Journal of Computational Mathematics, Vol.20, No.1, 2002, 89–96.

A NOTE ON THE CONSTRUCTION OF SYMPLECTIC SCHEMES FOR SPLITABLE HAMILTONIAN $H = H^{(1)} + H^{(2)} + H^{(3)}$ *1)

Yi-fa Tang

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

Abstract

In this note, we will give a proof for the uniqueness of 4th-order time-reversible symplectic difference schemes of 13th-fold compositions of phase flows $\phi^t_{H^{(1)}}, \phi^t_{H^{(2)}}, \phi^t_{H^{(3)}}$ with different temporal parameters for splitable hamiltonian $H = H^{(1)} + H^{(2)} + H^{(3)}$.

Key words: Time-Reversible symplectic scheme, Splitable hamiltonian.

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, the *symplectic* difference schemes should be exclusively employed to integrate it [1, 2]. One can get this kind of schemes of any high order, however the high-order derivatives of the hamiltonian H must be used or a system of high-order algebraic equations must be solved [2]–[4], and usually the symplectic schemes are implicit, unless the hamiltonian H is special, say, variable-separable [1, 2, 5], symplectically separable (nilpotent) [6] or splitable (we call a hamiltonian *splitable* if it can be split into several parts, and each part can be explicitly integrated) [7]–[9]. On the other hand, people have already utilized the technique of composing lower-order symplectic scheme for several times with different stepsizes to get higher-order one [7]–[10]. Comparatively, this is an economic and practical way, especially, when the hamiltonian is splitable [11]–[16].

For a splitable hamiltonian[11]–[16]

$$H(p,q) = H^{(1)}(p,q) + H^{(2)}(p,q) + H^{(3)}(p,q), \quad p,q \in R^n, \tag{2}$$

if ϕ^t_1, ϕ^t_2, ϕ^t_3 are the phase flows of $H^{(1)}(p,q)$, $H^{(2)}(p,q)$, $H^{(3)}(p,q)$ respectively, the following schemes **S1** and **S2** are symplectic difference schemes of order 1 and 2 respectively [7]–[9]:

Scheme 1 (S1): 1st-order symplectic scheme

$$\widetilde{Z} = \Phi^t(Z) = \phi^t_3 \circ \phi^t_2 \circ \phi^t_1(Z), \tag{3}$$

Scheme 2 (S2): 2nd-order symplectic scheme

$$\widetilde{Z} = \Psi^t(Z) = \phi_1^{\frac{t}{2}} \circ \phi_2^{\frac{t}{2}} \circ \phi_3^{t} \circ \phi_2^{\frac{t}{2}} \circ \phi_1^{\frac{t}{2}}(Z). \tag{4}$$

* Received Novermber 1, 1999.

1)This research is partially support by Special Funds for Major State Basic Research Projects of China (No. G1999032801-10 and No. G19999032804), and by the knowledge innovation program of the Chinese Academy of Sciences and a grant (No. 19801034) from National Natural Sciences Foundation of China.

Explicitly, scheme **S2** is time-reversible (a scheme G^τ is said to be *time-reversible* if $G^{-\tau} \circ G^\tau = identity$[17]–[19]).

We have known that via multi-fold composition (with different parameters) of a time-reversible symplectic scheme (**RESS**), one can get a higher-order **RESS**. Precisely for instance, if ϕ^t is a 2nd-order **RESS** for Hamiltonian H, then $\phi^{\beta t} \circ \phi^{\alpha t} \circ \phi^{\beta t}$ is a 4th-order **RESS** for Hamiltonian H, here $\alpha = \frac{-\sqrt[3]{2}}{2-\sqrt[3]{2}}$, $\beta = \frac{1}{2-\sqrt[3]{2}}$. We have known on the other hand, if ϕ^t and ψ^t are the phase flows of Hamiltonians $H^{(1)}$ and $H^{(2)}$ respectively, then $\psi^{\frac{t}{2}} \circ \phi^t \circ \psi^{\frac{t}{2}}$ is a 2nd-order **RESS** for Hamiltonian $H = H^{(1)} + H^{(2)}$. Therefore

$$\begin{aligned}&\psi^{\frac{\beta t}{2}} \circ \phi^{\beta t} \circ \psi^{\frac{\beta t}{2}} \circ \psi^{\frac{\alpha t}{2}} \circ \phi^{\alpha t} \circ \psi^{\frac{\alpha t}{2}} \circ \psi^{\frac{\beta t}{2}} \circ \phi^{\beta t} \circ \psi^{\frac{\beta t}{2}} \\ &= \psi^{\frac{\beta t}{2}} \circ \phi^{\beta t} \circ \psi^{\frac{\gamma t}{2}} \circ \phi^{\alpha t} \circ \psi^{\frac{\gamma t}{2}} \circ \phi^{\beta t} \circ \psi^{\frac{\beta t}{2}}\end{aligned} \tag{5}$$

(here $\gamma = \alpha + \beta = \frac{1-\sqrt[3]{2}}{2-\sqrt[3]{2}}$) is a 4-order **RESS** for Hamiltonian $H = H^{(1)} + H^{(2)}$ [7]–[9]. Conversely, it is easy to prove (see *Corollary 1* in the *Proof of Theorem* later): if $\psi^{\lambda t} \circ \phi^{\mu t} \circ \psi^{\nu t} \circ \phi^{\delta t} \circ \psi^{\nu t} \circ \phi^{\mu t} \circ \psi^{\lambda t}$ (ϕ^t and ψ^t are the phase flows of Hamiltonians $H^{(1)}$ and $H^{(2)}$ respectively) is a 4th-order **RESS** for Hamiltonian $H = H^{(1)} + H^{(2)}$, then $\lambda = \frac{1}{2(2-\sqrt[3]{2})}$, $\mu = \frac{1}{2-\sqrt[3]{2}}$, $\nu = \frac{1-\sqrt[3]{2}}{2(2-\sqrt[3]{2})}$, $\delta = \frac{-\sqrt[3]{2}}{2-\sqrt[3]{2}}$.

Similarly, we know: if ϕ_1^t, ϕ_2^t and ϕ_3^t are the phase flows of Hamiltonians $H^{(1)}$, $H^{(2)}$ and $H^{(3)}$ respectively, then $\phi_1^{\frac{t}{2}} \circ \phi_2^{\frac{t}{2}} \circ \phi_3^t \circ \phi_2^{\frac{t}{2}} \circ \phi_1^{\frac{t}{2}}$ is a 2nd-order **RESS** for Hamiltonian $H = H^{(1)} + H^{(2)} + H^{(3)}$. Therefore,

$$\begin{aligned}&\phi_1^{\frac{\beta t}{2}} \circ \phi_2^{\frac{\beta t}{2}} \circ \phi_3^{\beta t} \circ \phi_2^{\frac{\beta t}{2}} \circ \phi_1^{\frac{\beta t}{2}} \circ \phi_1^{\frac{\alpha t}{2}} \circ \phi_2^{\frac{\alpha t}{2}} \circ \phi_3^{\alpha t} \circ \phi_2^{\frac{\alpha t}{2}} \circ \phi_1^{\frac{\alpha t}{2}} \circ \phi_1^{\frac{\beta t}{2}} \circ \phi_2^{\frac{\beta t}{2}} \circ \phi_3^{\beta t} \circ \phi_2^{\frac{\beta t}{2}} \circ \phi_1^{\frac{\beta t}{2}} \\ &= \phi_1^{\frac{\beta t}{2}} \circ \phi_2^{\frac{\beta t}{2}} \circ \phi_3^{\beta t} \circ \phi_2^{\frac{\beta t}{2}} \circ \phi_1^{\frac{\gamma t}{2}} \circ \phi_2^{\frac{\alpha t}{2}} \circ \phi_3^{\alpha t} \circ \phi_2^{\frac{\alpha t}{2}} \circ \phi_1^{\frac{\gamma t}{2}} \circ \phi_2^{\frac{\beta t}{2}} \circ \phi_3^{\beta t} \circ \phi_2^{\frac{\beta t}{2}} \circ \phi_1^{\frac{\beta t}{2}}\end{aligned} \tag{6}$$

(here $\gamma = \alpha + \beta = \frac{1-\sqrt[3]{2}}{2-\sqrt[3]{2}}$) is a 4th-order **RESS** for Hamiltonian $H = H^{(1)} + H^{(2)} + H^{(3)}$ [7, 8].

But *how about the converse proposition? Is it true?* That's just what we are to answer. For this purpose we establish the following theorem:

Theorem 1. *If*

$$\widetilde{Z} = \Theta^t(Z) = \phi_{n_7}^{\delta t} \circ \phi_{n_6}^{\alpha t} \circ \phi_{n_5}^{\beta t} \circ \phi_{n_4}^{\gamma t} \circ \phi_{n_3}^{\lambda t} \circ \phi_{n_2}^{\mu t} \circ \phi_{n_1}^{\nu t} \circ \phi_{n_4}^{\mu t} \circ \phi_{n_3}^{\lambda t} \circ \phi_{n_4}^{\gamma t} \circ \phi_{n_5}^{\beta t} \circ \phi_{n_6}^{\alpha t} \circ \phi_{n_7}^{\delta t}(Z) \tag{7}$$

where $n_1, n_2, n_3, n_4, n_5, n_6, n_7 \in \{1, 2, 3\}$ *and any two neighbouring numbers are different, is a 4th-order* **RESS** *for Hamiltonian* $H = H^{(1)} + H^{(2)} + H^{(3)}$, *then* $\delta = \alpha = \gamma = \frac{1}{2(2-\sqrt[3]{2})}$, $\beta = \frac{1}{2-\sqrt[3]{2}}$, $\lambda = \frac{1-\sqrt[3]{2}}{2(2-\sqrt[3]{2})}$, $\mu = \frac{-\sqrt[3]{2}}{2(2-\sqrt[3]{2})}$, $\nu = \frac{-\sqrt[3]{2}}{2-\sqrt[3]{2}}$. *That is to say,* Θ^t *is actually 3-fold composition of* Ψ^t *with different coefficients:* $\Theta^t = \Psi^{\kappa_2 t} \circ \Psi^{\kappa_1 t} \circ \Psi^{\kappa_2 t}$ *with* $\kappa_1 = \frac{-\sqrt[3]{2}}{2-\sqrt[3]{2}}$ *and* $\kappa_2 = \frac{1}{2-\sqrt[3]{2}}$.

For the proof of Theorem 1, at first let's prepare something.

If ϕ_2^t, ϕ_3^t are the phase flows of hamiltonian $H^{(2)}$, $H^{(3)}$ respectively, then we can write the following expansion:

$$\begin{aligned}&\phi_3^{\beta t} \circ \phi_2^{\gamma t} \circ \phi_3^{\lambda t} \circ \phi_2^{\mu t} \circ \phi_3^{\nu t} \circ \phi_2^{\mu t} \circ \phi_3^{\lambda t} \circ \phi_2^{\gamma t} \circ \phi_3^{\beta t} \\ &= I + tJ\nabla\{2(\gamma+\mu)H^{(2)} + (2\beta + 2\lambda + \nu)H^{(3)}\} \\ &\quad + \frac{t^2}{2} J\{2(\gamma+\mu)H^{(2)} + (2\beta + 2\lambda + \nu)H^{(3)}\}_{zz} J\nabla\{2(\gamma+\mu)H^{(2)} + (2\beta + 2\lambda + \nu)H^{(3)}\} \\ &\quad + \frac{4(\gamma+\mu)^3}{3} t^3 J[\nabla H^{(2)}]_{zz}[J\nabla H^{(2)}]^2\end{aligned}$$

$$
\begin{aligned}
&+ \frac{(\gamma+\mu)[2\beta^2+(2\lambda+\nu)(2\beta+2\lambda+\nu)]-2\lambda\mu(\lambda+\nu)}{2} t^3 J[\nabla H^{(2)}]_{zz}[J\nabla H^{(3)}]^2 \\
&+ \frac{(\gamma+\mu)^2(4\beta+2\lambda+\nu)+2\lambda\mu^2}{2} t^3 J[\nabla H^{(3)}]_{zz}[J\nabla H^{(2)}]^2 \\
&+ \frac{(2\beta+2\lambda+\nu)^3}{6} t^3 J[\nabla H^{(3)}]_{zz}[J\nabla H^{(3)}]^2 \\
&+ \frac{(\gamma+\mu)^2(4\beta+6\lambda+3\nu)-2\lambda\mu^2}{2} t^3 J[\nabla H^{(2)}]_{zz}[J\nabla H^{(2)}][J\nabla H^{(3)}] \\
&+ \frac{(\gamma+\mu)[6\beta^2+(2\lambda+\nu)(6\beta+2\lambda+\nu)]+2\lambda\mu(\lambda+\nu)}{2} t^3 J[\nabla H^{(3)}]_{zz}[J\nabla H^{(2)}][J\nabla H^{(3)}] \\
&+ \frac{4(\gamma+\mu)^3}{3} t^3 JH^{(2)}_{zz} JH^{(2)}_{zz} J\nabla H^{(2)} \\
&+ \frac{(\gamma+\mu)^2(4\beta+2\lambda+\nu)+2\lambda\mu^2}{2} t^3 JH^{(2)}_{zz} JH^{(2)}_{zz} J\nabla H^{(3)} \\
&+ [(\gamma+\mu)^2(2\lambda+\nu)-2\lambda\mu^2] t^3 JH^{(2)}_{zz} JH^{(3)}_{zz} J\nabla H^{(2)} \\
&+ \frac{(\gamma+\mu)[2\beta^2+(2\lambda+\nu)(2\beta+2\lambda+\nu)]-2\lambda\mu(\lambda+\nu)}{2} t^3 JH^{(2)}_{zz} JH^{(3)}_{zz} J\nabla H^{(3)} \\
&+ \frac{(\gamma+\mu)^2(4\beta+2\lambda+\nu)+2\lambda\mu^2}{2} t^3 JH^{(3)}_{zz} JH^{(2)}_{zz} J\nabla H^{(2)} \\
&+ [2\lambda\mu(\lambda+\nu)+2\beta(\gamma+\mu)(\beta+2\lambda+\nu)] t^3 JH^{(3)}_{zz} JH^{(2)}_{zz} J\nabla H^{(3)} \\
&+ \frac{(\gamma+\mu)[2\beta^2+(2\lambda+\nu)(2\beta+2\lambda+\nu)]-2\lambda\mu(\lambda+\nu)}{2} t^3 JH^{(3)}_{zz} JH^{(3)}_{zz} J\nabla H^{(2)} \\
&+ \frac{(2\beta+2\lambda+\nu)^3}{6} t^3 JH^{(3)}_{zz} JH^{(3)}_{zz} J\nabla H^{(3)}.
\end{aligned} \tag{8}
$$

For the notation, we set

$$JH^{(u)}_{zz} J\nabla H^{(v_1)} = J \sum_{j_1=1}^{2n} \frac{\partial[\nabla H^{(u)}]}{\partial z_{j_1}} [J\nabla H^{(v_1)}]_{(j_1)}$$

and

$$J[\nabla H^{(u)}]_{zz}[J\nabla H^{(v_1)}][J\nabla H^{(v_2)}] = J \sum_{j_1,j_2=1}^{2n} \frac{\partial^2[\nabla H^{(u)}]}{\partial z_{j_1}\partial z_{j_2}} [J\nabla H^{(v_1)}]_{(j_1)}[J\nabla H^{(v_2)}]_{(j_2)}$$

where $u, v_1, v_2 \in \{1,2,3\}$, z_{j_w} is the j_w-th component of $2n$-dim vector Z, and $[J\nabla H^{(v_w)}]_{(j_w)}$ stands for the j_w-th component of $2n$-dim vector $[J\nabla H^{(v_w)}]$, $w = 1, 2$.

Lemma 1. RESS

$$\widetilde{Z} = \phi^{\beta t}_{n_1} \circ \phi^{\gamma t}_{n_2} \circ \phi^{\lambda t}_{n_1} \circ \phi^{\mu t}_{n_2} \circ \phi^{\nu t}_{n_1} \circ \phi^{\mu t}_{n_2} \circ \phi^{\lambda t}_{n_1} \circ \phi^{\gamma t}_{n_2} \circ \phi^{\beta t}_{n_1}(Z) \tag{9}$$

is of at least order 4 *for* $H^{(n_1)} + H^{(n_2)}$ *iff*

$$\begin{cases} \gamma+\mu = \frac{1}{2}, & 2\beta+2\lambda+\nu = 1, \\ \frac{1}{2}\beta + 2\lambda\mu^2 = \frac{1}{12}, & \beta^2-\beta-2\lambda\mu(\lambda+\nu) = -\frac{1}{6}. \end{cases} \tag{10}$$

Proof. We can get (10), after observing (8).

Corollary 1. RESS

$$\widetilde{Z} = \phi^{\gamma t}_{n_2} \circ \phi^{\lambda t}_{n_1} \circ \phi^{\mu t}_{n_2} \circ \phi^{\nu t}_{n_1} \circ \phi^{\mu t}_{n_2} \circ \phi^{\lambda t}_{n_1} \circ \phi^{\gamma t}_{n_2}(Z) \tag{11}$$

is of order 4 *for* $H^{(n_1)} + H^{(n_2)}$ *iff*

$$\begin{cases} \gamma = \frac{1}{2(2-\sqrt[3]{2})}, & \lambda = \frac{1}{2-\sqrt[3]{2}}, \\ \mu = \frac{1-\sqrt[3]{2}}{2(2-\sqrt[3]{2})}, & \nu = \frac{-\sqrt[3]{2}}{2-\sqrt[3]{2}}. \end{cases} \tag{12}$$

Proof. Setting $\beta = 0$, solving (10), we obtain (12). On the other hand, if we set $\Omega^t(Z) = \phi_{n_2}^{\frac{t}{2}} \circ \phi_{n_1}^t \circ \phi_{n_2}^{\frac{t}{2}}(Z)$, then solution (12) means that $\widetilde{Z} = \Omega^{\lambda t} \circ \Omega^{\nu t} \circ \Omega^{\lambda t}(Z)$. From Corollary 1 in [20], we know (11) is exactly of order 4 for $H^{(n_1)} + H^{(n_2)}$.

Proof of Theorem 1

FIRST STEP:

Without lose of generality, we display all the 13th-fold compositions (for instance, $\{2,1,2,1,3,2,3,2,3,1,2,1,2\}$ stands for $\phi_2^{\delta t} \circ \phi_1^{\alpha t} \circ \phi_2^{\beta t} \circ \phi_1^{\gamma t} \circ \phi_3^{\lambda t} \circ \phi_2^{\mu t} \circ \phi_3^{\nu t} \circ \phi_2^{\mu t} \circ \phi_3^{\lambda t} \circ \phi_1^{\gamma t} \circ \phi_2^{\beta t} \circ \phi_1^{\alpha t} \circ \phi_2^{\delta t}$) as follows:

$\{2,1,2,1,3,2,3,2,3,1,2,1,2\}$; $\{3,1,2,1,3,2,3,2,3,1,2,1,3\}$ $(D1;\ D2)$

$\{1,3,2,1,3,2,3,2,3,1,2,3,1\}$; $\{2,3,2,1,3,2,3,2,3,1,2,3,2\}$ $(D3;\ D4)$

$\{2,1,3,1,3,2,3,2,3,1,3,1,2\}$; $\{3,1,3,1,3,2,3,2,3,1,3,1,3\}$ $(D5;\ D6)$

$\{1,2,3,1,3,2,3,2,3,1,3,2,1\}$; $\{3,2,3,1,3,2,3,2,3,1,3,2,3\}$ $(D7;\ D8)$

$\{1,2,1,2,3,2,3,2,3,2,1,2,1\}$; $\{3,2,1,2,3,2,3,2,3,2,1,2,3\}$ $(D9;\ D10)$

$\{1,3,1,2,3,2,3,2,3,2,1,3,1\}$; $\{2,3,1,2,3,2,3,2,3,2,1,3,2\}$ $(D11;\ D12)$

$\{2,1,3,2,3,2,3,2,3,2,3,1,2\}$; $\{3,1,3,2,3,2,3,2,3,2,3,1,3\}$ $(D13;\ D14)$

$\{1,2,3,2,3,2,3,2,3,2,3,2,1\}$; $\{3,2,3,2,3,2,3,2,3,2,3,2,3\}$ $(D15;\ D16)$

$\{1,2,1,2,1,2,3,2,1,2,1,2,1\}$; $\{3,2,1,2,1,2,3,2,1,2,1,2,3\}$ $(D17;\ D18)$

$\{1,3,1,2,1,2,3,2,1,2,1,3,1\}$; $\{2,3,1,2,1,2,3,2,1,2,1,3,2\}$ $(D19;\ D20)$

$\{2,1,3,2,1,2,3,2,1,2,3,1,2\}$; $\{3,1,3,2,1,2,3,2,1,2,3,1,3\}$ $(D21;\ D22)$

$\{1,2,3,2,1,2,3,2,1,2,3,2,1\}$; $\{3,2,3,2,1,2,3,2,1,2,3,2,3\}$ $(D23;\ D24)$

$\{1,2,1,3,1,2,3,2,1,3,1,2,1\}$; $\{3,2,1,3,1,2,3,2,1,3,1,2,3\}$ $(D25;\ D26)$

$\{1,3,1,3,1,2,3,2,1,3,1,3,1\}$; $\{2,3,1,3,1,2,3,2,1,3,1,3,2\}$ $(D27;\ D28)$

$\{2,1,2,3,1,2,3,2,1,3,2,1,2\}$; $\{3,1,2,3,1,2,3,2,1,3,2,1,3\}$ $(D29;\ D30)$

$\{1,3,2,3,1,2,3,2,1,3,2,3,1\}$; $\{2,3,2,3,1,2,3,2,1,3,2,3,2\}$ $(D31;\ D32)$

If (D1): $\{2,1,2,1,3,2,3,2,3,1,2,1,2\}$ is of order 4 for $H = H^{(1)} + H^{(2)} + H^{(3)}$, after removing the numbers "2" from sequence (D1) and merging the same neighbouring numbers, then we obtain a new sequence $\{1,3,1\}$ (standing for $\phi_1^{(\alpha+\gamma)t} \circ \phi_3^{(2\lambda+\nu)t} \circ \phi_1^{(\alpha+\gamma)t}$) should be of order 4 for $H = H^{(1)} + H^{(3)}$. However we know from Corollary 1 that this is impossible. So (D1) cannot be of order 4 for $H = H^{(1)} + H^{(2)} + H^{(3)}$, and it is deleted.

Similarly, (D2), (D4) *et al* are also deleted. We have (D3), (D7), (D21), (D23), (D25), (D29), (D30), (D31) as remainder (the corresponding composing parameters are below the numbers of the sequence respectively):

$$\begin{matrix}\{1, & 3, & 2, & 1, & 3, & 2, & 3, & 2, & 3, & 1, & 2, & 3, & 1\} \\ \{\delta, & \alpha, & \beta, & \gamma, & \lambda, & \mu, & \nu, & \mu, & \lambda, & \gamma, & \beta, & \alpha, & \delta\}\end{matrix} \tag{C3}$$

$$\begin{matrix}\{1, & 2, & 3, & 1, & 3, & 2, & 3, & 2, & 3, & 1, & 3, & 2, & 1\} \\ \{\delta, & \alpha, & \beta, & \gamma, & \lambda, & \mu, & \nu, & \mu, & \lambda, & \gamma, & \beta, & \alpha, & \delta\}\end{matrix} \tag{C7}$$

$$\begin{matrix}\{2, & 1, & 3, & 2, & 1, & 2, & 3, & 2, & 1, & 2, & 3, & 1, & 2\} \\ \{\delta, & \alpha, & \beta, & \gamma, & \lambda, & \mu, & \nu, & \mu, & \lambda, & \gamma, & \beta, & \alpha, & \delta\}\end{matrix} \tag{C21}$$

$$\begin{matrix}\{1, & 2, & 3, & 2, & 1, & 2, & 3, & 2, & 1, & 2, & 3, & 2, & 1\} \\ \{\delta, & \alpha, & \beta, & \gamma, & \lambda, & \mu, & \nu, & \mu, & \lambda, & \gamma, & \beta, & \alpha, & \delta\}\end{matrix} \tag{C23}$$

$$\begin{matrix}\{1, & 2, & 1, & 3, & 1, & 2, & 3, & 2, & 1, & 3, & 1, & 2, & 1\} \\ \{\delta, & \alpha, & \beta, & \gamma, & \lambda, & \mu, & \nu, & \mu, & \lambda, & \gamma, & \beta, & \alpha, & \delta\}\end{matrix} \tag{C25}$$

$$\begin{matrix}\{2, & 1, & 2, & 3, & 1, & 2, & 3, & 2, & 1, & 3, & 2, & 1, & 2\} \\ \{\delta, & \alpha, & \beta, & \gamma, & \lambda, & \mu, & \nu, & \mu, & \lambda, & \gamma, & \beta, & \alpha, & \delta\}\end{matrix} \tag{C29}$$

$$\begin{matrix}\{3, & 1, & 2, & 3, & 1, & 2, & 3, & 2, & 1, & 3, & 2, & 1, & 3\} \\ \{\delta, & \alpha, & \beta, & \gamma, & \lambda, & \mu, & \nu, & \mu, & \lambda, & \gamma, & \beta, & \alpha, & \delta\}\end{matrix} \tag{C30}$$

$$\begin{matrix}\{1, & 3, & 2, & 3, & 1, & 2, & 3, & 2, & 1, & 3, & 2, & 3, & 1\} \\ \{\delta, & \alpha, & \beta, & \gamma, & \lambda, & \mu, & \nu, & \mu, & \lambda, & \gamma, & \beta, & \alpha, & \delta\}\end{matrix} \tag{C31}$$

SECOND STEP:

After removing the numbers "1", "2" and "3" respectively from sequence (C3) and merging the same neighbouring numbers, then we obtain three new sequences (C3a), (C3b) and (C3c) respectively. For other sequences, we do the same things. Thus we have obtain the following 24 new sequences:

$$\begin{matrix}\{3, & 2, & 3, & 2, & 3, & 2, & 3, & 2, & 3\} \\ \{\alpha, & \beta, & \lambda, & \mu, & \nu, & \mu, & \lambda, & \beta, & \alpha\}\end{matrix} \tag{C3a}$$

$$\begin{matrix}\{1, & 3, & 1, & 3, & 1, & 3, & 1\}; \\ \{\delta, & \alpha, & \gamma, & 2\lambda+\nu, & \gamma, & \alpha, & \delta\};\end{matrix} \quad \begin{matrix}\{1, & 2, & 1, & 2, & 1, & 2, & 1\} \\ \{\delta, & \beta, & \gamma, & 2\mu, & \gamma, & \beta, & \delta\}\end{matrix} \tag{C3b; C3c}$$

$$\begin{matrix}\{2, & 3, & 2, & 3, & 2, & 3, & 2\} \\ \{\alpha, & \beta+\lambda, & \mu, & \nu, & \mu, & \lambda+\beta, & \alpha\}\end{matrix} \tag{C7a}$$

$$\begin{matrix}\{1, & 3, & 1, & 3, & 1, & 3, & 1\}; \\ \{\delta, & \beta, & \gamma, & 2\lambda+\nu, & \gamma, & \beta, & \delta\};\end{matrix} \quad \begin{matrix}\{1, & 2, & 1, & 2, & 1, & 2, & 1\} \\ \{\delta, & \alpha, & \gamma, & 2\mu, & \gamma, & \alpha, & \delta\}\end{matrix} \tag{C7b; C7c}$$

$$\begin{matrix}\{2, & 3, & 2, & 3, & 2, & 3, & 2\}; \\ \{\delta, & \beta, & \gamma+\mu, & \nu, & \mu+\gamma, & \beta, & \delta\};\end{matrix} \quad \begin{matrix}\{1, & 3, & 1, & 3, & 1, & 3, & 1\} \\ \{\alpha, & \beta, & \lambda, & \nu, & \lambda, & \beta, & \alpha\}\end{matrix} \tag{C21a; C21b}$$

$$\begin{matrix}\{2, & 1, & 2, & 1, & 2, & 1, & 2, & 1, & 2\} \\ \{\delta, & \alpha, & \gamma, & \lambda, & 2\mu, & \lambda, & \gamma, & \alpha, & \delta\}\end{matrix} \tag{C21c}$$

$$\begin{matrix}\{2, & 3, & 2, & 3, & 2, & 3, & 2\}; \\ \{\alpha, & \beta, & \gamma+\mu, & \nu, & \mu+\gamma, & \beta, & \alpha\};\end{matrix} \quad \begin{matrix}\{1, & 3, & 1, & 3, & 1, & 3, & 1\} \\ \{\delta, & \beta, & \lambda, & \nu, & \lambda, & \beta, & \delta\}\end{matrix} \tag{C23a; C23b}$$

$$\begin{matrix}\{1, & 2, & 1, & 2, & 1, & 2, & 1\} \\ \{\delta, & \alpha+\gamma, & \lambda, & 2\mu, & \lambda, & \gamma+\alpha, & \delta\}\end{matrix} \tag{C23c}$$

$$\begin{matrix}\{2, & 3, & 2, & 3, & 2, & 3, & 2\}; \\ \{\alpha, & \gamma, & \mu, & \nu, & \mu, & \gamma, & \alpha\};\end{matrix} \qquad \begin{matrix}\{1, & 3, & 1, & 3, & 1, & 3, & 1\} \\ \{\delta+\beta, & \gamma, & \lambda, & \nu, & \lambda, & \gamma, & \beta+\delta\}\end{matrix} \qquad (C25a; \quad C25b)$$

$$\begin{matrix}\{1, & 2, & 1, & 2, & 1, & 2, & 1\} \\ \{\delta, & \alpha, & \beta+\lambda, & 2\mu, & \lambda+\beta, & \alpha, & \delta\}\end{matrix} \qquad (C25c)$$

$$\begin{matrix}\{2, & 3, & 2, & 3, & 2, & 3, & 2\}; \\ \{\delta+\beta, & \gamma, & \mu, & \nu, & \mu, & \gamma, & \beta+\delta\};\end{matrix} \qquad \begin{matrix}\{1, & 3, & 1, & 3, & 1, & 3, & 1\} \\ \{\alpha, & \gamma, & \lambda, & \nu, & \lambda, & \gamma, & \alpha\}\end{matrix} \qquad (C29a; \quad C29b)$$

$$\begin{matrix}\{2, & 1, & 2, & 1, & 2, & 1, & 2, & 1, & 2\} \\ \{\delta, & \alpha, & \beta, & \lambda, & 2\mu, & \lambda, & \beta, & \alpha, & \delta\}\end{matrix} \qquad (C29c)$$

$$\begin{matrix}\{3, & 2, & 3, & 2, & 3, & 2, & 3, & 2, & 3\} \\ \{\delta, & \beta, & \gamma, & \mu, & \nu, & \mu, & \gamma, & \beta, & \delta\}\end{matrix} \qquad (C30a)$$

$$\begin{matrix}\{3, & 1, & 3, & 1, & 3, & 1, & 3, & 1, & 3\}; \\ \{\delta, & \alpha, & \gamma, & \lambda, & \nu, & \lambda, & \gamma, & \alpha, & \delta\};\end{matrix} \qquad \begin{matrix}\{1, & 2, & 1, & 2, & 1, & 2, & 1\} \\ \{\alpha, & \beta, & \lambda, & 2\mu, & \lambda, & \beta, & \alpha\}\end{matrix} \qquad (C30b; \quad C30c)$$

$$\begin{matrix}\{3, & 2, & 3, & 2, & 3, & 2, & 3, & 2, & 3\} \\ \{\alpha, & \beta, & \gamma, & \mu, & \nu, & \mu, & \gamma, & \beta, & \alpha\}\end{matrix} \qquad (C31a)$$

$$\begin{matrix}\{1, & 3, & 1, & 3, & 1, & 3, & 1\}; \\ \{\delta, & \alpha+\gamma, & \lambda, & \nu, & \lambda, & \gamma+\alpha, & \delta\};\end{matrix} \qquad \begin{matrix}\{1, & 2, & 1, & 2, & 1, & 2, & 1\} \\ \{\delta, & \beta, & \lambda, & 2\mu, & \lambda, & \beta, & \delta\}\end{matrix} \qquad (C31b; \quad C31c)$$

If (C7) is of order 4 for $H = H^{(1)} + H^{(2)} + H^{(3)}$, then (C7a), (C7b) and (C7c) are of order 4 for $H^{(2)} + H^{(3)}$, $H^{(1)} + H^{(3)}$ and $H^{(1)} + H^{(2)}$ respectively. According to Corollary 1, from (C7a) and (C7b) we know $\delta = \alpha$, and from (C7c) we should have $\alpha = 2\delta$, this means $\delta = \alpha = 0$. But that's impossible for a 4-th order (C7a). Thus (C7) is deleted. Similarly, (C25) is also removed.

THIRD STEP:

According to Lemma 1 and Corollary 1, from (C3a), (C3b) and (C3c) we have

$$\left\{\begin{array}{lll} \alpha = \beta = 2\delta, & \gamma + \delta = \frac{1}{2}, & 2\lambda + \nu = 2\mu, \\ \beta + \mu = \frac{1}{2}, & \beta\gamma^2 = \frac{1}{24}, & \frac{1}{2}\beta + 2\lambda\mu^2 = \frac{1}{12}, \\ \beta^2 + 2\lambda^2\mu = 0; & & \end{array}\right. \qquad (CC3)$$

from (C21a), (C21b) and (C21c) we have

$$\left\{\begin{array}{lll} \beta = 2\alpha = 2\delta, & 2\beta + \nu = 1, & \lambda = \gamma + \mu, \\ \alpha + \lambda = \frac{1}{2}, & \beta\lambda^2 = \frac{1}{24}, & \frac{1}{2}\delta + 2\gamma\lambda^2 = \frac{1}{12}, \\ \delta^2 + 2\gamma^2\lambda = 0; & & \end{array}\right. \qquad (CC21)$$

from (C23a), (C23b) and (C23c) we have

$$\left\{\begin{array}{lll} \beta = 2\alpha = 2\gamma = 2\delta, & \lambda = \gamma + \mu, & \nu = 2\mu, \\ \alpha + \lambda = \frac{1}{2}, & \beta\lambda^2 = \frac{1}{24}; & \end{array}\right. \qquad (CC23)$$

from (C29a), (C29b) and (C29c) we have

$$\left\{\begin{array}{lll} \gamma = 2\alpha = 2(\beta + \delta), & \lambda = \mu, & \alpha + \lambda = \frac{1}{2}, \\ 2\gamma + \nu = 1, & \gamma\lambda^2 = \frac{1}{24}, & \frac{1}{2}\delta + 2\beta\lambda^2 = \frac{1}{12}, \\ \delta^2 - 2\beta^2\lambda = 0; & & \end{array}\right. \qquad (CC29)$$

from (C30a), (C30b) and (C30c) we have

$$\begin{cases} \beta = 2\alpha, & \alpha + \lambda = \frac{1}{2}, & \beta + \mu = \frac{1}{2}, \\ 2\delta + 2\gamma + \nu = 1, & \beta\lambda^2 = \frac{1}{24}, & \frac{1}{2}\delta + 2\gamma\lambda^2 = \frac{1}{12}, \\ \delta^2 - \delta - 2\gamma\lambda(\gamma + \nu) = -\frac{1}{6}, & \frac{1}{2}\delta + 2\gamma\mu^2 = \frac{1}{12}, & \delta^2 - \delta - 2\gamma\mu(\gamma + \nu) = -\frac{1}{6}; \end{cases} \tag{CC30}$$

from (C31a), (C31b) and (C31c) we have

$$\begin{cases} \beta = \alpha + \gamma = 2\delta, & \nu = 2\mu, & \delta + \lambda = \frac{1}{2}, \\ \beta + \mu = \frac{1}{2}, & \beta\lambda^2 = \frac{1}{24}, & \frac{1}{2}\alpha + 2\gamma\mu^2 = \frac{1}{12}, \\ \alpha^2 - 2\gamma^2\mu = 0. \end{cases} \tag{CC31}$$

One can easily check that systems (CC3), (CC21), (CC29), (CC30) and (CC31) have no solutions, and system (CC23) has a unique solution

$$\begin{cases} \delta = \alpha = \gamma = \frac{1}{2(2-\sqrt[3]{2})}, & \\ \beta = \frac{1}{2-\sqrt[3]{2}}, & \lambda = \frac{1-\sqrt[3]{2}}{2(2-\sqrt[3]{2})}, \\ \mu = \frac{-\sqrt[3]{2}}{2(2-\sqrt[3]{2})}, & \nu = \frac{-\sqrt[3]{2}}{2-\sqrt[3]{2}}. \end{cases} \tag{13}$$

Therefore we have the only 4th-order **RESS** (C23) with parameters determined by (13), for hamiltonian $H = H^{(1)} + H^{(2)} + H^{(3)}$.

Acknowledgment. The author would like to thank Clint Scovel for his support and encouragement (during the author's stay in LANL: Sept 1995—June 1996).

References

[1] K. Feng, On Difference Schemes and Symplectic Geometry, In Proceedings of the 1984 Beijing Symposium on Differential Geometry and Differential Equations, Edited by K. Feng, Beijing: Science Press, 1985, 42-58.

[2] P.J. Channell, J.C. Scovel, Symplectic Integration of Hamiltonian Systems, *Nonlinearity,* **3**:2 (1990), 231-259.

[3] K. Feng, Difference Schemes for Hamiltonian Formalism and Symplectic Geometry, *J. Comp. Math.,* **4**:3, (1986), 279-289.

[4] J.M. Sanz-Serna, Runge-Kutta Schemes for Hamiltonian-Systems, *BIT,* **28**:4, (1988), 877-883.

[5] M.Z. Qin, D.L. Wang, M.Q. Zhang, Explicit symplectic difference schemes for separable Hamiltonian systems, *J. Comp. Math.,* **9**:3, (1991), 211-221.

[6] K. Feng, D.L. Wang, Variations on a Theme by Euler, Computing Center, Chinese Academy of Sciences, Preprint, (1991). Also in Collected Works of Feng Kang (II), National Defence Industry Press, Beijing, 1995, 264-273.

[7] E. Forest and R.D. Ruth, Fourth-Order Symplectic Integration, *Physica D,* **43** (1990), 105-117.

[8] M. Suzuki, Fractal Decomposition of Exponential Operators with Applications to Many-Body Theories and Monte Carlo Simulations, *Phys Lett A,* **146**:6 (1990), 319-323.

[9] H. Yoshida, Construction of Higher-Order Symplectic Integrators, *Phys Lett A,* **150**:5-7 (1990), 262-268.

[10] D.L. Wang, Symplectic Numerical Methods for Hamiltonian Systems, Ph.D. Dissertation (in Chinese), Computing Center, Chinese Academy of Sciences, 1988.

[11] J.C. Scovel, Personal communications, 1996.

[12] Y.F. Tang, Splitting Symplectic Methods for the Nonlinear Schrödinger Equation, preprint, 1996.

[13] V.I. Arnold, Remarks on Quasicrystallic Symmetries, *Physica D*, **33**:21 (1988).

[14] V.V. Beloshapkin, A.A. Chernikov, M. Natenzon, B.A. Petrovichev, R.Z. Sagdeev, G.M. Zaslavsky, Chaotic Streamlines in Pre-turbulent States, *Nature*, **337**:12 (1989), 133-137.

[15] A.A. Chernikov, R.Z. Sagdeev and G.M. Zaslavsky, Stochastic Webs, *Physica D*, **33** (1988), 65-76.

[16] M. Hénon, C. Heiles, The Applicability of the Third Integral of Motion: Some Numerical Experiments, *Astron J,* **69**:73 (1964).

[17] K. Feng, D.L. Wang, Dynamical Systems and Geometric Construction of Algorothms, In Contemporary Mathematics, Series **163**, (Edited by Z C Shi and C C Yang), Providence, R I: American Mathematical Society, (1994), 1-32.

[18] J.C. Scovel, Symplectic Numerical Integration of Hamiltonian Systems, In The Geometry of Hamiltonian Systems, **MSRI** Series **22**, Edited by T. Ratiu, Springer-Verlag, New York, (1991), 463-496.

[19] D.M. Stoffer, Some Geometric and Numerical Methods for Perturbed Integrable Systems, PhD Thesis, ETH-Zürich, 1988.

[20] Y.F. Tang, Y.H. Long, Formal Energy of Symplectic Scheme for Hamiltonian Systems and its Applications (II), *Computers Math Applic,* **27**:12 (1994), 31-39.