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NON-EXISTENCE OF CONJUGATE-SYMPLECTIC MULTI-STEP METHODS OF ODD ORDER*

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Abstract

We prove that any linear multi-step method G_1^τ of the form

$$\sum_{k=0}^{m} \alpha_k Z_k = \tau \sum_{k=0}^{m} \beta_k J^{-1} \nabla H(Z_k)$$

with odd order u ($u \geq 3$) cannot be conjugate to a symplectic method G_2^τ of order w ($w \geq u$) via any generalized linear multi-step method G_3^τ of the form

$$\sum_{k=0}^{m} \alpha_k Z_k = \tau \sum_{k=0}^{m} \beta_k J^{-1} \nabla H(\sum_{l=0}^{m} \gamma_{kl} Z_l).$$

We also give a necessary condition for this kind of generalized linear multi-step methods to be conjugate-symplectic. We also demonstrate that these results can be easily extended to the case when G_3^τ is a more general operator.

Mathematics subject classification: 65L06.
Key words: Linear multi-step method, Generalized linear multi-step method, Step-transition operator, Infinitesimally symplectic, Conjugate-symplectic.

1. Introduction

For a Hamiltonian system

$$\frac{dZ}{dt} = J^{-1} \nabla H(Z), \quad Z \in \mathbb{R}^{2n}, \tag{1.1}$$

where

$$J = \begin{bmatrix} 0_n & I_n \\ -I_n & 0_n \end{bmatrix},$$

∇ stands for the gradient operator, and $H : \mathbb{R}^{2n} \to \mathbb{R}^1$ is a smooth function (*Hamiltonian*), the symplecticity of any compatible linear m-step method (LMSM)

$$\sum_{k=0}^{m} \alpha_k Z_k = \tau \sum_{k=0}^{m} \beta_k J^{-1} \nabla H(Z_k) \quad \text{with} \quad \sum_{k=0}^{m} \beta_k \neq 0 \tag{1.2}$$

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can be defined via its step-transition operator (STO) G (also denoted by G^τ): $\mathbb{R}^{2n} \to \mathbb{R}^{2n}$ satisfying

$$\sum_{k=0}^{m} \alpha_k G^k = \tau \sum_{k=0}^{m} \beta_k J^{-1} (\nabla H) \circ G^k, \tag{1.3}$$

where G^k stands for k-fold composition of G: $G \circ G \cdots \circ G$.

Definition 1.1. ([4, 7, 12]) *An LMSM* (1.2) *is said to be symplectic for the Hamiltonian system* (1.1) *iff its STO G defined by* (1.3) *is symplectic, i.e.,*

$$\left[\frac{\partial G(Z)}{\partial Z}\right]^\top J \left[\frac{\partial G(Z)}{\partial Z}\right] = J \tag{1.4}$$

for any Hamiltonian function H and any sufficiently small step-size τ.

Naturally, one can define an STO for any compatible difference scheme for any ordinarily differential equation and expand the STO as a power series in τ [6, 14]. In particular, the STO G^τ of any LMSM of order s was written as [12]:

$$G^\tau(Z) = \sum_{i=0}^{+\infty} \frac{\tau^i}{i!} Z^{[i]} + aZ^{[s+1]}\tau^{s+1} + \mathcal{O}(\tau^{s+2}), \tag{1.5}$$

where

$$Z^{[0]} = Z, \quad Z^{[1]} = J^{-1}\nabla H(Z), \quad Z^{[k+1]} = \frac{\partial Z^{[k]}}{\partial Z} Z^{[1]} = Z_z^{[k]} Z^{[1]}$$

for $k = 1, 2, \cdots$, $a \neq 0$ is a real number.

There have been some interesting negative results on the symplecticity of the STOs [7, 12] or even in a weak sense the step-transition mappings [2] for LMSMs. We will concentrate on the conjugate symplecticity of LMSMs and a kind of general linear methods in the sequel.

The following interesting relation was first found by Dahlquist [1] and was introduced to one of the authors (Tang) by Feng [5], and by Scovel [11] in a stimulating discussion on symplectic multistep methods.

For the general ordinary differential equation

$$\frac{dZ}{dt} = f(Z), \quad Z \in \mathbb{R}^p, \tag{1.6}$$

the 2nd-order trapezoidal rule (denoted by $G_{tz}^\tau : Z_0 \to Z_1$)

$$Z_1 = Z_0 + \frac{\tau}{2}[f(Z_1) + f(Z_0)] \tag{1.7}$$

is related to the 2nd-order mid-point rule (denoted by $G_{mp}^\tau : Z_0 \to Z_1$)

$$Z_1 - Z_0 = \tau f\left(\frac{Z_1 + Z_0}{2}\right) \tag{1.8}$$

via the 1st-order Euler-forward scheme (denoted by $G_{ef}^\tau : Z_0 \to Z_1$)

$$Z_1 = Z_0 + \tau f(Z_0). \tag{1.9}$$

More precisely,

$$G_{ef}^{\frac{\tau}{2}} \circ G_{tz}^\tau = G_{mp}^\tau \circ G_{ef}^{\frac{\tau}{2}}. \tag{1.10}$$

It is known [3, 8, 10] that the midpoint rule G_{mp}^{τ} is a 2nd-order symplectic scheme for the Hamiltonian system (1.1). In the sense of the step-transition operator, Eq. (1.10) shows that the trapezoidal rule is also symplectic up to a coordinate transformation which is close to the identity. We will call this kind of methods *conjugate-symplectic schemes* or *schemes of conjugate symplecticity.*

Definition 1.2. ([6, 13]) *If three difference schemes G_1^{τ}, G_2^{τ} and G_3^{τ} compatible with Eq.* (1.6) *satisfy*

$$G_3^{\lambda\tau} \circ G_1^{\tau} = G_2^{\tau} \circ G_3^{\lambda\tau} \tag{1.11}$$

for some real number λ and for any smooth function H and any sufficiently small step-size τ, then G_1^{τ} and G_2^{τ} are said to be a Dahlquist pair or a conjugate pair via G_3^{τ}. We call Eq. (1.11) *a conjugate relation. A Dahlquist pair G_1^{τ} and G_2^{τ} is said to be symplectic if G_1^{τ} or G_2^{τ} is symplectic for the Hamiltonian system* (1.1). *In this case when one of G_1^{τ} and G_2^{τ} is symplectic, we also call the other conjugate-symplectic.*

It has been shown [6, 13] that there is an order barrier for Dahlquist pairs: the orders of G_1^{τ}, G_2^{τ} and G_3^{τ} in (1.11) are 2, 2 and 1 respectively when both G_1^{τ} and G_3^{τ} are LMSMs, and G_2^{τ} is a symplectic method.

In the present paper, we study the case when G_1^{τ} is an LMSM (1.2) or the following generalized linear multi-step method (GLMSM):

$$\sum_{k=0}^{m} \alpha_k Z_k = \tau \sum_{k=0}^{m} \beta_k J^{-1} \nabla H\Big(\sum_{l=0}^{m} \gamma_{kl} Z_l\Big) \tag{1.12a}$$

with

$$\sum_{l=0}^{m} \gamma_{kl} = 1, \quad k = 0, \cdots, m, \tag{1.12b}$$

G_3^{τ} is a GLMSM and G_2^{τ} is a symplectic method. We will obtain some negative results for odd-order G_1^{τ}.

2. Preliminary Lemmas

Assume that the orders of G_1^{τ}, G_2^{τ} and G_3^{τ} are u, v and $w-1$ respectively with $u \geq 1$, $v \geq 1$ and $w \geq 2$ (due to the compatibility). We write their expansions as follows:

$$G_1^{\tau}(Z) = \sum_{i=0}^{+\infty} \frac{\tau^i}{i!} Z^{[i]} + \tau^{u+1} A(Z) + \mathcal{O}(\tau^{u+2}), \tag{2.1}$$

$$G_2^{\tau}(Z) = \sum_{i=0}^{+\infty} \frac{\tau^i}{i!} Z^{[i]} + \tau^{v+1} M(Z) + \mathcal{O}(\tau^{v+2}), \tag{2.2}$$

$$G_3^{\tau}(Z) = \sum_{i=0}^{+\infty} \frac{\tau^i}{i!} Z^{[i]} + \tau^{w} B(Z) + \mathcal{O}(\tau^{w+1}), \tag{2.3}$$

where $A(Z) \neq \mathbf{0}$, $M(Z) \neq \mathbf{0}$ and $B(Z) \neq \mathbf{0}$.

Lemma 2.1. *If $u = v = w$, then expanding both sides of Eq.* (1.11) *yields*

$$\lambda^w B_z Z^{[1]} + A = M + \lambda^w Z_z^{[1]} B. \tag{2.4}$$

Remark 2.1. In Lemma 2.1, if the condition $u = v = w$ is removed, then Eq. (2.4) will be changed too. More precisely,

- if $u = v < w$, then (2.4) changes to
$$A = M; \tag{2.5a}$$
- if $u = w < v$, then (2.4) changes to
$$A + \lambda^w B_z Z^{[1]} = \lambda^w Z_z^{[1]} B; \tag{2.5b}$$
- if $v = w < u$, then (2.4) changes to
$$\lambda^w B_z Z^{[1]} = \lambda^w Z_z^{[1]} B + M; \tag{2.5c}$$
- if $u < v < w$ or $u < w < v$, then (2.4) changes to
$$A = \mathbf{0}; \tag{2.5d}$$
- if $v < u < w$ or $v < w < u$, then (2.4) changes to
$$M = \mathbf{0}; \tag{2.5e}$$
- if $w < u < v$ or $w < v < u$, then (2.4) changes to
$$\lambda^w B_z Z^{[1]} = \lambda^w Z_z^{[1]} B. \tag{2.5f}$$

Definition 2.1. *A transformation $W\colon \mathbb{R}^{2n} \to \mathbb{R}^{2n}$ is said to be infinitesimally symplectic iff its Jacobian W_z satisfies $W_z^T J + J W_z = \mathbf{0}$.*

Lemma 2.2. *In* (2.2)*, if $G_2^\tau\colon \mathbb{R}^{2n} \to \mathbb{R}^{2n}$ is symplectic, then $M\colon \mathbb{R}^{2n} \to \mathbb{R}^{2n}$ is infinitesimally symplectic.*

Lemma 2.3. ([12]) *In the expansion* (2.2)*, if v is odd and*
$$M = \cdots + \kappa Z_z^{[1]} Z_z^{[1]} \cdots Z_z^{[1]} Z^{[1]} + \cdots$$
with $\kappa \neq 0$, then M cannot be infinitesimally symplectic and G_2^τ cannot be symplectic.

Lemma 2.4. ([7, 12]) *Under Definition* 1.1*, any LMSM* (1.2) *cannot be symplectic for the Hamiltonian system* (1.1)*.*

3. Results and Conjecture

Theorem 3.1. *It is impossible for an LMSM with odd order u (≥ 3) to be conjugate to a symplectic method with order v ($\geq u$) via any GLMSM.*

Proof. We suppose that Eq. (1.11) is satisfied with G_2^τ being symplectic. Since $A(Z) \neq \mathbf{0}$, $M(Z) \neq \mathbf{0}$ and $w \geq 2$, the cases (2.5d) and (2.5e) are impossible. When $\lambda \neq 0$, it is easy to check that the case (2.5f) is impossible; when $\lambda = 0$, Eq. (1.11) becomes $G_1^\tau(Z) = G_2^\tau(Z)$, that means that the LMSM G_1^τ is also symplectic which contradicts Lemma 2.4. If $v \geq u$, we need only to consider the cases (2.4), (2.5a) and (2.5b). We know from (1.5),

$$A = aZ^{[u+1]} = \cdots + aZ_z^{[1]} Z_z^{[1]} \cdots Z_z^{[1]} Z^{[1]} + \cdots$$

with $a \neq 0$. Consequently, Eq. (2.5b) cannot be satisfied. Moreover, for both cases (2.4) and (2.5a), we have

$$M = \cdots + aZ_z^{[1]} Z_z^{[1]} \cdots Z_z^{[1]} Z^{[1]} + \cdots$$

with $a \neq 0$, M cannot be infinitesimally symplectic according to Lemma 2.3, which contradicts the assumption that G_2^τ is symplectic. Thus both cases (2.4) and (2.5a) are also impossible. This completes the proof of this theorem.

Theorem 3.2. *It is impossible for a GLMSM of form* (1.12) *with odd order* u (≥ 3) *satisfying*

$$\sum_{k=0}^{m} \left[\beta_k \sum_{l=0}^{m} \frac{\gamma_{kl} l^u}{u!} - \alpha_k \frac{k^{u+1}}{(u+1)!} \right] \neq 0 \tag{3.1}$$

to be conjugate to a symplectic method with order v ($\geq u$) *via another GLMSM.*

Proof. Similarly, any GLMSM of form (1.12) can be characterized by the corresponding step-transition operator G satisfying

$$\sum_{k=0}^{m} \alpha_k G^k = \tau \sum_{k=0}^{m} \beta_k J(\nabla H) \circ (\sum_{l=0}^{m} \gamma_{kl} G^l). \tag{3.2}$$

Since (1.12) is of order u, one can write (see [12])

$$G^k(Z) = \sum_{i=0}^{u+1} \frac{k^i Z^{[i]}}{i!} \tau^i + k\Theta(Z)\tau^{u+1} + \mathcal{O}(\tau^{u+2}), \quad k = 1, 2, \cdots,$$

and,

$$\begin{aligned} &\sum_{k=0}^{m} \alpha_k \left[\sum_{i=0}^{u+1} \frac{k^i Z^{[i]}}{i!} \tau^i + k\Theta(Z)\tau^{u+1} + \mathcal{O}(\tau^{u+2}) \right] \\ &= \tau \sum_{k=0}^{m} \beta_k J(\nabla H) \circ \left(\sum_{j=0}^{m} \gamma_{kj} \left[\sum_{i=0}^{u+1} \frac{j^i Z^{[i]}}{i!} \tau^i + j\Theta(z)\tau^{u+1} + \mathcal{O}(\tau^{u+2}) \right] \right) \\ &= \tau \sum_{k=0}^{m} \beta_k J(\nabla H) \circ \left(Z + \sum_{i=1}^{u} \sum_{j=0}^{m} \frac{\gamma_{kj} j^i}{i!} Z^{[i]} \tau^i + \mathcal{O}(\tau^{u+1}) \right). \end{aligned} \tag{3.3}$$

Consequently,

$$\sum_{k=0}^{m} k\alpha_k \Theta(Z) = \cdots + \sum_{k=0}^{m} \left[\beta_k \sum_{l=0}^{m} \frac{\gamma_{kl} l^u}{u!} - \alpha_k \frac{k^{u+1}}{(u+1)!} \right] Z_z^{[1]} Z_z^{[1]} \cdots Z_z^{[1]} Z^{[1]} + \cdots. \tag{3.4}$$

Since $\sum_{k=0}^{m} k\alpha_k \neq 0$ is required by the compatibility of scheme (1.12), the condition (3.1) means that in (2.4) or (2.5a) $M(Z)$ cannot be infinitesimally symplectic because it contains the term $Z_z^{[1]} Z_z^{[1]} \cdots Z_z^{[1]} Z^{[1]}$ ("$u+1$"-fold "$Z^{[1]}$").

Remark 3.1. The results of Theorems 3.1 and 3.2 may not be true for even u. When $u=4$ and $A=aZ^{[u+1]}$ or simply $Z^{[5]}$, we set

$$\lambda^w B = bZ^{[1]}_{z^3}(Z^{[1]})^3 + 3cZ^{[1]}_{z^2}(Z^{[1]}Z^{[2]}) + dZ^{[1]}_z Z^{[3]}.$$

Then in (2.4)

$$\begin{aligned} M &= Z^{[u+1]} + \lambda^w(B_z Z^{[1]} - Z^{[1]}_z B) \\ &= (1+b)Z^{[1]}_{z^4}(Z^{[1]})^4 + 3(2+b+c)Z^{[1]}_{z^3}[(Z^{[1]})^2 Z^{[2]}] + 3(1+c)Z^{[1]}_{z^2}(Z^{[2]})^2 \\ &\quad +(4+3c+d)Z^{[1]}_{z^2}(Z^{[1]}Z^{[3]}) + (1-b+d)Z^{[1]}_z Z^{[1]}_{z^3}(Z^{[1]})^3 \\ &\quad +3(1-c+d)Z^{[1]}_z Z^{[1]}_{z^2}(Z^{[1]}Z^{[2]}) + Z^{[1]}_z Z^{[1]}_z Z^{[3]}, \end{aligned} \tag{3.5}$$

and

$$\begin{aligned} M_z &= (1+b)(Z^{[1]}_z)_{z^4}(Z^{[1]})^4 + 4(1+b)(Z^{[1]}_z)_{z^3}(Z^{[1]})^3 Z^{[1]}_z \\ &\quad +3(2+b+c)(Z^{[1]}_z)_{z^3}[(Z^{[1]})^2 Z^{[2]}] + 6(2+b+c)(Z^{[1]}_z)_{z^2}(Z^{[1]}Z^{[2]})Z^{[1]}_z \\ &\quad +3(2+b+c)(Z^{[1]}_z)_{z^2}(Z^{[1]})^2(Z^{[1]}_z)_z Z^{[1]} + 3(2+b+c)(Z^{[1]}_z)_{z^2}(Z^{[1]})^2 Z^{[1]}_z Z^{[1]}_z \\ &\quad +3(1+c)(Z^{[1]}_z)_{z^2}(Z^{[2]})^2 + 6(1+c)(Z^{[1]}_z)_z Z^{[2]}(Z^{[1]}_z)_z Z^{[1]} \\ &\quad +6(1+c)(Z^{[1]}_z)_z Z^{[2]} Z^{[1]}_z Z^{[1]}_z + (4+3c+d)(Z^{[1]}_z)_{z^2}(Z^{[1]}Z^{[3]}) \\ &\quad +(4+3c+d)(Z^{[1]}_z)_z Z^{[3]} Z^{[1]}_z + (4+3c+d)(Z^{[1]}_z)_z Z^{[1]}(Z^{[1]}_z)_{z^2}(Z^{[1]})^2 \\ &\quad +2(4+3c+d)(Z^{[1]}_z)_z Z^{[1]}(Z^{[1]}_z)_z Z^{[1]} Z^{[1]}_z + (4+3c+d)(Z^{[1]}_z)_z Z^{[1]}(Z^{[1]}_z)_z Z^{[2]} \\ &\quad +(4+3c+d)(Z^{[1]}_z)_z Z^{[1]} Z^{[1]}_z (Z^{[1]}_z)_z Z^{[1]} + (4+3c+d)(Z^{[1]}_z)_z Z^{[1]} Z^{[1]}_z Z^{[1]}_z Z^{[1]}_z \\ &\quad +(1-b+d)(Z^{[1]}_z)_z[Z^{[1]}_{z^3}(Z^{[1]})^3] + (1-b+d)Z^{[1]}_z(Z^{[1]}_z)_{z^3}(Z^{[1]})^3 \\ &\quad +3(1-b+d)Z^{[1]}_z(Z^{[1]}_z)_{z^2}(Z^{[1]})^2 Z^{[1]}_z + 3(1-c+d)(Z^{[1]}_z)_z[Z^{[1]}_{z^2}(Z^{[1]}Z^{[2]})] \\ &\quad +3(1-c+d)Z^{[1]}_z(Z^{[1]}_z)_{z^2}(Z^{[1]}Z^{[2]}) + 3(1-c+d)Z^{[1]}_z(Z^{[1]}_z)_z Z^{[2]} Z^{[1]}_z \\ &\quad +3(1-c+d)Z^{[1]}_z(Z^{[1]}_z)_z Z^{[1]}(Z^{[1]}_z)_z Z^{[1]} + 3(1-c+d)Z^{[1]}_z(Z^{[1]}_z)_z Z^{[1]} Z^{[1]}_z Z^{[1]}_z \\ &\quad +(Z^{[1]}_z)_z(Z^{[1]}_z Z^{[3]}) + Z^{[1]}_z(Z^{[1]}_z)_z Z^{[3]} + Z^{[1]}_z Z^{[1]}_z (Z^{[1]}_z)_{z^2}(Z^{[1]})^2 \\ &\quad +2Z^{[1]}_z Z^{[1]}_z (Z^{[1]}_z)_z Z^{[1]} Z^{[1]}_z + Z^{[1]}_z Z^{[1]}_z (Z^{[1]}_z)_z Z^{[2]} + Z^{[1]}_z Z^{[1]}_z Z^{[1]}_z (Z^{[1]}_z)_z Z^{[1]} \\ &\quad +Z^{[1]}_z Z^{[1]}_z Z^{[1]}_z Z^{[1]}_z Z^{[1]}_z. \end{aligned} \tag{3.6}$$

It can be verified that if

$$b = -\frac{5}{6}, \quad c = -\frac{5}{6}, \quad d = -\frac{5}{2}, \tag{3.7}$$

then M is infinitesimally symplectic.

Nevertheless, to make the result of Theorem 3.1 be untrue for even u, besides the conditions mentioned above, there are more equations to be satisfied. So we still believe that the result is true for even u. In particular, we have

Conjecture 3.1. *If a GLMSM of form* (1.12) *with order* u (≥ 1) *is conjugate-symplectic via another GLMSM, then it must be conjugate to the* 2*nd-order mid-point rule* (1.8).

Remark 3.2. It is easy to check from the proofs that the results of Theorems 3.1 and 3.2 are also true when G^τ_3 is a more general operator, say, a general linear method or a B-series (for the details about general linear methods and B-series, see [8, 9].

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