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CONJUGATE-SYMPLECTICITY OF LINEAR MULTISTEP METHODS*

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Abstract

For the numerical treatment of Hamiltonian differential equations, symplectic integrators are the most suitable choice, and methods that are conjugate to a symplectic integrator share the same good long-time behavior. This note characterizes linear multistep methods whose underlying one-step method is conjugate to a symplectic integrator. The boundedness of parasitic solution components is not addressed.

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1. Main Result

For the numerical integration of $\dot{y} = f(y)$ we consider the linear multistep method

$$\sum_{j=0}^{k} \alpha_j y_{n+j} \;=\; h \sum_{j=0}^{k} \beta_j f(y_{n+j}), \tag{1.1}$$

and we denote its generating polynomials by

$$\rho(\zeta) = \sum_{j=0}^{k} \alpha_j \zeta^j, \quad \sigma(\zeta) = \sum_{j=0}^{k} \beta_j \zeta^j.$$

We assume throughout this note that the method is consistent (i.e., $\rho(1) = 0$ and $\rho'(1) = \sigma(1) \neq 0$) and irreducible (i.e., $\rho(\zeta)$ and $\sigma(\zeta)$ do not have a common factor).

Since the discrete flow of a multistep method evolves on a product of k copies of the phase space, definitions like that for symplecticity are not straightforward. It was first suggested by Feng Kang [3] (see also [2, pp. 274-283]) to study the symplecticity of a linear multistep method via its *underlying one-step method* (also called step-transition operator). This is a mapping $y \mapsto \Phi_h(y)$, such that the iterates $y_n = \Phi_h^n(y_0)$ satisfy the recursion (1.1). The existence of this underlying one-step method as a formal B-series is discussed in [4, 10], see also [6, Sect. XV.2]. Unfortunately, multistep methods are non symplectic with respect to this definition of symplecticity [9].

A method $\Phi_h(y)$ is called conjugate-symplectic [8] if there exists a transformation $\chi_h(y)$ which is $\mathcal{O}(h)$ close to the identity (and represented by a formal B-series), such that $\chi_h^{-1} \circ \Phi_h \circ \chi_h$ is a (formal) symplectic transformation when $f(y)$ is a Hamiltonian vector field. Although such a method does not need to be symplectic, it shares the long-time behavior of a symplectic integrator because $(\chi_h^{-1} \circ \Phi_h \circ \chi_h)^n = \chi_h^{-1} \circ \Phi_h^n \circ \chi_h$.

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Theorem 1.1. *The underlying one-step method of the linear multistep method* (1.1) *is conjugate-symplectic if and only if* (1.1) *is symmetric, i.e.,* $\alpha_j = -\alpha_{k-j}$ *and* $\beta_j = \beta_{k-j}$ *for all* j.

Since the order of symmetric methods is always even and since we consider arbitrary B-series for the conjugacy mapping χ_h, this provides a new proof for the main result of [7], which states that the underlying one-step method of a method (1.1) with odd order $u \geq 3$ cannot be conjugate to a symplectic method with order $v \geq u$ via any generalized linear multistep method (GLMSM). In that article, a GLMSM denotes a difference formula like (1.1), where $f(y_{n+j})$ is replaced by $f\big(\sum_{l=0}^{k} \gamma_{jl} y_{n+l}\big)$.

In [7] it is furthermore conjectured that if a GLMSM (and in particular also (1.1)) is conjugate-symplectic via another GLMSM, then it must be conjugate to the 2nd order mid-point rule. The requirement on the conjugacy mapping seems very strong, because any B-series for χ_h would imply as well the good long-time behavior of the method. If we relax this requirement and admit arbitrary B-series for χ_h, Theorem 1.1 proves the existence of conjugate-symplectic methods (1.1) of arbitrarily high order.

The proof of Theorem 1.1 is a concatenation of various results that have been proved in a different context by several authors.

2. Proof of Necessity

It suffices to consider the harmonic oscillator which can be written as $\dot{y} = \lambda y$ with $\lambda = \mathrm{i}$ (put $y = p + \mathrm{i}q$). In this situation $\Phi_h(y) = \zeta(\lambda h) y$, where $\zeta = \zeta(z)$ is the solution of

$$\rho(\zeta) - z\,\sigma(\zeta) = 0 \tag{2.1}$$

which is the analytic continuation of $\zeta(0) = 1$. For the harmonic oscillator, conjugate-symplecticity as well as symplecticity and area preservation are equivalent to

$$|\zeta(\mathrm{i}h)|^2 = \zeta(\mathrm{i}h)\zeta(-\mathrm{i}h) = 1.$$

It is proved in [8] and in [3] (see also [2, pp. 274-283]) that this property implies the symmetry of the method (1.1): substituting $-z$ for z and ζ^{-1} for ζ in (2.1) shows that the adjoint mapping $\zeta^*(z) = \zeta(-z)^{-1}$ satisfies the relation $\rho^*(\zeta^*) + z\,\sigma^*(\zeta^*) = 0$ with $\rho^*(\zeta) = \zeta^k \rho(\zeta^{-1})$ and $\sigma^*(\zeta) = \zeta^k \sigma(\zeta^{-1})$. The condition $\zeta(\mathrm{i}h)\zeta(-\mathrm{i}h) = 1$ therefore implies that $\zeta = \zeta(\mathrm{i}h)$ satisfies

$$\rho(\zeta) - \mathrm{i}h\,\sigma(\zeta) = 0, \quad \rho^*(\zeta) + \mathrm{i}h\,\sigma^*(\zeta) = 0$$

for all sufficiently small h. Consequently, we have

$$\rho(\zeta)\,\sigma^*(\zeta) = -\rho^*(\zeta)\,\sigma(\zeta)$$

for $\zeta = \zeta(\mathrm{i}h)$ and, by analytic continuation, for all complex ζ. Since $\rho(\zeta)$ and $\sigma(\zeta)$ do not have common factors, and $\sigma(1) = \sigma^*(1) \neq 0$, this yields $\rho^*(\zeta) = -\rho(\zeta)$ and $\sigma^*(\zeta) = \sigma(\zeta)$ what is equivalent to the symmetry of the method.

3. Proof of Sufficiency

a) The following result has been proved in [5] for multistep methods for second order differential equations and in [6, Sect. XV.4.4] for methods (1.1): if $Q(y)$ is a quadratic first integral