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

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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

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

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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 $k \geq 1$,

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