrices) satisfies:

$$M^T \begin{bmatrix} O & -I_{2n} \\ I_{2n} & O \end{bmatrix} M = \mu \begin{bmatrix} -J_{2n} & O \\ O & J_{2n} \end{bmatrix} M \tag{5}$$

for some $\mu \neq 0$. The inverse of M is denoted by $M^{-1} = \begin{bmatrix} A^v & B^v \\ C^v & D^v \end{bmatrix}$. If Hamiltonian $H(Z)$ depends analytically on Z, then the generating function $\phi(w,t)$ is expressible as a convergent power series in t for sufficiently small $|t|$, with the recursively determined coefficients:

$$\phi(w,t) = \sum_{k=0}^{+\infty} \phi^{(k)}(w) t^k,$$

$$\phi^{(0)}(w) = \frac{1}{2} w^T N w, \quad N = (A+B)(C+D)^{-1},$$

$$\phi^{(1)}(w) = -\mu H(Ew), \quad E = (C+D)^{-1}, \tag{6}$$

for $k \geq 1$,

$$\begin{aligned} \phi^{(k+1)}(w) = \ & -\tfrac{\mu}{k+1} \textstyle\sum_{m=1}^{k} \frac{1}{m!} \sum_{i_1,\cdots,i_m=1}^{2n} \sum_{\substack{j_1+\cdots+j_m=k \\ j_l \geq 1}} \\ & H_{z_{i_1}\cdots z_{i_m}}(Ew) \left[A^v \nabla \phi^{(j_1)}\right]_{i_1} \cdots \left[A^v \nabla \phi^{(j_m)}\right]_{i_m}. \end{aligned} \tag{7}$$

Set

$$\psi^{(s)}(w,\tau)=\sum_{k=0}^{s}\phi^{(k)}(w)\tau^k, \quad s=1,2,\cdots, \tag{8}$$

then

$$A\widetilde{Z}+BZ=\nabla\psi^{(s)}(C\widetilde{Z}+DZ,\tau) \tag{9}$$

defines an implicit symplectic scheme: $Z\to\widetilde{Z}$ of order s.

Example 1. *If we choose* $M=\begin{bmatrix}-J_{2n} & J_{2n}\\ \frac{1}{2}I_{2n} & \frac{1}{2}I_{2n}\end{bmatrix}$ *and* $\mu=1$*, then we can obtain from (9) the following symplectic schemes of order* 2 *and order* 4*, by taking* $s=2$ *and* $s=4$ *respectively [6]:*

2nd-order mid-point rule:

$$\widetilde{Z}=Z+\tau J\nabla H\left(\frac{\widetilde{Z}+Z}{2}\right); \tag{10}$$

4th-order mid-point rule:

$$\widetilde{Z}=Z+\tau J\nabla H\left(\frac{\widetilde{Z}+Z}{2}\right)+\frac{\tau^3}{24}J\nabla\left[(J\nabla H)^T H_{zz}(J\nabla H)\right]\left(\frac{\widetilde{Z}+Z}{2}\right) \tag{11}$$

These two schemes are both revertible.

Example 2. *If we choose* $M=\begin{bmatrix}O & O & -I_n & O\\ O & -I_n & O & O\\ O & O & O & I_n\\ I_n & O & O & O\end{bmatrix}$ *and* $\mu=1$*, then we can obtain from (9) the following symplectic schemes of order* 1 *and order* 2*, by taking* $s=1$ *and* $s=2$ *respectively* ($Z=(p_1,\cdots,p_n;q_1,\cdots,q_n)^T$) *[6]:*

1st-order scheme:

$$\begin{cases}\tilde{p}=p-\tau H_q(\tilde{p},q),\\ \tilde{q}=q+\tau H_p(\tilde{p},q);\end{cases} \tag{12}$$

2nd-order scheme:

$$\begin{cases}\tilde{p}=p-\tau H_q(\tilde{p},q)-\frac{\tau^2}{2}H_{qp}H_q(\tilde{p},q)-\frac{\tau^2}{2}H_{qq}H_p(\tilde{p},q),\\ \tilde{q}=q+\tau H_p(\tilde{p},q)+\frac{\tau^2}{2}H_{pp}H_q(\tilde{p},q)+\frac{\tau^2}{2}H_{pq}H_p(\tilde{p},q).\end{cases} \tag{13}$$

For Newtonian system

$$m\frac{d^2x}{dt^2}=F(x), \tag{14}$$

whose energy is

$$E=\frac{1}{2}m\left(\frac{dx}{dt}\right)^2+U(x), \tag{15}$$

where $F=-dU/dx$, and U is the potential.

The corresponding Hamiltonian is

$$H(p,q) = \frac{1}{2m}p^2 + U(q), \tag{16}$$

where $p = \frac{dx}{dt}$ and $q = x$.

For this kind of special Hamiltonians, symplectic schemes (12) and (13) are explicit, their computation formulae for (16) are

$$\begin{cases} \tilde{p} = p - \tau U', \\ \tilde{q} = q + \tau \frac{p-\tau U'}{m}; \end{cases} \tag{17}$$

and

$$\begin{cases} \tilde{p} = \frac{p-\tau U'}{1+\frac{\tau^2}{2m}U''}, \\ \tilde{q} = q + \frac{\tau}{m}\frac{p-\tau U'}{1+\frac{\tau^2}{2m}U''} + \frac{\tau^2}{2m}U' \end{cases} \tag{18}$$

respectively.

Obviously, scheme (11) is scheme (10) and something more, and scheme (13) is scheme (12) and something more, to obtain them in fact, the higher-order terms of the generating functions are used respectively. One may ask: is it possible to obtain scheme (11) from scheme (10) directly, and obtain scheme (13) from (12) directly?

In the sequel, we will give a theorem to prove that one can improve the order of any symplectic scheme by modifying the Hamiltonian symbol H, for this the formal energy of the symplectic scheme plays the crucial role (*Theorem 1*). We will show through examples that this action exactly and directly simplifies Feng's way of construction of higher-order symplectic schemes by using higher-order terms of generating functions. So, from a symplectic scheme, one can obtain (through formal energies) another one of arbitrarily high order.[2)]

2. Formal Energies of Symplectic Schemes

On investigating the calculus of generating functions, Feng showed the existence of formal energies of symplectic schemes constructed via generating functions, and gave complete formulae for computation of the formal energies [7]. Transforming the symplecticity of a difference scheme into the closedness of some differential 1-forms and using Poincaré's Lemma on closed differential forms, Tang deduced directly the existence of formal energy of any symplectic scheme, and also gave some formulae for calculation of the formal energy [8].

[2)] It is noted that Stoffer used another technique to construct a new Hamiltonian function for the 2nd-order mid-point rule, and got a 4th-order reversible symplectic scheme. That's also very interesting, for details one can refer to [4-5].

For other techniques for the formal energies (perturbed Hamiltonian functions) of symplectic schemes applied to Hamiltonian systems, one can also refer to Hairer [9], Yoshida [10].

In fact, for the 2nd-order mid-point rule (10), the formal energy is [8]

$$\begin{aligned}\widetilde{H} &= H - \tfrac{\tau^2}{24}H_{z^2}\left(Z^{[1]}\right)^2 \\ &+\tfrac{7\tau^4}{5760}H_{z^4}\left(Z^{[1]}\right)^4 + \tfrac{\tau^4}{480}H_{z^3}\left(Z^{[1]}\right)^2 Z^{[2]} + \tfrac{\tau^4}{160}H_{z^2}\left(Z^{[2]}\right)^2 \\ &+O(\tau^6);\end{aligned} \tag{19}$$

and for the 4th-order mid-point rule (11), the formal energy is [8]

$$\begin{aligned}\widetilde{H} &= H - \tfrac{\tau^4}{1920}H_{z^4}\left(Z^{[1]}\right)^4 + \tfrac{\tau^4}{480}H_{z^3}\left(Z^{[1]}\right)^2 Z^{[2]} - \tfrac{\tau^4}{240}H_{z^2}\left(Z^{[2]}\right)^2 \\ &+O(\tau^6).\end{aligned} \tag{20}$$

And we have

Lemma 1. (see [8]) *If a symplectic scheme G_H^τ is of order s, then its formal energy can be expressed as $\widetilde{H} = H + \tau^s H_s + \tau^{s+1}H_{s+1} + \tau^{s+2}H_{s+2} + \cdots$, and G_H^τ is revertible iff the terms with odd subscripts in the sequence H_s, H_{s+1}, H_{s+2}, $\cdots$ are zero.*

Corollary 1. (see [8]) *Any revertible scheme is of even order.*

If we denote the formal energy of a symplectic scheme as

$$\widetilde{H}(p,q) = H^{(0)} + \sum_{k=1}^{+\infty} \tau^k H^{(k)}(p,q),$$

then it is not difficult to calculate for scheme (12),

$$H^{(1)} = -\frac{1}{2}H_q^T H_p, \tag{21}$$

and

$$H^{(2)} = \frac{1}{12}H_{pp}H_q^2 + \frac{1}{12}H_{qq}H_p^2 + \frac{1}{3}H_{qp}H_pH_q; \tag{22}$$

and for scheme (13),

$$H^{(2)} = -\frac{1}{6}H_{pp}H_q^2 - \frac{1}{6}H_{qq}H_p^2 - \frac{1}{6}H_{qp}H_pH_q, \tag{23}$$

$$\begin{aligned}H^{(3)} = &\tfrac{1}{24}(H_{ppp}H_q^3 + H_{qqq}H_p^3) + \tfrac{1}{8}(H_{ppq}H_q^2H_p + H_{pqq}H_qH_p^2) \\ &+\tfrac{1}{8}(H_{pp}H_q + H_{pq}H_p)^T(H_{qp}H_q + H_{qq}H_p).\end{aligned} \tag{24}$$

For the special Hamiltonian (16), (21)-(24) become into

$$H^{(1)} = -\frac{pU'}{2m}, \tag{25}$$

$$H^{(2)} = \frac{p^2U''}{12m^2} + \frac{(U')^2}{12m}; \tag{26}$$

and

$$H^{(2)} = -\frac{p^2 U''}{6m^2} - \frac{(U')^2}{6m}, \tag{27}$$

$$H^{(3)} = \frac{p^3 U^{(3)}}{24m^3} + \frac{pU'U''}{8m^2} \tag{28}$$

respectively.

3. Fundamental Theorem

Theorem 1. *If symplectic scheme G_H^τ is of order u, and its formal energy is expressed as*

$$\widetilde{H} = H + \tau^u H_u + \tau^{u+1} H_{u+1} + \tau^{u+2} H_{u+2} + \cdots, \tag{29}$$

then $G_{\hat{H}}^\tau$ is symplectic with order $\hat{u} \geq u+1$, where $\hat{H} = H - \tau^u H_u$. Furthermore, if G_H^τ is time-revertible, i.e., $G_H^{-\tau} \circ G_H^\tau =$ identity, then $G_{\hat{H}}^\tau$ is time-revertible too, and $\hat{u} \geq u+2$.

Proof. According to the definition of symplectic schemes, the symplecticity of G_H^τ does not depend on H. So G_H^τ is symplectic implies that $G_{\hat{H}}^\tau$ is symplectic too. And the formal energy of $G_{\hat{H}}^\tau$ comes out to be

$$\begin{aligned} \bar{H} = & \left.\widetilde{H}\right|_{H=\hat{H}} \\ = & \left.\{H + \tau^u H_u + O(\tau^{u+1})\}\right|_{H=\hat{H}} \\ = & H - \tau^u H_u + \tau^u H_u + O(\tau^{u+1}) \\ = & H + O(\tau^{u+1}), \end{aligned} \tag{30}$$

thus the order of $G_{\hat{H}}^\tau$ should be $\hat{u} \geq u+1$.

If G_H^τ is time-revertible, then according to **Lemma 1**, as functions of τ, $\widetilde{H}$ and $\hat{H}$ actually depend on τ^2 only, so does $\bar{H}$. Thus $G_{\hat{H}}^\tau$ is time-revertible too. And according to **Corollary 1** u and $\hat{u} \geq u+1$ are both even, so $\hat{u} \geq u+2$.

4. Examples of Modification

Example i. *It is easy to see, if H is changed into $H + \frac{\tau^2}{24} H_{z^2} \left(Z^{[1]}\right)^2$, we obtain the 4th-order mid-point rule (11) from the 2nd-order one (10), On the other hand then, the formal energy (19) should become into (20), in fact,*

$$\begin{aligned} \bar{H} = & \left.\widetilde{H}\right|_{H=H+\frac{\tau^2}{24}H_{z^2}\left(Z^{[1]}\right)^2} \\ = & H + \frac{\tau^2}{24} H_{z^2} \left(Z^{[1]}\right)^2 \\ & - \frac{\tau^2}{24} \left\{H + \frac{\tau^2}{24} H_{z^2} \left(Z^{[1]}\right)^2\right\}_{z^2} \left\{Z^{[1]} + J\nabla \frac{\tau^2}{24} H_{z^2} \left(Z^{[1]}\right)^2\right\}^2 \end{aligned}$$

$$
\begin{aligned}
&+\frac{7\tau^4}{5760}H_{z^4}\left(Z^{[1]}\right)^4+\frac{\tau^4}{480}H_{z^3}\left(Z^{[1]}\right)^2Z^{[2]}+\frac{\tau^4}{160}H_{z^2}\left(Z^{[2]}\right)^2\\
&+O(\tau^6)\\
=&H+\frac{\tau^2}{24}H_{z^2}\left(Z^{[1]}\right)^2\\
&-\frac{\tau^2}{24}H_{z^2}\left\{Z^{[1]}+\frac{\tau^2}{24}Z^{[1]}_{z^2}\left(Z^{[1]}\right)^2-\frac{\tau^2}{12}Z^{[1]}_{z}Z^{[2]}\right\}^2\\
&-\frac{\tau^4}{576}\left\{H_{z^4}\left(Z^{[1]}\right)^4+4H_{z^3}\left(Z^{[1]}\right)^2Z^{[2]}+2H_{z^2}Z^{[1]}Z^{[1]}_{z^2}\left(Z^{[1]}\right)^2+2H_{z^2}\left(Z^{[2]}\right)^2\right\}\\
&+\frac{7\tau^4}{5760}H_{z^4}\left(Z^{[1]}\right)^4+\frac{\tau^4}{480}H_{z^3}\left(Z^{[1]}\right)^2Z^{[2]}+\frac{\tau^4}{160}H_{z^2}\left(Z^{[2]}\right)^2\\
&+O(\tau^6)\\
=&H-\frac{\tau^2}{24}H_{z^2}\left\{\frac{\tau^2}{12}Z^{[1]}Z^{[1]}_{z^2}\left(Z^{[1]}\right)^2-\frac{\tau^2}{6}Z^{[1]}Z^{[1]}_{z}Z^{[2]}\right\}\\
&-\frac{\tau^4}{576}H_{z^4}\left(Z^{[1]}\right)^4-\frac{\tau^4}{144}H_{z^3}\left(Z^{[1]}\right)^2Z^{[2]}\\
&-\frac{\tau^4}{288}H_{z^2}Z^{[1]}Z^{[1]}_{z^2}\left(Z^{[1]}\right)^2-\frac{\tau^4}{288}H_{z^2}\left(Z^{[2]}\right)^2\\
&+\frac{7\tau^4}{5760}H_{z^4}\left(Z^{[1]}\right)^4+\frac{\tau^4}{480}H_{z^3}\left(Z^{[1]}\right)^2Z^{[2]}+\frac{\tau^4}{160}H_{z^2}\left(Z^{[2]}\right)^2\\
&+O(\tau^6) \qquad\qquad (31)\\
=&H+\frac{\tau^4}{288}H_{z^3}\left(Z^{[1]}\right)^2Z^{[2]}-\frac{\tau^4}{144}H_{z^2}\left(Z^{[2]}\right)^2\\
&-\frac{\tau^4}{576}H_{z^4}\left(Z^{[1]}\right)^4-\frac{\tau^4}{144}H_{z^3}\left(Z^{[1]}\right)^2Z^{[2]}\\
&+\frac{\tau^4}{288}H_{z^3}\left(Z^{[1]}\right)^2Z^{[2]}-\frac{\tau^4}{288}H_{z^2}\left(Z^{[2]}\right)^2\\
&+\frac{7\tau^4}{5760}H_{z^4}\left(Z^{[1]}\right)^4+\frac{\tau^4}{480}H_{z^3}\left(Z^{[1]}\right)^2Z^{[2]}+\frac{\tau^4}{160}H_{z^2}\left(Z^{[2]}\right)^2\\
&+O(\tau^6)\\
=&H-\frac{\tau^4}{1920}H_{z^4}\left(Z^{[1]}\right)^4+\frac{\tau^4}{480}H_{z^3}\left(Z^{[1]}\right)^2Z^{[2]}-\frac{\tau^4}{240}H_{z^2}\left(Z^{[2]}\right)^2+O(\tau^6).
\end{aligned}
$$

Example ii. *Obviously, if H is replaced by $H+\frac{\tau}{2}H_q^TH_p$, then we get the 2nd-order scheme (13) from the 1st-order one (12). Similarly as before, the corresponding formal energy should be also replaced, in fact,*

$$
\begin{aligned}
\bar{H}=&\widetilde{H}\Big|_{H=H+\frac{\tau}{2}H_q^TH_p}\\
=&H+\frac{\tau}{2}H_q^TH_p-\frac{\tau}{2}\left\{H+\frac{\tau}{2}H_q^TH_p\right\}_q^T\left\{H+\frac{\tau}{2}H_q^TH_p\right\}_p\\
&+\frac{\tau^2}{12}H_{pp}H_q^2+\frac{\tau^2}{12}H_{qq}H_p^2+\frac{\tau^2}{3}H_{qp}H_pH_q+O(\tau^3)
\end{aligned}
$$

$$
\begin{aligned}
=&H+\frac{\tau}{2}H_q^T H_p-\frac{\tau}{2}\left\{H_q^T+\frac{\tau}{2}H_{qq}H_p+\frac{\tau}{2}H_{qp}H_q\right\}\left\{H_p+\frac{\tau}{2}H_{pq}H_p+\frac{\tau}{2}H_{pp}H_q\right\}\\
&+\frac{\tau^2}{12}H_{pp}H_q^2+\frac{\tau^2}{12}H_{qq}H_p^2+\frac{\tau^2}{3}H_{qp}H_pH_q+O(\tau^3) \qquad (32)\\
=&H+\frac{\tau}{2}H_q^T H_p-\frac{\tau}{2}H_q^T H_p-\frac{\tau^2}{4}H_{pq}H_qH_p-\frac{\tau^2}{4}H_{pp}H_q^2-\frac{\tau^2}{4}H_{qq}H_p^2\\
&-\frac{\tau^2}{4}H_{qp}H_pH_q+\frac{\tau^2}{12}H_{pp}H_q^2+\frac{\tau^2}{12}H_{qq}H_p^2+\frac{\tau^2}{3}H_{qp}H_pH_q+O(\tau^3)\\
=&-\frac{1}{6}H_{pp}H_q^2-\frac{1}{6}H_{qq}H_p^2-\frac{1}{6}H_{qp}H_pH_q+O(\tau^3).
\end{aligned}
$$

(32) shows that (25) becomes into (27).

From examples i, ii one can imagine, by the help of the "formal energies" only, we can obtain symplectic scheme of arbitrarily high order from any symplectic scheme. Comparatively, one can find that this action exactly and directly simplifies Feng's way of construction of higher-order symplectic schemes by using higher-order terms of generating functions.

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