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SYMPLECTIC COMPUTATION OF HAMILTONIAN SYSTEMS (I)*1)

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Abstract

We get τ^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 ∇ 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 τ^{2k} in (3) for general k ?

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

(c). How about the absolute values of the coefficients of the terms of τ^{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. τ^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

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

$$+ 15Z^{[1]}_{z^3}\left((Z^{[1]})^2 Z^{[4]}\right) + 60Z^{[1]}_{z^3}\left(Z^{[1]}Z^{[2]}Z^{[3]}\right) + 15Z^{[1]}_{z^3}(Z^{[2]})^3$$
$$+ 6Z^{[1]}_{z^2}\left(Z^{[1]}Z^{[5]}\right) + 15Z^{[1]}_{z^2}\left(Z^{[2]}Z^{[4]}\right) + 10Z^{[1]}_{z^2}(Z^{[3]})^2 + Z^{[1]}_{z}Z^{[6]}$$

and we have

Lemma 1. *$Z^{[n+1]}$, $n \geq 1$ has the following expansion:*

$$\begin{aligned} Z^{[n+1]} =& \sum_{j=1}^{n} \sum_{l_1+\cdots+l_j=n; l_u \geq 1} d_{l_1\cdots l_j} J(\nabla H)_{z^j} Z^{[l_1]} \cdots Z^{[l_j]} \\ =& A_n Z^{[1]}_{z^n}(Z^{[1]})^n \\ &+ B_n Z^{[1]}_{z^{n-1}}(Z^{[1]})^{n-2} Z^{[2]} \\ &+ C_n Z^{[1]}_{z^{n-2}}(Z^{[1]})^{n-4}(Z^{[2]})^2 \\ &+ \cdots\cdots \end{aligned} \tag{6}$$

where $d_{l_1\cdots l_j} > 0$ for all $l_1, \cdots, l_j$ and

$$A_n = 1, \quad n \geq 1; \tag{7.1}$$

$$B_n = \binom{n-1}{2} = \frac{(n-1)(n-2)}{2}, \quad n \geq 1; \tag{7.2}$$

$$C_n = 3\binom{n-1}{4} = \frac{(n-1)(n-2)(n-3)(n-4)}{8}, \quad n \geq 1. \tag{7.3}$$

Proof. Using the notation introduced above, from (6) we obtain

$$\begin{aligned} Z^{[n+2]} =& A_n Z^{[1]}_{z^{n+1}}(Z^{[1]})^{n+1} \\ &+ (nA_n + B_n) Z^{[1]}_{z^n}(Z^{[1]})^{n-2} Z^{[2]} \\ &+ [(n-2)B_n + C_n] Z^{[1]}_{z^{n-1}}(Z^{[1]})^{n-4}(Z^{[2]})^2 \\ &+ \cdots\cdots, \end{aligned} \tag{8}$$

then we have the recursive relations

$$A_{n+1} = A_n; \tag{9.1}$$

$$B_{n+1} = nA_n + B_n; \tag{9.2}$$

$$C_{n+1} = (n-2)B_n + C_n. \tag{9.3}$$

One can easily deduce (7.1-7.3) from (9.1-9.3).

After some calculation, one can expand the mid-point rule (2) as follows:

$$\widetilde{Z} = Z + \sum_{k=1}^{7} \tau^k R_k + O(\tau^8) \tag{10}$$

where

$$R_1 = Z^{[1]}; \tag{10.1}$$

$$R_2 = \frac{1}{2} Z^{[2]}; \tag{10.2}$$

$$R_3 = \frac{1}{8} Z^{[1]}_{z^2}(Z^{[1]})^2 + \frac{1}{4} Z^{[1]}_{z} Z^{[2]}; \tag{10.3}$$

$$R_4 = \frac{1}{48} Z^{[1]}_{z^3}(Z^{[1]})^3 + \frac{1}{8} Z^{[1]}_{z^2} Z^{[1]} Z^{[2]} \tag{10.4}$$

$$+\frac{1}{16}Z^{[1]}_{z}Z^{[1]}_{z^2}(Z^{[1]})^2+\frac{1}{8}Z^{[1]}_{z}Z^{[1]}_{z}Z^{[2]};$$

$$\begin{aligned}R_5=&\frac{1}{384}Z^{[1]}_{z^4}(Z^{[1]})^4+\frac{1}{32}Z^{[1]}_{z^3}(Z^{[1]})^2Z^{[2]}+\frac{1}{32}Z^{[1]}_{z^2}Z^{[1]}Z^{[1]}_{z^2}(Z^{[1]})^2\\&+\frac{1}{16}Z^{[1]}_{z^2}Z^{[1]}Z^{[1]}_{z}Z^{[2]}+\frac{1}{32}Z^{[1]}_{z^2}(Z^{[2]})^2+\frac{1}{96}Z^{[1]}_{z}Z^{[1]}_{z^3}(Z^{[1]})^3\\&+\frac{1}{16}Z^{[1]}_{z}Z^{[1]}_{z^2}Z^{[1]}Z^{[2]}+\frac{1}{32}Z^{[1]}_{z}Z^{[1]}_{z}Z^{[1]}_{z^2}(Z^{[1]})^2+\frac{1}{16}Z^{[1]}_{z}Z^{[1]}_{z}Z^{[1]}_{z}Z^{[2]};\end{aligned}\tag{10.5}$$

$$\begin{aligned}R_6=&\frac{1}{3840}Z^{[1]}_{z^5}(Z^{[1]})^5+\frac{1}{192}Z^{[1]}_{z^4}(Z^{[1]})^3Z^{[2]}\\&+\frac{1}{128}Z^{[1]}_{z^3}(Z^{[1]})^2Z^{[1]}_{z^2}(Z^{[1]})^2+\frac{1}{64}Z^{[1]}_{z^3}(Z^{[1]})^2Z^{[1]}_{z}Z^{[2]}+\frac{1}{64}Z^{[1]}_{z^3}Z^{[1]}(Z^{[2]})^2\\&+\frac{1}{192}Z^{[1]}_{z^2}Z^{[1]}Z^{[1]}_{z^3}(Z^{[1]})^3+\frac{1}{32}Z^{[1]}_{z^2}Z^{[1]}Z^{[1]}_{z^2}Z^{[1]}Z^{[2]}+\frac{1}{64}Z^{[1]}_{z^2}Z^{[1]}Z^{[1]}_{z}Z^{[1]}_{z^2}(Z^{[1]})^2\\&+\frac{1}{32}Z^{[1]}_{z^2}Z^{[1]}Z^{[1]}_{z}Z^{[1]}_{z}Z^{[2]}+\frac{1}{64}Z^{[1]}_{z^2}Z^{[2]}Z^{[1]}_{z^2}(Z^{[1]})^2+\frac{1}{32}Z^{[1]}_{z^2}Z^{[2]}Z^{[1]}_{z}Z^{[2]}\\&+\frac{1}{768}Z^{[1]}_{z}Z^{[1]}_{z^4}(Z^{[1]})^4+\frac{1}{64}Z^{[1]}_{z}Z^{[1]}_{z^3}(Z^{[1]})^2Z^{[2]}+\frac{1}{64}Z^{[1]}_{z}Z^{[1]}_{z^2}Z^{[1]}Z^{[1]}_{z^2}(Z^{[1]})^2\\&+\frac{1}{32}Z^{[1]}_{z}Z^{[1]}_{z^2}Z^{[1]}Z^{[1]}_{z}Z^{[2]}+\frac{1}{64}Z^{[1]}_{z}Z^{[1]}_{z^2}(Z^{[2]})^2+\frac{1}{192}Z^{[1]}_{z}Z^{[1]}_{z}Z^{[1]}_{z^3}(Z^{[1]})^3\\&+\frac{1}{32}Z^{[1]}_{z}Z^{[1]}_{z}Z^{[1]}_{z^2}Z^{[1]}Z^{[2]}+\frac{1}{64}Z^{[1]}_{z}Z^{[1]}_{z}Z^{[1]}_{z}Z^{[1]}_{z^2}(Z^{[1]})^2+\frac{1}{32}Z^{[1]}_{z}Z^{[1]}_{z}Z^{[1]}_{z}Z^{[1]}_{z}Z^{[2]};\end{aligned}\tag{10.6}$$

and

$$\begin{aligned}R_7=&\frac{1}{720\times 64}Z^{[1]}_{z^6}(Z^{[1]})^6+\frac{1}{1536}Z^{[1]}_{z^5}(Z^{[1]})^4Z^{[2]}\\&+\frac{1}{768}Z^{[1]}_{z^4}(Z^{[1]})^3Z^{[1]}_{z^2}(Z^{[1]})^2+\frac{1}{384}Z^{[1]}_{z^4}(Z^{[1]})^3Z^{[1]}_{z}Z^{[2]}\\&+\frac{1}{256}Z^{[1]}_{z^4}(Z^{[1]})^2(Z^{[2]})^2+\frac{1}{768}Z^{[1]}_{z^3}(Z^{[1]})^2Z^{[1]}_{z^3}(Z^{[1]})^3\\&+\frac{1}{128}Z^{[1]}_{z^3}(Z^{[1]})^2Z^{[1]}_{z^2}Z^{[1]}Z^{[2]}+\frac{1}{256}Z^{[1]}_{z^3}(Z^{[1]})^2Z^{[1]}_{z}Z^{[1]}_{z^2}(Z^{[1]})^2\\&+\frac{1}{128}Z^{[1]}_{z^3}(Z^{[1]})^2Z^{[1]}_{z}Z^{[1]}_{z}Z^{[2]}+\frac{1}{128}Z^{[1]}_{z^3}Z^{[1]}Z^{[2]}Z^{[1]}_{z^2}(Z^{[1]})^2\\&+\frac{1}{64}Z^{[1]}_{z^3}Z^{[1]}Z^{[2]}Z^{[1]}_{z}Z^{[2]}+\frac{1}{384}Z^{[1]}_{z^3}(Z^{[2]})^3\\&+\frac{1}{1536}Z^{[1]}_{z^2}Z^{[1]}Z^{[1]}_{z^4}(Z^{[1]})^4+\frac{1}{128}Z^{[1]}_{z^2}Z^{[1]}Z^{[1]}_{z^3}(Z^{[1]})^2Z^{[2]}\\&+\frac{1}{128}Z^{[1]}_{z^2}Z^{[1]}Z^{[1]}_{z^2}Z^{[1]}Z^{[1]}_{z^2}(Z^{[1]})^2+\frac{1}{64}Z^{[1]}_{z^2}Z^{[1]}Z^{[1]}_{z^2}Z^{[1]}Z^{[1]}_{z}Z^{[2]}\\&+\frac{1}{128}Z^{[1]}_{z^2}Z^{[1]}Z^{[1]}_{z^2}(Z^{[2]})^2+\frac{1}{384}Z^{[1]}_{z^2}Z^{[1]}Z^{[1]}_{z}Z^{[1]}_{z^3}(Z^{[1]})^3\\&+\frac{1}{64}Z^{[1]}_{z^2}Z^{[1]}Z^{[1]}_{z}Z^{[1]}_{z^2}Z^{[1]}Z^{[2]}+\frac{1}{128}Z^{[1]}_{z^2}Z^{[1]}Z^{[1]}_{z}Z^{[1]}_{z}Z^{[1]}_{z^2}(Z^{[1]})^2\\&+\frac{1}{64}Z^{[1]}_{z^2}Z^{[1]}Z^{[1]}_{z}Z^{[1]}_{z}Z^{[1]}_{z}Z^{[2]}+\frac{1}{384}Z^{[1]}_{z^2}Z^{[2]}Z^{[1]}_{z^3}(Z^{[1]})^3\\&+\frac{1}{64}Z^{[1]}_{z^2}Z^{[2]}Z^{[1]}_{z^2}Z^{[1]}Z^{[2]}+\frac{1}{128}Z^{[1]}_{z^2}Z^{[2]}Z^{[1]}_{z}Z^{[1]}_{z^2}(Z^{[1]})^2\\&+\frac{1}{64}Z^{[1]}_{z^2}Z^{[2]}Z^{[1]}_{z}Z^{[1]}_{z}Z^{[2]}+\frac{1}{512}Z^{[1]}_{z^2}\left(Z^{[1]}_{z^2}(Z^{[1]})^2\right)^2\end{aligned}\tag{10.7}$$

$$
\begin{aligned}
&+\frac{1}{128}Z_{z^2}^{[1]}\left(Z_{z^2}^{[1]}(Z^{[1]})^2\right)\left(Z_z^{[1]}Z^{[2]}\right)+\frac{1}{128}Z_{z^2}^{[1]}\left(Z_z^{[1]}Z^{[2]}\right)^2\\
&+\frac{1}{7680}Z_z^{[1]}Z_{z^5}^{[1]}(Z^{[1]})^5+\frac{1}{384}Z_z^{[1]}Z_{z^4}^{[1]}(Z^{[1]})^3Z^{[2]}\\
&+\frac{1}{256}Z_z^{[1]}Z_{z^3}^{[1]}(Z^{[1]})^2Z_{z^2}^{[1]}(Z^{[1]})^2+\frac{1}{128}Z_z^{[1]}Z_{z^3}^{[1]}(Z^{[1]})^2Z_z^{[1]}Z^{[2]}\\
&+\frac{1}{128}Z_z^{[1]}Z_{z^3}^{[1]}Z^{[1]}(Z^{[2]})^2+\frac{1}{384}Z_z^{[1]}Z_{z^2}^{[1]}Z^{[1]}Z_{z^3}^{[1]}(Z^{[1]})^3\\
&+\frac{1}{64}Z_z^{[1]}Z_{z^2}^{[1]}Z^{[1]}Z_{z^2}^{[1]}Z^{[1]}Z^{[2]}+\frac{1}{128}Z_z^{[1]}Z_{z^2}^{[1]}Z^{[1]}Z_z^{[1]}Z_{z^2}^{[1]}(Z^{[1]})^2\\
&+\frac{1}{64}Z_z^{[1]}Z_{z^2}^{[1]}Z^{[1]}Z_z^{[1]}Z_z^{[1]}Z^{[2]}+\frac{1}{128}Z_z^{[1]}Z_{z^2}^{[1]}Z^{[2]}Z_{z^2}^{[1]}(Z^{[1]})^2\\
&+\frac{1}{64}Z_z^{[1]}Z_{z^2}^{[1]}Z^{[1]}Z_z^{[1]}Z^{[2]}+\frac{1}{1536}Z_z^{[1]}Z_z^{[1]}Z_{z^4}^{[1]}(Z^{[1]})^4\\
&+\frac{1}{128}Z_z^{[1]}Z_z^{[1]}Z_{z^3}^{[1]}(Z^{[1]})^2Z^{[2]}+\frac{1}{128}Z_z^{[1]}Z_z^{[1]}Z_{z^2}^{[1]}Z^{[1]}Z_{z^2}^{[1]}(Z^{[1]})^2\\
&+\frac{1}{64}Z_z^{[1]}Z_z^{[1]}Z_{z^2}^{[1]}Z^{[1]}Z_z^{[1]}Z^{[2]}+\frac{1}{128}Z_z^{[1]}Z_z^{[1]}Z_{z^2}^{[1]}(Z^{[2]})^2\\
&+\frac{1}{384}Z_z^{[1]}Z_z^{[1]}Z_z^{[1]}Z_{z^3}^{[1]}(Z^{[1]})^3+\frac{1}{64}Z_z^{[1]}Z_z^{[1]}Z_z^{[1]}Z_{z^2}^{[1]}Z^{[1]}Z^{[2]}\\
&+\frac{1}{128}Z_z^{[1]}Z_z^{[1]}Z_z^{[1]}Z_z^{[1]}Z_{z^2}^{[1]}(Z^{[1]})^2+\frac{1}{64}Z_z^{[1]}Z_z^{[1]}Z_z^{[1]}Z_z^{[1]}Z_z^{[1]}Z^{[2]}.
\end{aligned}
$$

Similar to (10.7), we can rewrite $\frac{Z^{[7]}}{7!}$ as

$$
\begin{aligned}
\frac{Z^{[7]}}{7!}=&\frac{1}{720\times 7}Z_{z^6}^{[1]}(Z^{[1]})^6+\frac{1}{48\times 7}Z_{z^5}^{[1]}(Z^{[1]})^4Z^{[2]}\\
&+\frac{1}{36\times 7}Z_{z^4}^{[1]}(Z^{[1]})^3Z_{z^2}^{[1]}(Z^{[1]})^2+\frac{1}{36\times 7}Z_{z^4}^{[1]}(Z^{[1]})^3Z_z^{[1]}Z^{[2]}\\
&+\frac{1}{16\times 7}Z_{z^4}^{[1]}(Z^{[1]})^2(Z^{[2]})^2+\frac{1}{48\times 7}Z_{z^3}^{[1]}(Z^{[1]})^2Z_{z^3}^{[1]}(Z^{[1]})^3\\
&+\frac{1}{16\times 7}Z_{z^3}^{[1]}(Z^{[1]})^2Z_{z^2}^{[1]}Z^{[1]}Z^{[2]}+\frac{1}{48\times 7}Z_{z^3}^{[1]}(Z^{[1]})^2Z_z^{[1]}Z_{z^2}^{[1]}(Z^{[1]})^2\\
&+\frac{1}{48\times 7}Z_{z^3}^{[1]}(Z^{[1]})^2Z_z^{[1]}Z_z^{[1]}Z^{[2]}+\frac{1}{12\times 7}Z_{z^3}^{[1]}Z^{[1]}Z^{[2]}Z_{z^2}^{[1]}(Z^{[1]})^2\\
&+\frac{1}{12\times 7}Z_{z^3}^{[1]}Z^{[1]}Z^{[2]}Z_z^{[1]}Z^{[2]}+\frac{1}{48\times 7}Z_{z^3}^{[1]}(Z^{[2]})^3\\
&+\frac{1}{120\times 7}Z_{z^2}^{[1]}Z^{[1]}Z_{z^4}^{[1]}(Z^{[1]})^4+\frac{1}{20\times 7}Z_{z^2}^{[1]}Z^{[1]}Z_{z^3}^{[1]}(Z^{[1]})^2Z^{[2]}\\
&+\frac{1}{30\times 7}Z_{z^2}^{[1]}Z^{[1]}Z_{z^2}^{[1]}Z^{[1]}Z_{z^2}^{[1]}(Z^{[1]})^2+\frac{1}{30\times 7}Z_{z^2}^{[1]}Z^{[1]}Z_{z^2}^{[1]}Z^{[1]}Z_z^{[1]}Z^{[2]}\\
&+\frac{1}{40\times 7}Z_{z^2}^{[1]}Z^{[1]}Z_{z^2}^{[1]}(Z^{[2]})^2+\frac{1}{120\times 7}Z_{z^2}^{[1]}Z^{[1]}Z_z^{[1]}Z_{z^3}^{[1]}(Z^{[1]})^3\\
&+\frac{1}{40\times 7}Z_{z^2}^{[1]}Z^{[1]}Z_z^{[1]}Z_{z^2}^{[1]}Z^{[1]}Z^{[2]}+\frac{1}{120\times 7}Z_{z^2}^{[1]}Z^{[1]}Z_z^{[1]}Z_z^{[1]}Z_{z^2}^{[1]}(Z^{[1]})^2\\
&+\frac{1}{120\times 7}Z_{z^2}^{[1]}Z^{[1]}Z_z^{[1]}Z_z^{[1]}Z_z^{[1]}Z^{[2]}+\frac{1}{48\times 7}Z_{z^2}^{[1]}Z^{[2]}Z_{z^3}^{[1]}(Z^{[1]})^3\\
&+\frac{1}{16\times 7}Z_{z^2}^{[1]}Z^{[2]}Z_{z^2}^{[1]}Z^{[1]}Z^{[2]}+\frac{1}{48\times 7}Z_{z^2}^{[1]}Z^{[2]}Z_z^{[1]}Z_{z^2}^{[1]}(Z^{[1]})^2\\
&+\frac{1}{48\times 7}Z_{z^2}^{[1]}Z^{[2]}Z_z^{[1]}Z_z^{[1]}Z^{[2]}+\frac{1}{72\times 7}Z_{z^2}^{[1]}\left(Z_{z^2}^{[1]}(Z^{[1]})^2\right)^2 \qquad (11)
\end{aligned}
$$

$$+\frac{1}{36\times 7}Z^{[1]}_{z^2}\left(Z^{[1]}_{z^2}(Z^{[1]})^2\right)\left(Z^{[1]}_{z}Z^{[2]}\right)+\frac{1}{72\times 7}Z^{[1]}_{z^2}\left(Z^{[1]}_{z}Z^{[2]}\right)^2$$
$$+\frac{1}{720\times 7}Z^{[1]}_{z}Z^{[1]}_{z^5}(Z^{[1]})^5+\frac{1}{72\times 7}Z^{[1]}_{z}Z^{[1]}_{z^4}(Z^{[1]})^3Z^{[2]}$$
$$+\frac{1}{72\times 7}Z^{[1]}_{z}Z^{[1]}_{z^3}(Z^{[1]})^2Z^{[1]}_{z^2}(Z^{[1]})^2+\frac{1}{72\times 7}Z^{[1]}_{z}Z^{[1]}_{z^3}(Z^{[1]})^2Z^{[1]}_{z}Z^{[2]}$$
$$+\frac{1}{48\times 7}Z^{[1]}_{z}Z^{[1]}_{z^3}Z^{[1]}(Z^{[2]})^2+\frac{1}{144\times 7}Z^{[1]}_{z}Z^{[1]}_{z^2}Z^{[1]}Z^{[1]}_{z^3}(Z^{[1]})^3$$
$$+\frac{1}{48\times 7}Z^{[1]}_{z}Z^{[1]}_{z^2}Z^{[1]}Z^{[1]}_{z^2}Z^{[1]}Z^{[2]}+\frac{1}{144\times 7}Z^{[1]}_{z}Z^{[1]}_{z^2}Z^{[1]}Z^{[1]}_{z}Z^{[1]}_{z^2}(Z^{[1]})^2$$
$$+\frac{1}{144\times 7}Z^{[1]}_{z}Z^{[1]}_{z^2}Z^{[1]}Z^{[1]}_{z}Z^{[1]}_{z}Z^{[2]}+\frac{1}{72\times 7}Z^{[1]}_{z}Z^{[1]}_{z^2}Z^{[2]}Z^{[1]}_{z^2}(Z^{[1]})^2$$
$$+\frac{1}{72\times 7}Z^{[1]}_{z}Z^{[1]}_{z^2}Z^{[2]}Z^{[1]}_{z}Z^{[2]}+\frac{1}{720\times 7}Z^{[1]}_{z}Z^{[1]}_{z}Z^{[1]}_{z^4}(Z^{[1]})^4$$
$$+\frac{1}{120\times 7}Z^{[1]}_{z}Z^{[1]}_{z}Z^{[1]}_{z^3}(Z^{[1]})^2Z^{[2]}+\frac{1}{180\times 7}Z^{[1]}_{z}Z^{[1]}_{z}Z^{[1]}_{z^2}Z^{[1]}Z^{[1]}_{z^2}(Z^{[1]})^2$$
$$+\frac{1}{180\times 7}Z^{[1]}_{z}Z^{[1]}_{z}Z^{[1]}_{z^2}Z^{[1]}Z^{[1]}_{z}Z^{[2]}+\frac{1}{240\times 7}Z^{[1]}_{z}Z^{[1]}_{z}Z^{[1]}_{z^2}(Z^{[2]})^2$$
$$+\frac{1}{720\times 7}Z^{[1]}_{z}Z^{[1]}_{z}Z^{[1]}_{z}Z^{[1]}_{z^3}(Z^{[1]})^3+\frac{1}{240\times 7}Z^{[1]}_{z}Z^{[1]}_{z}Z^{[1]}_{z}Z^{[1]}_{z^2}Z^{[1]}Z^{[2]}$$
$$+\frac{1}{720\times 7}Z^{[1]}_{z}Z^{[1]}_{z}Z^{[1]}_{z}Z^{[1]}_{z}Z^{[1]}_{z^2}(Z^{[1]})^2+\frac{1}{720\times 7}Z^{[1]}_{z}Z^{[1]}_{z}Z^{[1]}_{z}Z^{[1]}_{z}Z^{[1]}_{z}Z^{[2]}.$$

Proof of Theorem 1. According to the definition of formal energy of symplectic scheme [6],

$$\widetilde{Z}=Z+\sum_{k=1}^{+\infty}\tau^k\widetilde{Z}^{[k]} \tag{12}$$

where $\widetilde{Z}^{[1]}=J\nabla\widetilde{H}$, and $\widetilde{Z}^{[k+1]}=\frac{\partial\widetilde{Z}^{[k]}}{\partial Z}\widetilde{Z}^{[1]}$ for $k=1,2,\cdots$, then after comparing the terms of τ^7 on the right sides of (10) and (12) we obtain

$$\begin{aligned}
&R_7-\frac{Z^{[7]}}{7!}\\
&=J\nabla H_6+\frac{1}{6}Z^{[2]}_{z}J\nabla H_4+\frac{1}{6}\left[Z^{[1]}_{z}J\nabla H_2\right]_z J\nabla H_2+\frac{1}{6}\left[J(\nabla H_2)_z Z^{[1]}\right]_z J\nabla H_2\\
&\quad+\frac{1}{6}\left[Z^{[1]}_{z}J\nabla H_4\right]_z Z^{[1]}+\frac{1}{6}\left[J(\nabla H_2)_z J\nabla H_2\right]_z Z^{[1]}+\frac{1}{6}\left[J(\nabla H_4)_z Z^{[1]}\right]_z Z^{[1]}\\
&\quad+\frac{1}{120}Z^{[4]}_{z}J\nabla H_2+\frac{1}{120}\left[Z^{[3]}_{z}J\nabla H_2\right]_z Z^{[1]}+\frac{1}{120}\left[\left(Z^{[2]}_{z}J\nabla H_2\right)_z Z^{[1]}\right]_z Z^{[1]}\\
&\quad+\frac{1}{120}\left\{\left[\left(Z^{[1]}_{z}J\nabla H_2\right)_z Z^{[1]}\right]_z Z^{[1]}\right\}_z Z^{[1]}+\frac{1}{120}\left\{\left(\left[J(\nabla H_2)_z Z^{[1]}\right]_z Z^{[1]}\right)_z Z^{[1]}\right\}_z Z^{[1]}.
\end{aligned} \tag{13}$$

Since we have known the expressions for H_2 and H_4 as in (3) or in (4.1-4.2), from (13) we can obtain the expression (4.3) for H_6. The procedure is tedious but straightforward calculus, we omit it here.

Remark 1. One can find from (4.1-4.3) that

(i). In the expression of the formal energy of the mid-point rule, for τ^2, τ^4 and τ^6, the number of the terms are 1, 3 and 11 resectively, these are exactly the numbers of free unlabeled trees of 3 vertices, 5 vertices and 7 vertices respectively.

(ii). In the expression of the formal energy of the mid-point rule, for τ^2, τ^4 and τ^6, the maxium absolute values of the coefficients of the terms are $\frac{1}{24}=\frac{1}{2^3\times 3}$, $\frac{1}{160}=\frac{1}{2^5\times 5}$ are $\frac{9}{24^2\times 2\times 7}=$

$\frac{1}{2^7\times 7}$ respectively.

In fact for (i) there is a general result, that is, *in the expansion (4) of the formal energy of the mid-point rule, the number of the terms in* τ^{2k} *is exactly the number of the free unlabeled trees of* $2k+1$ *vertices* (refer to [8,13,15,19]).

And for (ii) let's give the following

Conjecture 1. *In the expression of the formal energy of the mid-point rule, the maximum absolute value of the coefficients of the terms in* τ^{2k} *is exactly* $\frac{1}{2^{2k+1}\times(2k+1)}$ *(refer to [13,15,19]).*

Remark 2. If the Hamiltonian is linear, i.e., $H=\frac{1}{2}Z^TMZ$ where M is a $2n\times 2n$ symmetric matrix, then (refer to (5)) $Z^{[r]}=(JM)^rZ$, $r=1,2,\cdots$, and (refer to (4))

$$\begin{aligned}\widetilde{H}=&H-\frac{\tau^2}{24}H_{z^2}\left(Z^{[1]}\right)^2+\frac{\tau^4}{160}H_{z^2}\left(Z^{[2]}\right)^2-\frac{9\tau^6}{24^2\times 2\times 7}H_{z^2}\left(Z_z^{[1]}Z^{[2]}\right)^2+O(\tau^8)\\=&\frac{1}{2}Z^T(M)Z+\frac{\tau^2}{2^3\times 3}Z^T(MJMJM)Z+\frac{\tau^4}{2^5\times 5}Z^T(MJMJMJMJM)Z\\&+\frac{\tau^6}{2^7\times 7}Z^T(MJMJMJMJMJMJM)Z+O(\tau^8)\\=&\frac{1}{2}Z^T(\widetilde{M})Z+O(\tau^8)\end{aligned}\tag{14}$$

where $\widetilde{M}=\sum_{k=0}^{+\infty}\frac{1}{2^{2k}\times(2k+1)}M\left(\tau JM\right)^{2k}$.

On the other hand, substituting $H=\frac{1}{2}Z^TMZ$ into (2) we directly get

$$\widetilde{Z}=\left[I-\frac{\tau}{2}JM\right]^{-1}\left[I+\frac{\tau}{2}JM\right]Z.\tag{15}$$

But

$$\begin{aligned}\ln\left\{\left[I-\frac{\tau}{2}JM\right]^{-1}\left[I+\frac{\tau}{2}JM\right]\right\}&=-\ln\left[I-\frac{\tau}{2}JM\right]+\ln\left[I+\frac{\tau}{2}JM\right]\\&=\sum_{k=0}^{+\infty}\frac{1}{2^{2k}\times(2k+1)}\left(\tau JM\right)^{2k+1}\\&=\tau J\widetilde{M}.\end{aligned}\tag{16}$$

One can find the coincideince between (14) and (16), and furthermore in fact, the tail $O(\tau^8)$ in (14) can be cancelled [13,15].

3. The Mathematical Pendulum

The mathematical pendulum has a hamiltonian

$$H=H_0=\frac{1}{2}p^2-\omega^2\cos q,\tag{17.1}$$

where ω is a constant. When $-\omega^2<h<\omega^2$ its motion is *periodic* (see [1,2]) with period (see [10,11])

$$T=4\sqrt{2}\int_0^{\frac{\pi}{2}}\frac{d\theta}{\sqrt{(\omega^2-h)+(\omega^2+h)\sin^2\theta}},\tag{18}$$

where h is the constant value of the hamiltonian. According to (4.1-4.3), one can obtain by calculation the following:

$$H_2=-\frac{1}{24}\omega^2(p^2\cos q+\omega^2\sin^2 q);\tag{17.2}$$

$$H_4 = -\frac{7}{5760}p^4\omega^2\cos q + \frac{1}{480}p^2\omega^4\sin^2 q + \frac{1}{160}\omega^4\cos q(p^2\cos q + \omega^2\sin^2 q); \tag{17.3}$$

$$\begin{aligned} H_6 = &- \frac{31}{24^3 \times 10 \times 7}p^6\omega^2\cos q + \frac{1}{24^2 \times 2 \times 7}p^4\omega^4(1 + 2\cos^2 q) \\ &+ \frac{51}{24^2 \times 20 \times 7}p^2\omega^6\sin^2 q\cos q - \frac{1}{24^2 \times 10 \times 7}\omega^8\sin^4 q \\ &- \frac{9}{24^2 \times 2 \times 7}\omega^6\cos^2 q(p^2\cos q + \omega^2\sin^2 q). \end{aligned} \tag{17.4}$$

4. Numerical Experiments

If we set in expression (4) of the formal energy of the mid-point rule

$$H^{(2k)} = \sum_{i=0}^{k}\tau^{2i}H_{2i} = H_0 + \tau^2 H_2 + \cdots + \tau^{2k}H_{2k}, \quad k = 0, 1, \cdots, \tag{19}$$

($H^{(2k)}$ is also denoted by $H_\tau^{(2k)}$ for stepsize τ in the sequel) then

$$H^{(2k)} = \widetilde{H} + O(\tau^{2(k+1)}), \quad k = 0, 1, \cdots, \tag{20}$$

that is to say, $H^{(0)}$, $H^{(2)}$, $H^{(4)}$ and $H^{(6)}$ are approximations of order 0, 2, 4 and 6 respectively (of order 1, 3, 5 and 7 respectively in fact, because there are no odd-order terms in expression (4)) to the formal energy $\widetilde{H}$.

We choose $\omega = 3.0$ and $h = 7.5$, then the period of motion $T = 3.552256$. In the following we will call $Err(A)(t) = A(t) - A(0)$ for any variable A.

We use the mid-point rule with the different stepsizes $\tau_1 = T/60 = 0.059204$, $\tau_2 = \tau_1/2 = 0.029602$, to simulate the motion of the mathematical pendulum for 67,560 steps and $540,480 = 8 * 67,560$ steps respectively, Figure 1–8 plot the numerical results for variation of $Err(H^{(0)})$ (Figure 1–2), $Err(H^{(2)})$ (Figure 3–4), $Err(H^{(4)})$ (Figure 5–6) and $Err(H^{(6)})$ (Figure 7–8) respectively.

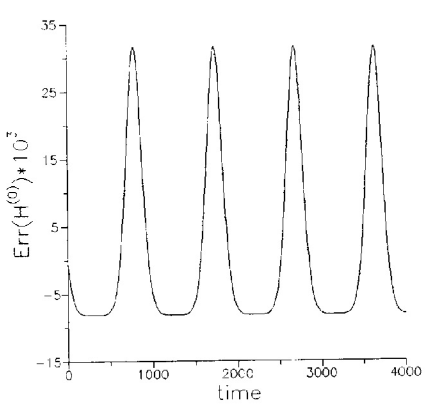

Figure 1: variation of formal energy's approximation $H^{(0)}$ (order 1) for midpoint rule (order 2) stepsize=0.0592, 67,560 steps

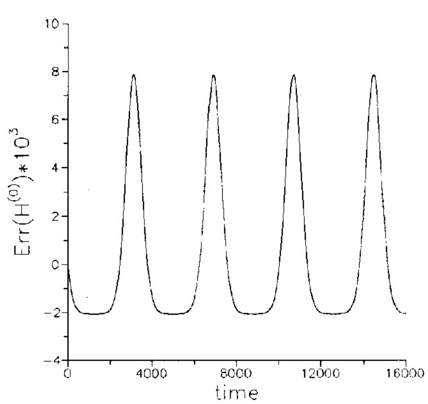

Figure 2: variation of formal energy's approximation $H^{(0)}$ (order 1) for midpoint rule (order 2) stepsize=0.0296, 540,480 steps

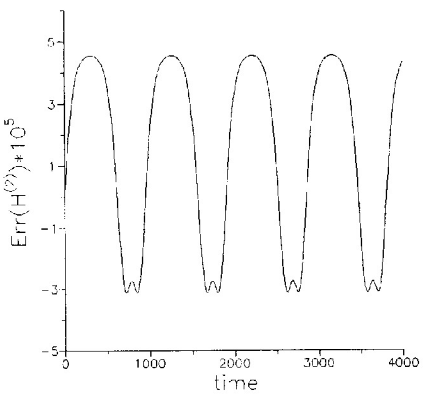

Figure 3: variation of formal energy's approximation $H^{(2)}$ (order 3) for midpoint rule (order 2) stepsize=0.0592, 67,560 steps

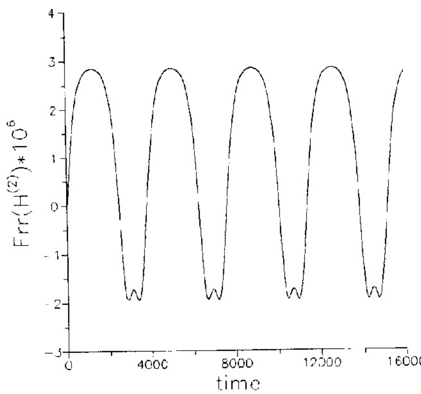

Figure 4: variation of formal energy's approximation $H^{(2)}$ (order 3) for midpoint rule (order 2) stepsize=0.0296, 540,480 steps

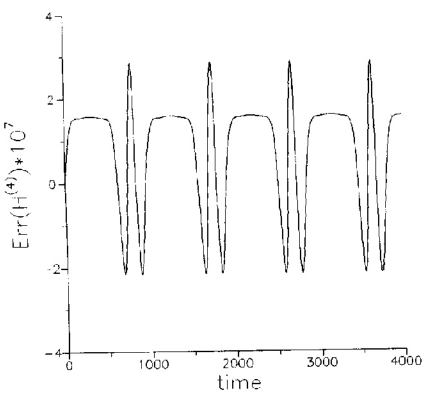

Figure 5: variation of formal energy's approximation $H^{(4)}$ (order 5) for midpoint rule (order 2) stepsize=0.0592, 67,560 steps

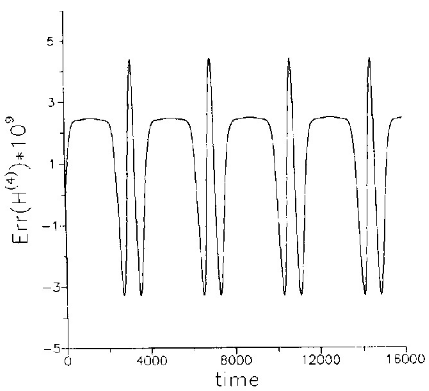

Figure 6: variation of formal energy's approximation $H^{(4)}$ (order 5) for midpoint rule (order 2) stepsize=0.0296, 540,480 steps

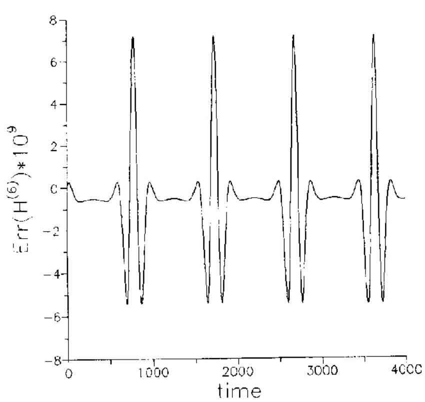

Figure 7: variation of formal energy's approximation $H^{(6)}$ (order 7) for midpoint rule (order 2) stepsize=0.0592, 67,560 steps

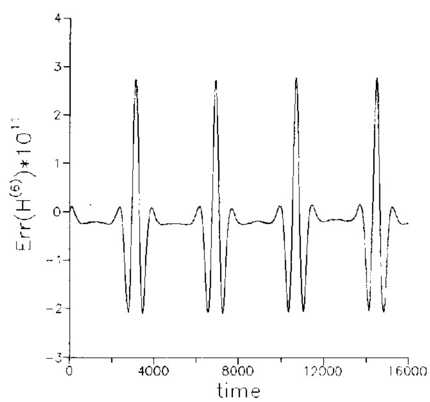

Figure 8: variation of formal energy's approximation $H^{(6)}$ (order 7) for midpoint rule (order 2) stepsize=0.0296, 540,480 steps

One can easily find something interesting: Figure 1 and Figure 2, Figure 3 and Figure 4, Figure 5 and Figure 6, Figure 7 and Figure 8, have the same configurations respectively and, in Figure 1 $Err(H^{(0)})*10^3 \in [-8.151787, 31.601730] \approx 2^2*[-2.049836, 7.890028](\ni Err(H^{(0)})*10^3$ in Figure 2); in Figure 3 $Err(H^{(2)})*10^5 \in [-3.111049, 4.556480] \approx 2^4/10*[-1.942975, 2.837876](\ni Err(H^{(2)})*10^6$ in Figure 4); in Figure 5 $Err(H^{(4)})*10^7 \in [-2.153531, 2.861244] \approx 2^6/100*[-3.297866, 4.393560](\ni Err(H^{(4)})*10^9$ in Figure 6); in Figure 7 $Err(H^{(6)})*10^9 \in [-5.458335, 7.198202] \approx 2^8/100*[-2.102585, 2.793943](\ni Err(H^{(6)})*10^{11}$ in Figure 8). That is to say,

$$Err\left(H_{\tau}^{(2k)}\right)(t) \approx 2^{2(k+1)} * Err\left(H_{\tau/2}^{(2k)}\right)(2^2 * t) \tag{21}$$

for $k = 0, 1, 2, 3$.

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