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ON CONJUGATE SYMPLECTICITY OF MULTI-STEP METHODS*[1)]

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Dedicated to Feng Kang on his 80th birthday

Abstract

In this paper, we solve a problem on the existence of conjugate symplecticity of linear multi-step methods (**LMSM**), the negative result is obtained.

Key words: Conjugate symplecticity, Multi-step method

1. Introduction

For an ordinary differential equation

$$\frac{dZ}{dt} = f(Z), \quad Z \in R^p, \tag{1}$$

any compatible linear m-step difference scheme (for simplicity, denoted by **LMSM**):

$$\sum_{k=0}^{m} \alpha_k Z_k = \tau \sum_{k=0}^{m} \beta_k f(Z_k) \quad (\sum_{k=0}^{m} \beta_k \neq 0) \tag{2}$$

can be characterized by a step-transition operator G (also denoted by G^τ): $R^p \to R^p$ satisfying

$$\sum_{k=0}^{m} \alpha_k G^k = \tau \sum_{k=0}^{m} \beta_k f \circ G^k, \tag{3}$$

where G^k stands for k-time composition of G: $G \circ G \cdots \circ G$ (refer to [1-4]).

The operator G defined by (3) can be represented as a power series in τ with first term equal to identity I. More precisely, it is shown[4] that

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Lemma A. *If scheme (2) is of order s, then the corresponding operator G can be written as the following form:*

$$G(Z) = \sum_{i=0}^{s+1} \tau^i \frac{Z^{[i]}}{i!} + aZ^{[s+1]}\tau^{s+1} + O(\tau^{s+2}), \tag{4}$$

where $Z^{[0]} = Z, Z^{[1]} = f(Z), Z^{[k+1]} = \frac{\partial Z^{[k]}}{\partial Z} Z^{[1]}, k = 1, 2, \cdots,$ *and a is a constant* $(\neq 0)$.

Thus, the step-transition operator completely characterizes the multi-step scheme as: $Z_1 = G(Z_0), \cdots, Z_m = G(Z_{m-1}) = G^m(Z_0), \cdots$.

When equation (2) is a hamiltonian system, i.e., $p = 2n$ and $f(Z) = J\nabla H(Z)$, here $J = \begin{bmatrix} 0_n & -I_n \\ I_n & 0_n \end{bmatrix}$, ∇ stands for gradient operator, and $H : R^{2n} \to R^1$ is a (smooth) hamiltonian function, (1), (2) and (3) become

$$\frac{dZ}{dt} = J\nabla H(Z), \quad z \in R^{2n}, \tag{5}$$

$$\sum_{k=0}^{m} \alpha_k Z_k = \tau \sum_{k=0}^{m} \beta_k J\nabla H(Z_k) \quad (\sum_{k=0}^{m} \beta_k \neq 0), \tag{6}$$

$$\sum_{k=0}^{m} \alpha_k G^k = \tau \sum_{k=0}^{m} \beta_k J(\nabla H) \circ G^k. \tag{7}$$

And one can rewrite

$$\begin{aligned}
&Z^{[0]} = Z, \\
&Z^{[1]} = J\nabla H, \\
&Z^{[2]} = JH_{zz}J\nabla H = Z_z^{[1]} Z^{[1]}, \\
&Z^{[3]} = Z_{z^2}^{[1]}(Z^{[1]})^2 + Z_z^{[1]} Z^{[2]}, \\
&Z^{[4]} = Z_{z^3}^{[1]}(Z^{[1]})^3 + 3Z_{z^2}^{[1]}(Z^{[1]}Z^{[2]}) + Z_z^{[1]}Z^{[3]}, \\
&Z^{[5]} = Z_{z^4}^{[1]}(Z^{[1]})^4 + 6Z_{z^3}^{[1]}\left((Z^{[1]})^2 Z^{[2]}\right) \\
&\qquad +3Z_{z^2}^{[1]}(Z^{[2]})^2 + 4Z_{z^2}^{[1]}(Z^{[1]}Z^{[3]}) + Z_z^{[1]}Z^{[4]},
\end{aligned} \tag{8}$$

or generally,

$$Z^{[s+1]} = \sum_{j=1}^{s} \sum_{l_1+\cdots+l_j=s; l_u \geq 1} d_{l_1\cdots l_j} J(\nabla H)_{z^j} Z^{[l_1]} \cdots Z^{[l_j]}, \tag{9}$$

where $d_{l_1\cdots l_j} > 0$ for all $l_1, \cdots, l_j$ and $(\nabla H)_{z^j} Z^{[l_1]} \cdots Z^{[l_j]}$ stands for the multi-linear form

$$\sum_{1 \leq t_1, \cdots, t_j \leq 2n} \frac{\partial^j (\nabla H(Z))}{\partial Z_{(t_1)} \cdots \partial Z_{(t_j)}} Z_{(t_1)}^{[l_1]} \cdots Z_{(t_j)}^{[l_j]}$$

($Z_{(t_v)}^{[l_u]}$ stands for the t_v-th component of the $2n$-dim vector $Z^{[l_u]}$).