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

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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

$$\widetilde{Z} = \Psi^t(Z) = \phi^{\frac{t}{2}}_1 \circ \phi^{\frac{t}{2}}_2 \circ \phi^t_3 \circ \phi^{\frac{t}{2}}_2 \circ \phi^{\frac{t}{2}}_1(Z). \tag{4}$$

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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:

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