Journal of Computational Mathematics, Vol.20, No.3, 2002, 267–276.

# SYMPLECTIC COMPUTATION OF HAMILTONIAN SYSTEMS (I)[*1)]

Yi-fa Tang
(*LSEC, ICMSEC, Academy of Mathematics and System Sciences, Chinese Academy of Sciences, Beijing 100080, China*)

**Abstract**

We get $\tau^6$-terms of the formal energy of the mid-point rule, and use the mathematical pendulum to test the convergence of the formal energy.

*Key words*: Mid-point rule, Formal energy.

## 1. Introduction

For a *hamiltonian* system

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

(where $J = \begin{bmatrix} O & -I_n \\ I_n & O \end{bmatrix}$, $I_n$ is $n \times n$ identity matrix, $H : R^{2n} \to R$ is a smooth function and $\nabla$ is the gradient operator), any *symplectic* scheme has a *formal energy* [3,6,8,12,20], which takes a most important part in the study of the scheme itself [14-18]. For instance, the mid-point rule

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

is a 2nd-order, revertible, symplectic scheme. It preserves any quadratic invariant of the Hamiltonian $H$ [5,7,12], and its formal energy has an expression [12]

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

where $Z^{[1]} = J\nabla H(Z)$, $Z^{[2]} = \frac{\partial Z^{[1]}}{\partial Z}Z^{[1]}$. For the notation for example,

$$H_{z^3}\left(Z^{[1]}\right)^2 Z^{[2]} = \sum_{i,j,k=1}^{2n} \frac{\partial^3 H}{\partial z_i \partial z_j \partial z_k}\left[Z^{[1]}\right]_{(i)}\left[Z^{[1]}\right]_{(j)}\left[Z^{[2]}\right]_{(k)},$$

where $z_i$ is the $i$-th component of $2n$-dim vector $Z$, and $\left[Z^{[1]}\right]_{(j)}$ stands for the $j$-th component of $2n$-dim vector $Z^{[1]}$.

Naturally, there would be the following questions:

(a). What are the terms of $\tau^{2k}$ in (3) for general $k$ ?

* Received January 11, 1999; Final revised March 28, 2001.

1) This research is supported by Special Funds for Major State Basic Research Projects of China (No. G1999032801-10 and No. G1999032804), and by the knowledge innovation program of the Chinese Academy of Sciences and a grant (No. 19801034) from National Natural Science Foundation of China.

(b). How many terms for $\tau^{2k}$ in (3), just like 1 for $\tau^2$ and 3 for $\tau^4$ ?

(c). How about the absolute values of the coefficients of the terms of $\tau^{2k}$ for general $k$? Is there a bound for them?

Obviously, the questions above are very interesting, to answer them must be involved in the study of formal energies of general symplectic schemes for Hamiltonian systems, although they are specifically offered to the mid-point rule. For question (b), people have already had the answer (refer to [8,13,15,19]) which is *the number of free unlabeled trees of* $2k+1$ *vertices* (for an introduction to *free unlabeled tree*, one can refer to [4,9]). In the present paper, we answer question (a) for the special case $k=3$ (§2, **Theorem 1**), give a conjecture for question (c) (§2, **Conjecture 1**), and use the *mathematical pendulum* to test the convergence of the expansion (3) (§3 − §4).

## 2. $\tau^6$-Terms of Formal Energy of Mid-Point Rule

**Theorem 1.** *For Hamiltonian (1), the formal energy of the mid-point rule (2) can be written as*

$$\widetilde{H} = H + \tau^2 H_2 + \tau^4 H_4 + +\tau^6 H_6 + O(\tau^8) \tag{4}$$

*where*

$$H_2 = -\frac{1}{24} H_{z^2} \left(Z^{[1]}\right)^2; \tag{4.1}$$

$$H_4 = \frac{7}{5760} H_{z^4} \left(Z^{[1]}\right)^4 + \frac{1}{480} H_{z^3} \left(Z^{[1]}\right)^2 Z^{[2]} + \frac{1}{160} H_{z^2} \left(Z^{[2]}\right)^2; \tag{4.2}$$

$$\begin{aligned} H_6 = &- \frac{31}{24^3\times 10\times 7} H_{z^6}(Z^{[1]})^6 - \frac{53}{24^2\times 40\times 7} H_{z^5}(Z^{[1]})^4 Z^{[2]} \\ &- \frac{19}{24^2\times 20\times 7} H_{z^4}(Z^{[1]})^3 Z^{[1]}_{z^2}(Z^{[1]})^2 + \frac{3}{24^2\times 2\times 7} H_{z^4}(Z^{[1]})^3 Z^{[1]}_{z} Z^{[2]} \\ &- \frac{23}{24\times 160\times 7} H_{z^4}(Z^{[1]})^2 (Z^{[2]})^2 - \frac{39}{24^2\times 10\times 7} H_{z^3} Z^{[1]} Z^{[2]} Z^{[1]}_{z^2}(Z^{[1]})^2 \\ &- \frac{18}{24^2\times 10\times 7} H_{z^3} Z^{[1]} Z^{[2]} Z^{[1]}_{z} Z^{[2]} - \frac{1}{24^2\times 10\times 7} H_{z^3}(Z^{[2]})^3 \\ &- \frac{33}{24^2\times 40\times 7} H_{z^2}\left(Z^{[1]}_{z^2}(Z^{[1]})^2\right)^2 - \frac{27}{24^2\times 10\times 7} H_{z^2}\left(Z^{[1]}_{z^2}(Z^{[1]})^2\right)\left(Z^{[1]}_{z} Z^{[2]}\right) \\ &- \frac{9}{24^2\times 2\times 7} H_{z^2}\left(Z^{[1]}_{z} Z^{[2]}\right)^2 \end{aligned} \tag{4.3}$$

*(refer to [13,15]).*

If we set $Z^{[k+1]} = \frac{\partial Z^{[k]}}{\partial Z} Z^{[1]}$ for $k = 1, 2, \cdots$, then we can write

$$\begin{aligned} Z^{[1]} &= J\nabla H \\ Z^{[2]} &= Z^{[1]}_{z} Z^{[1]} = J H_{zz} J\nabla H \\ Z^{[3]} &= Z^{[1]}_{z^2}(Z^{[1]})^2 + Z^{[1]}_{z} Z^{[2]} \\ Z^{[4]} &= Z^{[1]}_{z^3}(Z^{[1]})^3 + 3Z^{[1]}_{z^2}(Z^{[1]} Z^{[2]}) + Z^{[1]}_{z} Z^{[3]} \\ Z^{[5]} &= Z^{[1]}_{z^4}(Z^{[1]})^4 + 6Z^{[1]}_{z^3}\left((Z^{[1]})^2 Z^{[2]}\right) + 3Z^{[1]}_{z^2}(Z^{[2]})^2 + 4Z^{[1]}_{z^2}(Z^{[1]} Z^{[3]}) + Z^{[1]}_{z} Z^{[4]} \\ Z^{[6]} &= Z^{[1]}_{z^5}(Z^{[1]})^5 + 10Z^{[1]}_{z^4}\left((Z^{[1]})^3 Z^{[2]}\right) + 15Z^{[1]}_{z^3}\left(Z^{[1]}(Z^{[2]})^2\right) + 10Z^{[1]}_{z^3}\left((Z^{[1]})^2 Z^{[3]}\right) \\ &\quad + 10Z^{[1]}_{z^2}\left(Z^{[2]} Z^{[3]}\right) + 5Z^{[1]}_{z^2}\left(Z^{[1]} Z^{[4]}\right) + Z^{[1]}_{z} Z^{[5]} \\ Z^{[7]} &= Z^{[1]}_{z^6}(Z^{[1]})^6 + 15Z^{[1]}_{z^5}\left((Z^{[1]})^4 Z^{[2]}\right) + 45Z^{[1]}_{z^4}\left((Z^{[1]})^2 (Z^{[2]})^2\right) + 20Z^{[1]}_{z^4}\left((Z^{[1]})^3 Z^{[3]}\right) \end{aligned} \tag{5}$$