An International Journal
computers & mathematics with applications

PERGAMON Computers and Mathematics with Applications 43 (2002) 1171–1181
www.elsevier.com/locate/camwa

Is the Formal Energy of the Mid-Point Rule Convergent?

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(Received March 2000; revised and accepted November 2000)

Abstract—We obtain some formulae for calculation of the coefficients of four special types of terms in τ^{2k}, $k = 1, 2, \dots$ (1-1 corresponding to four type of $(2k+1)$-vertex free unlabeled trees, $k = 1, 2, \dots$, respectively), for a fixed step size τ, in the tree-expansion of the formal energy of the mid-point rule. And, we give an estimate of the difference between the formal energy $\tilde{H}$ and the standard Hamiltonian H in some domain Ω under the assumptions

(i) H is smooth and bounded in Ω, and
(ii) the absolute values of the coefficients of the terms in τ^{2k} are uniformly bounded by $\eta\sigma^{2k}$ for some constants $\eta \geq 1$, $\sigma > 0$ and for any $k \geq 1$.

Keywords—Mid-point rule, Formal energy, Tree-expansion.

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Subsidized by the Special Funds for Major State Basic Research Projects (No. G1999032800), also by a grant (No. 19801034) from National Natural Science Foundation of China and a grant for *innovation* (for the project "*Geometrical Integration of Dynamical Systems*") from Academy of Mathematics and Systems Sciences, Academia Sinica.
We are indebted to the referee for his valuable recommendations and corrections.

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PII: S0898-1221(01)00353-4

1. INTRODUCTION

For a *Hamiltonian* system

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

(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), it has been suggested that the *symplectic* difference schemes should be employed to integrate it [1,2]. A great deal of numerical experiment has shown the superiority of symplectic schemes over the nonsymplectic ones, especially in structural, global, and long-term tracking capabilities [1,3,4]. Except for some trivial cases, a symplectic scheme will not preserve the Hamiltonian energy H [1,2,4]. However, one of the striking outcomes of the symplectic simulation is that the numerically resulted values for H at the discrete temporal points, always undulate up and down in a very small neighborhood of the original identical value of H [1,4,5]. And, in fact, for a fixed-step size, any *symplectic* scheme has a *formal energy* (or *nearby energy*, or *perturbed Hamiltonian function*) [6–10] which is the "*exact Hamiltonian*" for the symplectic scheme to be the "*formal phase flow*" when evaluated at the discrete temporal points [7]. And, the expansions of the formal energies have found some remarkable applications, say, in construction of higher-order symplectic schemes and in delicate test of the long-term behavior of the schemes [11–13]. Such being the case, the theoretical study of the convergence of the formal energy of a symplectic scheme, and of the difference between the formal energy and the original Hamiltonian H has come out to be most interesting and most important.

For instance, the mid-point rule

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

is a second-order time-reversible symplectic scheme that preserves any quadratic invariants of the Hamiltonian H [4,14,15], and its formal energy has an expansion [13]

$$\tilde{H} = H + \tau^2 H_2 + \tau^4 H_4 + +\tau^6 H_6 + \cdots, \tag{3}$$

where

$$H_2 = -\frac{1}{24} H_{z^2}\left(Z^{[1]}\right)^2; \tag{3.1}$$

$$H_4 = \frac{7}{5760} H_{z^4}\left(Z^{[1]}\right)^4 + \frac{1}{480} H_{z^3}\left(Z^{[1]}\right)^2 Z^{[2]} + \frac{1}{160} H_{z^2}\left(Z^{[2]}\right)^2; \tag{3.2}$$

$$\begin{aligned} H_6 = &-\frac{31}{967680} H_{z^6}\left(Z^{[1]}\right)^6 - \frac{53}{161280} H_{z^5}\left(Z^{[1]}\right)^4 Z^{[2]} \\ &- \frac{19}{80640} H_{z^4}\left(Z^{[1]}\right)^3 Z^{[1]}_{z^2}\left(Z^{[1]}\right)^2 + \frac{1}{2688} H_{z^4}\left(Z^{[1]}\right)^3 Z^{[1]}_{z} Z^{[2]} \\ &- \frac{23}{26880} H_{z^4}\left(Z^{[1]}\right)^2\left(Z^{[2]}\right)^2 - \frac{13}{13440} H_{z^3} Z^{[1]} Z^{[2]} Z^{[1]}_{z^2}\left(Z^{[1]}\right)^2 \\ &- \frac{1}{2240} H_{z^3} Z^{[1]} Z^{[2]} Z^{[1]}_{z} Z^{[2]} - \frac{1}{40320} H_{z^3}\left(Z^{[2]}\right)^3 \\ &- \frac{11}{53760} H_{z^2}\left(Z^{[1]}_{z^2}\left(Z^{[1]}\right)^2\right)^2 - \frac{3}{4480} H_{z^2}\left(Z^{[1]}_{z^2}\left(Z^{[1]}\right)^2\right)\left(Z^{[1]}_{z} Z^{[2]}\right) \\ &- \frac{1}{896} H_{z^2}\left(Z^{[1]}_{z} Z^{[2]}\right)^2, \end{aligned} \tag{3.3}$$

where $Z^{[1]} = J\nabla H(Z)$, $Z^{[k+1]} = \frac{\partial Z^{[k]}}{\partial Z} Z^{[1]}$ for $k = 1, 2, \ldots$. We use the notation

$$A_{z^r}(V_1)\ldots(V_r) = \sum_{j_1,\ldots,j_r=1}^{2n} \frac{\partial^r A}{\partial z_{j_1}\ldots\partial z_{j_r}} [V_1]_{(j_1)} \cdots [V_r]_{(j_r)},$$

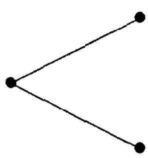
where A is a variable of any dimension (say, H or $Z^{[1]}$), V_i is a $2n$-dim variable (say, $Z^{[1]}$, $Z^{[2]}$ *et al.*) for $i = 1, \dots, r$, z_{j_u} is the j_u^{th} component of $2n$-dim vector Z, and $[V_u]_{(j_u)}$ stands for the j_u^{th} component of $2n$-dim vector V_u, $u = 1, \dots, r$.

For example, in (3.3),

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

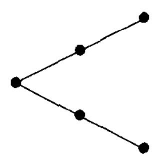
In the expansion of (3), just like 1 for τ^2, 3 for τ^4, and 11 for τ^6 in (3.1)–(3.3), respectively, the number of terms for τ^{2k} is exactly *the number of free unlabeled trees of* $2k+1$ *vertices* and there is a 1-1 correspondence between the terms in H_{2k} and the $(2k+1)$-vertex free unlabeled trees, for $k \geq 1$ [8,13].

(T-δ_2)



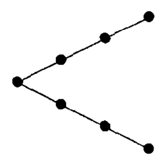
$H_{Z^2}\,(Z^{[1]})^2$

(T-δ_4)



$H_{Z^2}\,(Z^{[2]})^2$

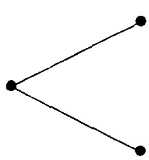
(T-δ_6)



$H_{Z^2}\left(Z_z^{[1]} Z^{[2]}\right)^2$

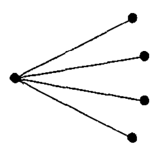
For example, the above free unlabeled trees: (T-δ_2), (T-δ_4), and (T-δ_6) correspond to the terms in (3.1)–(3.3): $-(1/24)\,H_{z^2}(Z^{[1]})^2$, $(1/160)\,H_{z^2}(Z^{[2]})^2$, and $-(1/896)\,H_{z^2}(Z_z^{[1]}Z^{[2]})^2$, respectively. They also correspond to the δ_2-, δ_4-, and δ_6-terms, respectively, in (12) in Theorem 1 in Section 3.

(T-λ_2)



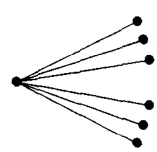
$H_{Z^2}\,(Z^{[1]})^2$

(T-λ_4)



$H_{Z^4}\,(Z^{[1]})^4$

(T-λ_6)

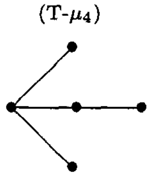


$H_{Z^6}\,(Z^{[1]})^6$

The above free unlabeled trees: (T-λ_2), (T-λ_4), and (T-λ_6) correspond to the terms in (3.1)–(3.3): $-(1/24)\,H_{z^2}(Z^{[1]})^2$, $(7/5760)\,H_{z^4}(Z^{[1]})^4$, and $-(31/967680)\,H_{z^6}(Z^{[1]})^6$, respectively. They also correspond to the λ_2-, λ_4-, and λ_6-terms, respectively, in (17) in Theorem 2 in Section 3.

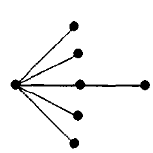
The following free unlabeled trees: (T-μ_4) and (T-μ_6) correspond to the terms in (3.2),(3.3): $(1/480)\,H_{z^3}(Z^{[1]})^2 Z^{[2]}$ and $-(53/161280)\,H_{z^5}(Z^{[1]})^4 Z^{[2]}$, respectively. (T-$\mu_4$), (T-$\mu_6$), and (T-$\mu_8$) also correspond to the μ_4-, μ_6-, and μ_8-terms, respectively, in (17) in Theorem 2 in Section 3.

(T-μ_4)



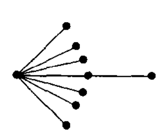
$H_{Z^3}\,(Z^{[1]})^2\,Z^{[2]}$

(T-μ_6)



$H_{Z^5}\,(Z^{[1]})^4\,Z^{[2]}$

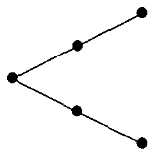
(T-μ_8)



$H_{Z^7}\,(Z^{[1]})^6\,Z^{[2]}$

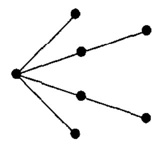
The following free unlabeled trees: (T-ν_4) and (T-ν_6) correspond to the terms in (3.2),(3.3): $(1/160)\, H_{z^2}(Z^{[2]})^2$ and $-(23/26880)\, H_{z^4}(Z^{[1]})^2(Z^{[2]})^2$, respectively. (T-$\nu_4$), (T-$\nu_6$), and (T-$\nu_8$) also correspond to the ν_4-, ν_6-, and ν_8-terms, respectively, in (17) in Theorem 2 in Section 3.

(T-ν_4)



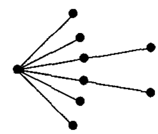
$H_{Z^2}\,(Z^{[2]})^2$

(T-ν_6)



$H_{Z^4}\,(Z^{[1]})^2\,(Z^{[2]})^2$

(T-ν_8)



$H_{Z^6}\,(Z^{[1]})^4\,(Z^{[2]})^2$

We call this kind of expansion of the formal energy a "*tree-expansion*" (for an introduction to *free unlabeled trees*, refer to [16,17]). On the other hand, for the number of coefficients of the terms in τ^{2k} for general k, there is no definite result. It is conjectured [13] that *the maximum absolute value of the coefficients of the terms in* τ^{2k} *is exactly* $1/(2^{2k+1} \times (2k+1))$.

In this paper, first we review the *generating functions for rooted unlabeled trees and free unlabeled trees*, and write out a rough bound for the number of the free unlabeled trees of $2k+1$ vertices v_{2k+1} (for $k \geq 1$). This is also a bound for the number of the terms for H_{2k} in the tree-expansion of the formal energy of the mid-point rule (Section 2, Remark 1). Second, we obtain some formulae for the coefficients of four special type of terms in τ^{2k}, $k = 1, 2, \dots$, in the tree-expansion of the formal energy of the mid-point rule. These four special types of terms, with coefficients $\{\delta_{2k}\}_1^{+\infty}$, $\{\lambda_{2k}\}_1^{+\infty}$, $\{\mu_{2k}\}_2^{+\infty}$, and $\{\nu_{2k}\}_2^{+\infty}$, are four different subsequences of the tree-expansion of the formal energy and exactly 1-1 corresponding to four type of $(2k+1)$-vertex free unlabeled trees, $k = 1, 2, \dots$, respectively, (Section 3, Theorems 1 and 2). And, according to these formulae, we give some estimates for the bounds of the coefficients (Section 3, Theorem 3). Finally, we give an estimate of the difference between the formal energy $\tilde{H}$ and the standard Hamiltonian H in a domain Ω under the assumptions

(i) H is smooth and bounded in Ω,

(ii) the absolute values of the coefficients of the terms in τ^{2k} are uniformly bounded by $\eta\sigma^{2k}$ for some constants $\eta \geq 1$, $\sigma > 0$, and for any $k \geq 1$ (Section 4, Theorem 4).

And, we indicate that this kind of analysis is also suitable for other type of terms (subsequences) of the tree-expansion of the formal energy of the mid-point rule, and possibly suitable for that of other symplectic methods (say, of Runge-Kutta type) (Section 5).

2. GENERATING FUNCTIONS FOR ROOTED UNLABELED TREES AND FREE UNLABELED TREES

If we expand the mid-point rule (2) as follows:

$$\tilde{Z} = Z + \sum_{k=1}^{+\infty} \tau^k R_k, \tag{4}$$

where

$$R_1 = Z^{[1]}; \tag{4.1}$$

$$R_2 = \frac{1}{2}\, Z^{[2]}; \tag{4.2}$$

$$R_3 = \frac{1}{8}\, Z^{[1]}_{z^2} \left(Z^{[1]}\right)^2 + \frac{1}{4}\, Z^{[1]}_{z} Z^{[2]}; \tag{4.3}$$

$$R_4 = \frac{1}{48}\, Z^{[1]}_{z^3} \left(Z^{[1]}\right)^3 + \frac{1}{8}\, Z^{[1]}_{z^2} Z^{[1]} Z^{[2]} + \frac{1}{16}\, Z^{[1]}_{z} Z^{[1]}_{z^2} \left(Z^{[1]}\right)^2 + \frac{1}{8}\, Z^{[1]}_{z} Z^{[1]}_{z} Z^{[2]}; \tag{4.4}$$

$$\vdots$$

then just like 1 for τ^1, 1 for τ^2, 2 for τ^3, and 4 for τ^4, the number of terms for τ^k is exactly *the number of rooted unlabeled trees of k vertices* and there is a 1-1 correspondence between the terms in R_k and the k-vertex rooted unlabeled trees, for $k \geq 1$ [8,13].

We know the generating function $u(x) = \sum_{r=1}^{+\infty} u_r x^r$ for rooted unlabeled trees has a recursive definition [16,17]

$$u(x) = x \exp\left\{\sum_{i=1}^{\infty} \frac{1}{i} u\left(x^i\right)\right\} = x\Pi_{r=1}^{+\infty}\left(1 - x^r\right)^{-u_r}, \tag{5}$$

and its expansion is

$$\begin{aligned}\sum_{r=1}^{+\infty} u_r x^r &= x + x^2 + 2x^3 + 4x^4 + 9x^5 + 20x^6 + 48x^7 + 115x^8 \\ &\quad + 286x^9 + 719x^{10} + 1842x^{11} + 4766x^{12} + 12486x^{13} \\ &\quad + 32973x^{14} + 87811x^{15} + 235381x^{16} + 634847x^{17} + \cdots .\end{aligned} \tag{6}$$

For the coefficients u_r, $r = 1, 2, \dots$, in [19] it is given that

$$u_n \sim \frac{\beta\alpha^{3/2}}{2\sqrt{\pi}} \frac{\alpha^{-n}}{n^{3/2}} = 0.4399237 \frac{\alpha^{-n}}{n^{3/2}} \tag{7}$$

with $\alpha = 0.3383219$, $\beta = 7.924780$.

The generating function $v(x)$ for free unlabeled trees can be expressed by that for rooted unlabeled trees $u(x)$ [18,19]

$$v(x) = u(x) - \frac{1}{2}\left[u^2(x) - u\left(x^2\right)\right], \tag{8}$$

and its expansion is

$$\begin{aligned}v(x) = \sum_{k=1}^{+\infty} v_k x^k &= x + x^2 + x^3 + 2x^4 + 3x^5 + 6x^6 + 11x^7 + 23x^8 \\ &\quad + 47x^9 + 106x^{10} + 235x^{11} + 551x^{12} + \cdots .\end{aligned} \tag{9}$$

In fact [19],

$$v_n \sim \frac{\beta^3\alpha^{9/2}}{4\sqrt{\pi}} \frac{\alpha^{-n}}{n^{5/2}} = 0.5349485 \frac{\alpha^{-n}}{n^{5/2}}. \tag{10}$$

From (10),

$$v_n \leq 3^n, \qquad n = 1, 2, \dots . \tag{11}$$

REMARK 1. As mentioned above, inequality (11) also gives a bound for the number of the terms of H_{2k} in the tree-expansion of the formal energy (3) of the mid-point rule (2), for any $k \geq 1$.

3. FORMULAE FOR THE COEFFICIENTS OF TERMS OF FOUR SPECIAL TYPES

THEOREM 1. *If the tree-expansion of (3) is written*

$$\begin{aligned}\tilde{H} = H &+ \delta_2\tau^2 H_{z^2}\left(Z^{[1]}\right)^2 \\ &+ \cdots + \delta_4\tau^4 H_{z^2}\left(Z_z^{[1]} Z^{[1]}\right)^2 \\ &+ \cdots \\ &+ \cdots + \delta_{2k}\tau^{2k} H_{z^2}\left(Z_z^{[1]} \dots Z_z^{[1]} Z^{[1]}\right)^2 \\ &+ \cdots ,\end{aligned} \tag{12}$$

then for any $s \geq 1$,

$$\delta_{2s} = \frac{(-1)^s}{2^{2s+1} \times (2s+1)}. \tag{13}$$

PROOF OF THEOREM 1. It's easy to check

$$\begin{aligned} &\left\{ H_{z^2} \left(Z_z^{[1]} \dots Z_z^{[1]} Z^{[1]} \right)^2 \right\}_{zz} \qquad (s - \text{time} - \text{“}Z\text{”}) \\ &= (-1)^s 2 H_{zz} J H_{zz} \dots J H_{zz} J H_{zz} J H_{zz} \dots J H_{zz} J H_{zz} + \cdots . \end{aligned} \tag{14}$$

Observing the expansions like (4.1)–(4.4) of R_{2s+1} in (4) and of $Z^{[2s+1]}$, we easily see that the term $Z_z^{[1]} Z_z^{[1]} \dots Z_z^{[1]} Z^{[1]} = J H_{zz} J H_{zz} \dots J H_{zz} J \nabla H$ (with $(2s+1)$—the number of “Z”) has the coefficients $1/2^{2s}$ and 1 for R_{2s+1} and $Z^{[2s+1]}$, respectively. So for any $s \geq 1$, $(\tau^{2s+1})/2^{2s}$ is the term of τ^{2s+1} in

$$\begin{aligned} &\tau \left(1 - 2\delta_2 \tau^2 + 2\delta_4 \tau^4 - \cdots \right) + \frac{\tau^3}{3!} \left(1 - 2\delta_2 \tau^2 + 2\delta_4 \tau^4 - \cdots \right)^3 \\ &+ \cdots + \frac{\tau^{2k+1}}{(2k+1)!} \left(1 - 2\delta_2 \tau^2 + 2\delta_4 \tau^4 - \cdots \right)^{2k+1} + \cdots \\ &= e^{\tau \left(1 - 2\delta_2 \tau^2 + 2\delta_4 \tau^4 - \cdots \right)}. \end{aligned} \tag{15}$$

If $\delta_2 = -1/24 = -1/(2^3 \times 3), \dots, \delta_{2k} = (-1)^k/(2^{2k+1} \times (2k+1))$, then (15) can be rewritten as

$$\begin{aligned} &e^{2\left[\tau/2 + (1/3)(\tau/2)^3 + \cdots + (1/2k+1)(\tau 2)^{2k+1} + \cdots\right]} + \left\{ \delta_{2(k+1)} - \frac{(-1)^{k+1}}{2^{2k+3} \times (2k+3)} \right\} \tau^{2k+3} \\ &+ O\left(\tau^{2k+5}\right) = \frac{1 + (\tau/2)}{1 - (\tau/2)} + \left\{ \delta_{2(k+1)} - (-1)^{k+1} \frac{1}{2^{2k+3} \times (2k+3)} \right\} \tau^{2k+3} + O\left(\tau^{2k+5}\right). \end{aligned} \tag{16}$$

Since in (16), the term of τ^{2k+3} is $(\tau^{2k+3})/(2^{2(k+1)})$, we should have $\delta_{2(k+1)} = (-1)^{k+1} (1/2^{2k+3} \times (2k+3))$. ∎

THEOREM 2. *If the tree-expansion of (3) is written*

$$\begin{aligned} \tilde{H} = {} & H + \lambda_2 \tau^2 H_{z^2} \left(Z^{[1]}\right)^2 \\ & + \lambda_4 \tau^4 H_{z^4} \left(Z^{[1]}\right)^4 + \mu_4 \tau^4 H_{z^3} \left(Z^{[1]}\right)^2 Z^{[2]} + \nu_4 \tau^4 H_{z^2} \left(Z^{[2]}\right)^2 \\ & + \lambda_6 \tau^6 H_{z^6} \left(Z^{[1]}\right)^6 + \mu_6 \tau^6 H_{z^5} \left(Z^{[1]}\right)^4 Z^{[2]} + \nu_6 \tau^6 H_{z^4} \left(Z^{[1]}\right)^2 \left(Z^{[2]}\right)^2 + \cdots \\ & + \cdots \\ & + \lambda_{2k} \tau^{2k} H_{z^{2k}} \left(Z^{[1]}\right)^{2k} + \mu_{2k} \tau^{2k} H_{z^{2k-1}} \left(Z^{[1]}\right)^{2k-2} Z^{[2]} \\ & + \nu_{2k} \tau^{2k} H_{z^{2k-2}} \left(Z^{[1]}\right)^{2k-4} \left(Z^{[2]}\right)^2 + \cdots \\ & + \cdots , \end{aligned} \tag{17}$$

then

$$\sum_{s=0}^{+\infty} \lambda_{2s} \tau^{2s} = \frac{\tau}{e^{\tau/2} - e^{-\tau/2}}, \tag{18}$$

$$\sum_{s=0}^{+\infty} \mu_{2s} \tau^{2s} = -\frac{\tau^2}{12} + \frac{\tau^3}{4\left(e^{\tau/2} - e^{-\tau/2}\right)} + \frac{\tau^3}{\left(e^{\tau/2} - e^{-\tau/2}\right)^3} - \frac{\tau^2 \left(e^{\tau/2} + e^{-\tau/2}\right)}{2\left(e^{\tau/2} - e^{-\tau/2}\right)^2}, \tag{19}$$

and

$$\sum_{s=0}^{+\infty} \nu_{2s}\tau^{2s} = \frac{\tau^5}{32\left(e^{\tau/2}-e^{-\tau/2}\right)} + \frac{3\tau^5}{4\left(e^{\tau/2}-e^{-\tau/2}\right)^3} - \frac{\tau^4\left(e^{\tau/2}+e^{-\tau/2}\right)}{8\left(e^{\tau/2}-e^{-\tau/2}\right)^2} + \frac{3\tau^5}{\left(e^{\tau/2}-e^{-\tau/2}\right)^5} - \frac{3\tau^4\left(e^{\tau/2}+e^{-\tau/2}\right)}{2\left(e^{\tau/2}-e^{-\tau/2}\right)^4}. \tag{20}$$

PROOF OF THEOREM 2. We can write out

$$\begin{aligned}
&\tau\tilde{Z}^{[1]} + \frac{\tau^3}{3!}\tilde{Z}^{[3]} + \frac{\tau^5}{5!}\tilde{Z}^{[5]} + \cdots + \frac{\tau^{2k-1}}{(2k-1)!}\tilde{Z}^{[2k-1]} + \frac{\tau^{2k+1}}{(2k+1)!}\tilde{Z}^{[2k+1]} + \cdots \\
&= \tau Z^{[1]} + \frac{\tau^3}{3!}Z^{[1]}_{z^2}\left(Z^{[1]}\right)^2 + \frac{\tau^5}{5!}Z^{[1]}_{z^4}\left(Z^{[1]}\right)^4 + \cdots \\
&+ \frac{\tau^{2k-1}}{(2k-1)!}Z^{[1]}_{z^{2k-2}}\left(Z^{[1]}\right)^{2k-2} + \frac{\tau^{2k+1}}{(2k+1)!}Z^{[1]}_{z^{2k}}\left(Z^{[1]}\right)^{2k} + \cdots \\
&+ \tau^3\lambda_2 Z^{[1]}_{z^2}\left(Z^{[1]}\right)^2 + \frac{\tau^5}{3!}\lambda_2 Z^{[1]}_{z^4}\left(Z^{[1]}\right)^4 + \cdots \\
&+ \frac{\tau^{2k+1}}{(2k-1)!}\lambda_2 Z^{[1]}_{z^{2k}}\left(Z^{[1]}\right)^{2k} + \frac{\tau^{2k+3}}{(2k+1)!}\lambda_2 Z^{[1]}_{z^{2k+2}}\left(Z^{[1]}\right)^{2k+2} + \cdots \\
&+ \tau^5\lambda_4 Z^{[1]}_{z^4}\left(Z^{[1]}\right)^4 + \frac{\tau^7}{3!}\lambda_4 Z^{[1]}_{z^6}\left(Z^{[1]}\right)^6 + \cdots \\
&+ \frac{\tau^{2k+3}}{(2k-1)!}\lambda_4 Z^{[1]}_{z^{2k+2}}\left(Z^{[1]}\right)^{2k+2} + \frac{\tau^{2k+5}}{(2k+1)!}\lambda_4 Z^{[1]}_{z^{2k+4}}\left(Z^{[1]}\right)^{2k+4} + \cdots \\
&+ \cdots \\
&+ \tau^{1+2r}\lambda_{2r} Z^{[1]}_{z^{2r}}\left(Z^{[1]}\right)^{2r} + \frac{\tau^{3+2r}}{3!}\lambda_{2r} Z^{[1]}_{z^{2+2r}}\left(Z^{[1]}\right)^{2+2r} + \cdots \\
&+ \frac{\tau^{2k-1+2r}}{(2k-1)!}\lambda_{2r} Z^{[1]}_{z^{2k-2+2r}}\left(Z^{[1]}\right)^{2k-2+2r} + \frac{\tau^{2k+1+2r}}{(2k+1)!}\lambda_{2r} Z^{[1]}_{z^{2k+2r}}\left(Z^{[1]}\right)^{2k+2r} + \cdots \\
&+ \cdots .
\end{aligned} \tag{21}$$

And, it is easily shown that in the expansion of R_{k+1} in (4), the term $Z^{[1]}_{z^k}(Z^{[1]})^k$ has coefficient $\tau^{k+1}/k!2^k$.

Thus, we have

$$\sum_{r=0}^{+\infty} \frac{\tau^{2r+1}}{(2r)!2^{2r}} = \sum_{r=0}^{+\infty} \frac{\tau^{2r+1}}{(2r+1)!} \sum_{s=0}^{+\infty} \lambda_{2s}\tau^{2s}, \tag{22}$$

i.e.,

$$\frac{\tau}{2}\left\{e^{\tau/2}+e^{-\tau/2}\right\} = \frac{1}{2}\left\{e^{\tau}-e^{-\tau}\right\}\sum_{s=0}^{+\infty}\lambda_{2s}\tau^{2s}. \tag{23}$$

So we obtain (18). Similarly, and a little more tediously, one can get (19) and (20). ∎

THEOREM 3. *With the notation above, we have the following inequalities:* $|\lambda_{2l}| \le |\delta_{2l}|$ *for* $l = 1, 2, \ldots$; $|\mu_{2l}| \le |\delta_{2l}|$ *and* $|\nu_{2l}| \le \rho^l|\delta_{2l}|$ *for* $l = 2, 3, \ldots$. *Here* $\rho = 1.2416154923235787$.

PROOF OF THEOREM 3. From (18) we have

$$\left\{\sum_{s=0}^{+\infty}\lambda_{2s}\tau^{2s}\right\}\left\{\sum_{r=0}^{+\infty}\frac{\tau^{2r}}{(2r+1)!2^{2r}}\right\} = 1, \tag{24}$$

so

$$\lambda_0 = 1; \tag{25.0}$$

$$\lambda_2 = -\frac{1}{24}; \tag{25.1}$$

$$\sum_{r=0}^{l+1} \frac{\lambda_{2(l+1-r)}}{(2r+1)!2^{2r}} = 0, \qquad l \geq 1. \tag{25.2}$$

If we set

$$\bar{\lambda}_0 = \lambda_0 = 1; \tag{26.0}$$

$$\bar{\lambda}_{2s} = \frac{\lambda_{2s}}{|\delta_{2s}|} = \lambda_{2s} \cdot 2^{2s+1}(2s+1), \qquad s = 1, 2, \dots, \tag{26.1}$$

then from (25.1), (26.0), and (26.1) we have

$$\bar{\lambda}_0 = 1; \tag{27.0}$$

$$\bar{\lambda}_2 = -1; \tag{27.1}$$

and for $l \geq 1$,

$$\bar{\lambda}_{2(l+1)} = -\frac{2}{(2l+2)!}\,\bar{\lambda}_0 - \sum_{r=1}^{l} \frac{2l+3}{(2r+1)\,[2(l-r)+3]!}\,\bar{\lambda}_{2r}. \tag{27.2}$$

If $|\lambda_{2s}| \leq |\delta_{2s}| = 1/(2^{2s+1} \times (2s+1))$, i.e., $|\bar{\lambda}_{2s}| \leq 1$ for $s = 1, 2, \dots, l$, then from (27.2) for $l \geq 1$,

$$|\bar{\lambda}_{2(l+1)}| \leq \frac{2}{(2l+2)!} + \frac{2l+3}{3(2l+1)!} + \cdots + \frac{2l+3}{(2r+1)\,[2(l-r)+3]!} + \cdots + \frac{2l+3}{(2l+1)3!} \equiv \Theta_l. \tag{28}$$

It is readily proven that $\{\Theta_l\}_1^{+\infty}$ monotonically decreases to $(1/2)\,[(e-e^{-1})-2]$ as l increases to $+\infty$. And, $(1/2)\,[(e-e^{-1})-2] = 0.1752011936438016$. Thus,

$$|\lambda_{2(l+1)}| \leq |\delta_{2(l+1)}|, \qquad l = 0, 1, \dots. \tag{29}$$

From (19), we have

$$\left\{\sum_{s=2}^{+\infty} \mu_{2s}\tau^{2s}\right\}\left\{\sum_{r=1}^{+\infty} \frac{3^{2r+1}-3}{(2r+1)!2^{2r+1}}\,\tau^{2r}\right\} = \frac{\tau^2}{4}\left\{\sum_{r=1}^{+\infty} \frac{(2r-1)2^{2r+1}-3^{2r}+1}{(2r+1)!2^{2r+1}}\,\tau^{2r}\right\}, \tag{30}$$

so

$$\mu_4 = \frac{1}{480}; \tag{31.2}$$

$$\sum_{r=1}^{l} \mu_{2(l+2-r)}\,\frac{3^{2r+1}-3}{(2r+1)!2^{2r+1}} = \frac{(2l+1)2^{2l+3}-3^{2(l+1)}+1}{(2l+3)!2^{2l+5}}, \qquad l \geq 1. \tag{31.3}$$

If we set

$$\bar{\mu}_{2s} = \frac{\mu_{2s}}{|\delta_{2s}|} = \mu_{2s} \cdot 2^{2s+1}(2s+1), \qquad s = 2, 3, \dots, \tag{32}$$

then from (31.2), (31.3), and (32) we have

$$\bar{\mu}_4 = \frac{1}{3}; \tag{33.2}$$

and for $l \geq 2$,

$$\bar{\mu}_{2(l+1)} = \frac{(2l+1)2^{2l+3}-3^{2(l+1)}+1}{2(2l+2)!} - \sum_{r=2}^{l} \frac{(2l+3)\left[3^{2(l-r)+5}-3\right]}{2^2(2r+1)[2(l-r)+5]!}\,\bar{\mu}_{2r}. \tag{33.3}$$

If $|\mu_{2s}| \leq |\delta_{2s}| = 1/(2^{2s+1} \times (2s+1))$, i.e., $|\bar{\mu}_{2s}| \leq 1$ for $s = 2, 3, \dots, l$, then from (33.3) for $l \geq 2$,

$$\begin{aligned} |\bar{\mu}_{2(l+1)}| \leq {} & \frac{(2l+1)2^{2l+3}+3^{2(l+1)}-1}{2(2l+2)!} + \frac{(2l+3)\left(3^{2l+1}-3\right)}{2^2 \cdot 5(2l+1)!} + \cdots \\ & + \frac{(2l+3)\left[3^{2(l-r)+5}-3\right]}{2^2(2r+1)[2(l-r)+5]!} + \cdots + \frac{(2l+3)\left(3^5-3\right)}{2^2(2l+1)5!} \equiv \Phi_l. \end{aligned} \tag{34}$$

It is readily proven that $\{\Phi_l\}_2^{+\infty}$ monotonically decreases to $(1/8)\left[(e-e^{-1})^3-8\right]$ as l increases to $+\infty$. And, $(1/8)\left[(e-e^{-1})^3-8\right]=0.6230678366196249$. Thus,

$$\left|\mu_{2(l+1)}\right| \le \left|\delta_{2(l+1)}\right|, \qquad l=1,2,\dots. \tag{35}$$

From (20), we have

$$\begin{aligned}&\left\{\sum_{s=2}^{+\infty}\nu_{2s}\tau^{2s}\right\}\left\{\sum_{r=2}^{+\infty}\frac{5^{2r+1}-5\cdot 3^{2r+1}+10}{(2r+1)!2^{2r+1}}\tau^{2r}\right\}\\ &=\frac{\tau^4}{32}\left\{\sum_{r=1}^{+\infty}\frac{2^{2r}(2r-7)+20(2r-1)}{(2r+1)!}\tau^{2r}\right\},\end{aligned} \tag{36}$$

so

$$\nu_4=\frac{1}{160}; \tag{37.2}$$

$$\sum_{r=2}^{l+1}\nu_{2(l+3-r)}P_{2r}=\frac{1}{32}Q_{2(l+1)}, \qquad l\ge 1, \tag{37.3}$$

where $P_{2r}=(5^{2r+1}-5\cdot 3^{2r+1}+10)/((2r+1)!2^{2r+1})$, $Q_{2r}=(2^{2r}(2r-7)+20(2r-1))/(2r+1)!$ for $r\ge 2$.

If we set

$$\bar{\nu}_{2s}=\frac{\nu_{2s}}{|\delta_{2s}|}=\nu_{2s}\cdot 2^{2s+1}(2s+1), \qquad s=2,3,\dots, \tag{38}$$

then, from (37.2), (37.3), and (38), we have

$$\bar{\nu}_4=1; \tag{39.2}$$

and, for $l\ge 2$,

$$\bar{\nu}_{2(l+1)}=\frac{(2l-5)2^{4l+1}+10(2l+1)2^{2l}}{(2l+2)!}-\sum_{r=2}^{l}\frac{(2l+3)\left[5^{2(l-r)+7}-5\cdot 3^{2(l-r)+7}+10\right]}{2^4(2r+1)\left[2(l-r)+7\right]!}\bar{\nu}_{2r}. \tag{39.3}$$

If $|\nu_{2s}|\le\rho^s|\delta_{2s}|=\rho^s/(2^{2s+1}\times(2s+1))$, i.e., $|\bar{\nu}_{2s}|\le\rho^s$ (where $\rho=(1/32)\left[(e-e^{-1})^5-32\right]=1.2416154923235787$) for $s=2,3,\dots,l$, then from (39.3) for $l\ge 2$,

$$\begin{aligned}\left|\bar{\nu}_{2(l+1)}\right|\le{}&\frac{(2l-5)2^{4l+1}+10(2l+1)2^{2l}}{(2l+2)!}\rho^l+\frac{(2l+3)\left[5^{2l+3}-5\cdot 3^{2l+3}+10\right]}{2^4\cdot 5(2l+3)!}\rho^l\\ &+\dots+\frac{(2l+3)\left[5^{2(l-r)+7}-5\cdot 3^{2(l-r)+7}+10\right]}{2^4(2r+1)\left[2(l-r)+7\right]!}\rho^l\\ &+\dots+\frac{(2l+3)\left(5^7-5\cdot 3^7+10\right)}{2^4(2l+1)7!}\rho^l\equiv\rho^l\Psi_l.\end{aligned} \tag{40}$$

It is readily proven that $\{\Psi_l\}_2^{+\infty}$ monotonically decreases to ρ as l increases to $+\infty$. Thus,

$$\left|\nu_{2(l+1)}\right|\le\rho^{l+1}\left|\delta_{2(l+1)}\right|, \qquad l=1,2,\dots. \tag{41}$$ ∎

REMARK 2. From (24), we have

$$\sum_{s=0}^{+\infty}(-1)^s\lambda_{2s}\tau^{2s}=\frac{\tau}{2\sin(\tau/2)}=\Pi_{r=1}^{+\infty}\frac{1}{1-(\tau^2/(4\pi^2r^2))}, \tag{42}$$

so $\sum_{s=0}^{\infty}\lambda_{2s}\tau^{2s}$ is an alternating series, i.e., $\lambda_0>0,\lambda_2<0,\dots,\lambda_{4k}>0,\lambda_{4k+2}<0,\dots$. Furthermore, according to the recursive relations (27.2), (33.3), and (39.3), the numerical calculation shows that the sequences of the beginning finite terms (at least 320 terms) of $\{\bar{\lambda}_{2s}\}_1^{+\infty}$, $\{\bar{\mu}_{2s}\}_2^{+\infty}$ and $\{\bar{\nu}_{2s}\}_2^{+\infty}$ are alternating, and monotonically and rapidly decrease to 0 as $s\to+\infty$, respectively. Unfortunately, we are not yet able to prove this strictly. This is an open problem.

4. ESTIMATE OF THE DIFFERENCE BETWEEN FORMAL ENERGY AND ORIGINAL HAMILTONIAN—A NOTE ON CONVERGENCE OF FORMAL ENERGY OF MID-POINT RULE

Theorems 1–3 and Remark 2 confirm to some extent the Conjecture (*the maximum absolute value of the coefficients of the terms in* τ^{2k} *is exactly* $1/(2^{2k+1} \times (2k+1))$) mentioned in Section 1. If this conjecture is true, even if only "*the maximum absolute value of the coefficients of the terms in* τ^{2k} *is less than* $\eta\sigma^{2k}$ *for some constants* $\eta \geq 1$, $\sigma > 0$ *and for any* $k \geq 1$", and the Hamiltonian H is sufficiently smooth and bounded in some domain Ω, i.e., there exists some constant $B > 0$, such that

$$\left|H_{z_{t_1}\cdots z_{t_j}}\right| = \left|\frac{\partial^j H}{\partial z_{t_1} \dots \partial z_{t_j}}\right| \leq B, \tag{43}$$

(here, z_{t_u} stands for the t_u-component of the $2n$-dim vector Z) for $Z \in O(\bullet, r^{2n}) \subset \Omega$, and $j \geq 0$ and $1 \leq t_1, \dots, t_j \leq 2n$, then, in the expansion (like (3.1)–(3.3)) of H_{2k} in formal energy (3), the absolute value of every single term is not greater than $\eta\sigma^{2k}B(2nB)^{2k}$, $k = 0, 1, 2, \dots$, and according to (11)

$$|H_{2k}| \leq 3^{2k+1}\eta\sigma^{2k}B(2nB)^{2k} = Ew^{2k}, \qquad k = 0, 1, 2, \dots, \tag{44}$$

where $E = 3\eta B$, $w = 6n\sigma B$.

Thus, we have the following.

THEOREM 4. *With condition (43), if the step size* τ *is sufficiently small, and in the tree-expansion of (3) the absolute values of the coefficients of the terms in* τ^{2k} *are uniformly bounded by* $\eta\sigma^{2k}$ *for some constants* $\eta \geq 1$, $\sigma > 0$ *and for any* $k \geq 1$, *then for the mid-point rule (2), we have the estimate:*

$$\left|\tilde{H} - H\right| \leq E\,\frac{(w\tau)^2}{1 - (w\tau)^2} \leq D_2\tau^2. \tag{45}$$

where D_2 *depends only on the Hamiltonian* H.

5. CONCLUSIONS AND FURTHER WORK

We have studied the tree-expansion for the formal energy of the fixed step size mid-point rule, and obtained the formulae and estimates for the coefficients of terms of four special types. With some assumptions on the smoothness of the Hamiltonian H and on the size of the coefficients of the terms in the tree-expansion, we have given an estimate of the difference between the formal energy and the original Hamiltonian, which implies the convergence of the formal energy $\tilde{H}$. Of course, our reasoning is incomplete because we could not deal with all the terms in the tree-expansion. So there is still much to be done. We hope this could be a starting point for the study of the convergence of the formal energies of the symplectic methods. Obviously, the techniques used here are also suitable for the coefficients of the terms of other types in the tree-expansion of the formal energy of the mid-point rule, and possibly suitable for that of other symplectic one-step methods.

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