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*Correction*

# Correction to "On a Class of Hermite-Obreshkov One-Step Methods with Continuous Spline Extension" [Axioms 7(3), 58, 2018]

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**Abstract:** The authors of the above mentioned paper specify that the considered class of one-step symmetric Hermite-Obreshkov methods satisfies the property of conjugate-symplecticity up to order $p+r$, where $r=2$ and $p$ is the order of the method. This generalization of conjugate-symplecticity states that the methods conserve quadratic first integrals and the Hamiltonian function over time intervals of length $O(h^{-r})$. Theorem 1 of the above mentioned paper is then replaced by a new one. All the other results in the paper do not change. Two new figures related to the already considered Kepler problem are also added.

**Keywords:** initial value problems; one-step methods; Hermite–Obreshkov methods; symplecticity; B-splines; BS methods

## Introduction

In paper [1] we analyzed the numerical solution of the first order Ordinary Differential Equation (ODE),

$$\mathbf{y}'(t) = \mathbf{f}(\mathbf{y}(t)), \ t \in [t_0, t_0+T], \tag{1}$$

associated with the initial condition:

$$\mathbf{y}(t_0) = \mathbf{y}_0, \tag{2}$$

where $\mathbf{f} : \mathbb{R}^m \to \mathbb{R}^m, m \geq 1$, is a $C^{R-1}, R \geq 1$, function on its domain and $\mathbf{y}_0 \in \mathbb{R}^m$ is assigned. In particular, we considered the numerical solution of Hamiltonian problems which in canonical form can be written as follows:

$$\mathbf{y}' = J\nabla H(\mathbf{y}), \qquad \mathbf{y}(t_0) = \mathbf{y}_0 \in \mathbb{R}^{2\ell}, \tag{3}$$

with

$$\mathbf{y} = \begin{pmatrix} \mathbf{q} \\ \mathbf{p} \end{pmatrix}, \quad \mathbf{q}, \mathbf{p} \in \mathbb{R}^{\ell}, \qquad J = \begin{pmatrix} O & I_\ell \\ -I_\ell & O \end{pmatrix}, \tag{4}$$

where $\mathbf{q}$ and $\mathbf{p}$ are the generalized coordinates and momenta, $H : \mathbb{R}^{2\ell} \to \mathbb{R}$ is the Hamiltonian function and $I_\ell$ stands for the identity matrix of dimension $\ell$. Note that the flow $\varphi_t : \mathbf{y}_0 \to \mathbf{y}(t)$ associated with the dynamical system (3) is symplectic; this means that its Jacobian satisfies:

$$\frac{\partial \varphi_t(\mathbf{y})}{\partial \mathbf{y}}^{\top} J \frac{\partial \varphi_t(\mathbf{y})}{\partial \mathbf{y}} = J, \quad \forall\, \mathbf{y} \in \mathbb{R}^{2\ell}. \tag{5}$$

We recall that a one-step numerical method $\Phi_h : \mathbb{R}^{2\ell} \to \mathbb{R}^{2\ell}$ with stepsize $h$ is symplectic if the discrete flow $\mathbf{y}_{n+1} = \Phi_h(\mathbf{y}_n), n \geq 0$, satisfies:

$$\frac{\partial \Phi_h(\mathbf{y})^\top}{\partial \mathbf{y}} J \frac{\partial \Phi_h(\mathbf{y})}{\partial \mathbf{y}} = J, \quad \forall\, \mathbf{y} \in \mathbb{R}^{2\ell}. \tag{6}$$

Two numerical methods $\Phi_h, \Psi_h$ are conjugate to each other if there exists a global change of coordinates $\chi_h$, such that:

$$\Psi_h = \chi_h \circ \Phi_h \circ \chi_h^{-1}$$

with $\chi_h(\mathbf{y}) = \mathbf{y} + O(h)$ uniformly for $\mathbf{y}$ varying in a compact set and $\circ$ denoting a composition operator [2]. A method which is conjugate to a symplectic method is said to be conjugate symplectic, this is a less strong requirement than symplecticity, which allows the numerical solution to have the same long-time behavior of a symplectic method. A more relaxed property, shared by a wider class of numerical schemes, is a generalization of the conjugate-symplecticity property, introduced in [3]. A method $\mathbf{y}_1 = \Psi_h(\mathbf{y}_0)$ of order $p$ is conjugate-symplectic up to order $p + r$, with $r \geq 0$, if a global change of coordinates $\chi_h(\mathbf{y}) = \mathbf{y} + O(h^p)$ exists such that $\Psi_h = \chi_h \circ \Phi_h \circ \chi_h^{-1}$, with the map $\Psi_h$ satisfying

$$\frac{\partial \Psi_h(\mathbf{y})^\top}{\partial \mathbf{y}} J \frac{\partial \Psi_h(\mathbf{y})}{\partial \mathbf{y}} = J + O(h^{p+r+1}). \tag{7}$$

A consequence of property (7) is that the method $\Psi_h(\mathbf{y})$ nearly conserves all quadratic first integrals and the Hamiltonian function over time intervals of length $O(h^{-r})$ (see [3]).

Recently, the class of Euler–Maclaurin Hermite–Obreshkov (EMHO) methods for the solution of Hamiltonian problems has been analyzed in [4] where the conjugate symplecticity up to order $p + 2$ of the $p$-th order methods was proven. In this paper, we fix Theorem 1 of [1] related to symmetric one-step BS Hermite–Obreshkov (BSHO) methods, proving that the conjugate-symplecticity property is satisfied by the $R$-th one-step symmetric Hermite–Obreshkov method up to order $2R + 2$.

Let $t_i, i = 0, \ldots, N$, be an assigned partition of the integration interval $[t_0\,, \, t_0 + T]$, and let us denote by $\mathbf{u}_i$ an approximation of $\mathbf{y}(t_i)$. We consider one-step symmetric BSHO method as follows, setting $\mathbf{u}_0 := \mathbf{y}_0$,

$$\mathbf{u}_{n+1} = \mathbf{u}_n + \sum_{j=1}^{R} h_n^j \, \beta_j^{(R)} \left( \mathbf{u}_n^{(j)} - (-1)^j \mathbf{u}_{n+1}^{(j)} \right), \; n = 0, \ldots, N-1, \tag{8}$$

where $h_n := t_{n+1} - t_n$, $\beta_j^{(R)} := \frac{1}{j!} \frac{R(R-1)\ldots(R-j+1)}{(2R)(2R-1)\ldots(2R-j+1)}$, and $\mathbf{u}_i^{(j)}$, for $j \geq 1$, denotes the $(j-1)$-th Lie derivative of $\mathbf{f}$ computed at $\mathbf{u}_i$,

$$\mathbf{u}_i^{(j)} := D_{j-1}\mathbf{f}(\mathbf{u}_i)\,, \quad j = 1, \ldots, R\,, \tag{9}$$

where $D_0 = I$ is the identity operator and $D_k\mathbf{f}(\mathbf{z})$ is defined as the $k$-th total derivative of $\mathbf{f}(\mathbf{y}(t))$ computed at $\mathbf{y}(t) = \mathbf{z}$, where for the computation of the total derivative it is assumed that $\mathbf{y}$ satisfies the differential equation in (1). Thus for example $D_1\mathbf{f}(\mathbf{z}) = \frac{\partial \mathbf{f}}{\partial \mathbf{y}}(\mathbf{z})\, \mathbf{f}(\mathbf{z})$, where $\frac{\partial \mathbf{f}}{\partial \mathbf{y}}$ is the $m \times m$ Jacobian matrix of $\mathbf{f}$. Note that we use the subscript to define the Lie operator to avoid confusion with the same order classical derivative operator in the following denoted as $D^k$. With this clarification on the definition of $\mathbf{u}_i^{(j)}$, following the lines of the proof given in [4], we can actually prove that the $R$-th one-step symmetric BSHO method is conjugate symplectic up to order $2R + 2$.

We show that the map $\mathbf{y}_1 = \Psi_h(\mathbf{y}_0)$ associated with the BSHO method is such that $\Psi_h(\mathbf{y}) = \Phi_h(\mathbf{y}) + O(h^{2R+3})$, where $\mathbf{y}_1 = \Phi_h(\mathbf{y}_0)$ is a suitable conjugate symplectic B-series integrator.

**Theorem 1.** *The map $\mathbf{u}_1 = \Psi_h(\mathbf{u}_0)$ associated with the one-step method (8) admits a B-series expansion and is conjugate to a symplectic B-series integrator up to order $2R + 2$.*

**Proof.** The existence of a $B$-series expansion for $\mathbf{y}_1 = \Psi_h(\mathbf{y}_0)$ is directly deduced from [5], where a $B$-series representation of a generic multi-derivative Runge-Kutta method has been obtained. By defining the two characteristic polynomials of the trapezoidal rule:

$$\rho(z) := z - 1, \qquad \sigma(z) := \frac{1}{2}(z+1)$$

and the shift operator $E(\mathbf{u}_n) := \mathbf{u}_{n+1}$, the $R$-th method described in (8) reads,

$$\rho(E)\mathbf{u}_n = \sum_{k=1}^{\lceil R/2 \rceil} 2\beta_{2k-1}^{(R)} h^{2k-1}\sigma(E)\mathbf{u}_n^{(2k-1)} - \sum_{k=1}^{\lfloor R/2 \rfloor} \beta_{2k}^{(R)} h^{2k}\rho(E)\mathbf{u}_n^{(2k)}. \tag{10}$$

We now consider a function $\mathbf{v}(t)$, a stepsize $h$ and the shift operator $E_h(\mathbf{v}(t)) := \mathbf{v}(t+h)$, and we look for a continuous function $\mathbf{v}(t)$ that satisfies (10) in the sense of formal series (a series where the number of terms is allowed to be infinite), using the relation $E_h = \sum_{j=0}^{\infty} \frac{h^j}{j!} D^j \equiv e^{hD}$ where $D = D^1$ is the classical derivative operator,

$$\rho(e^{hD})\mathbf{v}(t) = \sum_{k=1}^{\lceil R/2 \rceil} 2\beta_{2k-1}^{(R)} h^{2k-1}\sigma(e^{hD})D_{2k-2}\mathbf{f}(\mathbf{v}(t)) - \sum_{k=1}^{\lfloor R/2 \rfloor} \beta_{2k}^{(R)} h^{2k}\rho(e^{hD})D_{2k-1}\mathbf{f}(\mathbf{v}(t)).$$

By multiplying both sides of the previous equation by $D\rho(e^{hD})^{-1}$, we obtain:

$$D\mathbf{v}(t) = hD\rho(e^{hD})^{-1}\sigma(e^{hD}) \sum_{k=0}^{\lceil R/2 \rceil -1} 2\beta_{2k+1}^{(R)} h^{2k} D_{2k}\mathbf{f}(\mathbf{v}(t)) - \sum_{k=1}^{\lfloor R/2 \rfloor} \beta_{2k}^{(R)} h^{2k} DD_{2k-1}\mathbf{f}(\mathbf{v}(t)). \tag{11}$$

Now, since Bernoulli numbers define the Taylor expansion of the function $z/(e^z - 1)$ and $b_0 = 1, b_1 = -1/2$ and $b_j = 0$ for the other odd $j$, we have:

$$\frac{z\sigma(e^z)}{\rho(e^z)} = \frac{1}{2}\frac{z(e^z+1)}{e^z - 1} = \frac{z}{e^z-1} + \frac{z}{2} = 1 + \sum_{j=1}^{\infty} \frac{b_{2j}}{(2j)!} z^{2j}.$$

Thus, we can write (11) as

$$\dot{\mathbf{v}}(t) = \left( \left( I + \sum_{j=1}^{\infty} \frac{b_{2j}}{(2j)!} h^{2j} D^{2j} \right) \left( I + \sum_{k=1}^{\lceil R/2 \rceil -1} 2\beta_{2k+1}^{(R)} h^{2k} D_{2k} \right) - \sum_{k=1}^{\lfloor R/2 \rfloor} \beta_{2k}^{(R)} h^{2k} DD_{2k-1} \right) \mathbf{f}(\mathbf{v}(t)).$$

Adding and subtracting terms involving the classical derivative operator $D^{2k}, D^{2k-1}$, we get

$$\begin{aligned}\dot{\mathbf{v}}(t) = \Bigg( & \left( I + \sum_{j=1}^{\infty} \frac{b_{2j}}{(2j)!} h^{2j} D^{2j} \right) \\ & \left( I + \sum_{k=1}^{\lceil R/2 \rceil -1} 2\beta_{2k+1}^{(R)} h^{2k} D^{2k} + \sum_{k=1}^{\lceil R/2 \rceil -1} 2\beta_{2k+1}^{(R)} h^{2k} (D_{2k} - D^{2k}) \right) \\ & - \sum_{k=1}^{\lfloor R/2 \rfloor} \beta_{2k}^{(R)} h^{2k} DD^{2k-1} - \sum_{k=1}^{\lfloor R/2 \rfloor} \beta_{2k}^{(R)} h^{2k} D(D_{2k-1} - D^{2k-1}) \Bigg) \mathbf{f}(\mathbf{v}(t)).\end{aligned}$$

that we recast as

$$\dot{\mathbf{v}}(t) = \left(\left(I + \sum_{j=1}^{\infty} \frac{b_{2j}}{(2j)!} h^{2j} D^{2j}\right)\left(I + \sum_{k=1}^{\lceil R/2\rceil-1} 2\beta_{2k+1}^{(R)} h^{2k} D^{2k}\right) - \sum_{k=1}^{\lfloor R/2\rfloor} \beta_{2k}^{(R)} h^{2k} D^{2k}\right) \mathbf{f}(\mathbf{v}(t)) + \left(\left(I + \sum_{j=1}^{\infty} \frac{b_{2j}}{(2j)!} h^{2j} D^{2j}\right)\left(\sum_{k=1}^{\lceil R/2\rceil-1} 2\beta_{2k+1}^{(R)} h^{2k} (D_{2k} - D^{2k})\right) - \sum_{k=1}^{\lfloor R/2\rfloor} \beta_{2k}^{(R)} h^{2k} D(D_{2k-1} - D^{2k-1})\right) \mathbf{f}(\mathbf{v}(t)). \tag{12}$$

Since $\mathbf{v}(t) = \mathbf{y}(t) + O(h^{2R})$, due to the regularity conditions on the function $\mathbf{f}$, we see that $(D^i - D_i)\mathbf{f}(\mathbf{v}(t)) = O(h^{2R}), i = 1, \dots, R-1$ and hence the solution $\mathbf{v}(t)$ of (12) is $O(h^{2R+2})$-close to the solution of the following initial value problem

$$\dot{\mathbf{w}}(t) = \mathbf{f}(\mathbf{w}(t)) + \sum_{j=R}^{\infty} \delta_j h^{2j} D^{2j} \mathbf{f}(\mathbf{w}(t)), \tag{13}$$

with:

$$\delta_j := \sum_{k=0}^{\lceil R/2\rceil-1} \frac{b_{2(j-k)}}{(2(j-k))!} 2\beta_{2k+1}^{(R)}, \quad j \geq R.$$

that has been derived from (12) by neglecting the sums containing the derivatives $D_{2k}, D_{2k-1}$. Observe that $\delta_j = 0$ for $j = 1, \dots, R-1$, since the method is of order $2R$ (see [2], Theorem 3.1, page 340). We may interpret (13) as the modified equation of a one-step method $\mathbf{y}_1 = \Phi_h(\mathbf{y}_0)$, where $\Phi_h$ is evidently the time-$h$ flow associated with (13). Expanding the solution of (13) in Taylor series, we get the modified initial value differential equation associated with the numerical scheme by coupling (13) with the initial condition $\mathbf{w}(t_0) = \mathbf{y}_0$. Thus, $\Phi_h$ is a B-series integrators. The proof of the conjugated symplecticity of $\Phi_h$ follows exactly the same steps of the analogous proof in Theorem 1 of [4]. Since $\Psi_h(\mathbf{y}) = \Phi_h(\mathbf{y}) + O(h^{2R+3})$ and $\Phi_h$ is conjugate-symplectic, the result follows using the same global change of coordinates $\chi_h(\mathbf{y})$ associated to $\Phi_h$. □

We report in Figure 1 the bottom-rigth picture of Figure 2 of [1], related to the Kepler problem, where we noticed that the error in the second component of the Lenz vector was not correctly computed, for completness Figure 1 also reports the error in the first component of the Lenz vector. To stress that the methods show a good long time behavior for Hamiltonian problems, we report also, in Figure 2 the results using a longer integration interval of $10^5$ periods and all the other parameters unchanged. In the pictures we report the maximum error in each period for the Hamiltonian function, the angular mument and the Lenz vector. The results remain consistent, showing a linear grows in the error and in the Lenz vector and a near conservation of the Hamiltonian and of the angular moment.

All the other results in the paper do not change.

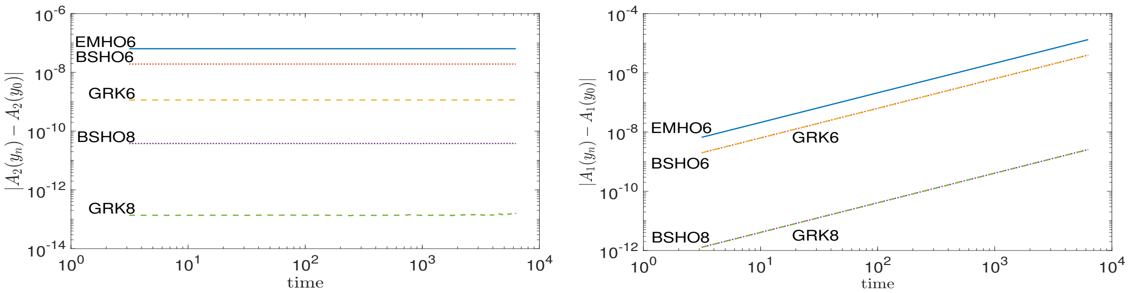


**Figure 1.** Kepler problem: results for the sixth (BSHO6, red dotted line) and eighth (BSHO8, purple dotted line) order BSHO methods, sixth order Euler–Maclaurin method (EMHO6, blue solid line) and sixth (Gauss–Runge–Kutta (GRK6), yellow dashed line) and eighth (GRK8-green dashed line) order Gauss methods. (**Left**) error in the second component of the Lenz vector; (**Right**) error in the first component of the Lenz vector.

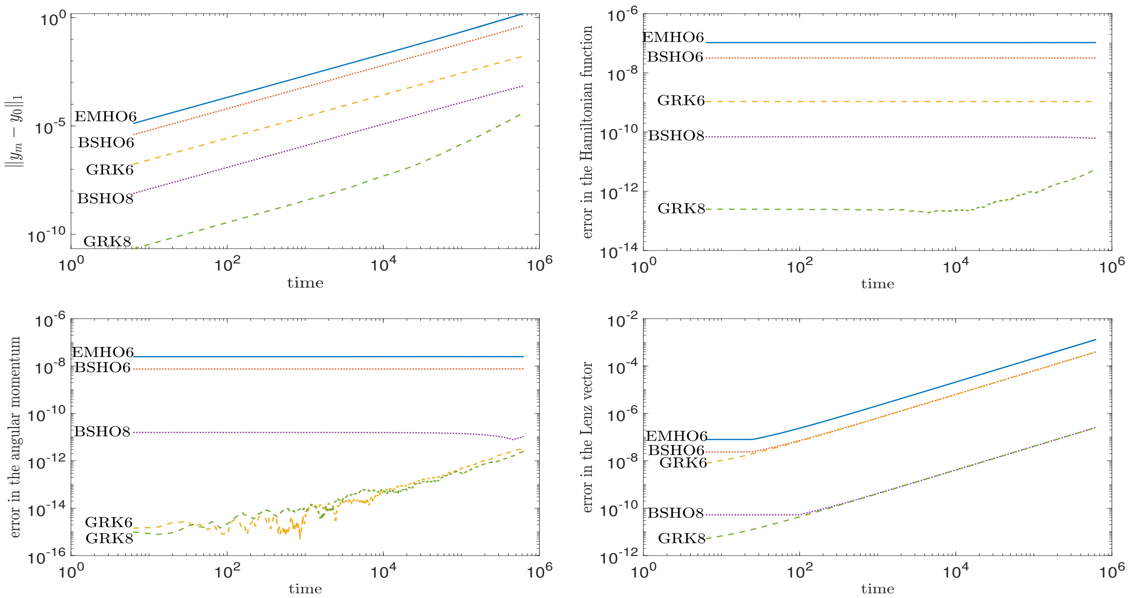


**Figure 2.** Kepler problem: results for the sixth (BSHO6, red dotted line) and eighth (BSHO8, purple dotted line) order BSHO methods, sixth order Euler–Maclaurin method (EMHO6, blue solid line) and sixth (Gauss–Runge–Kutta (GRK6), yellow dashed line) and eighth (GRK8-green dashed line) order Gauss methods. (**Top-left**) Absolute error of the numerical solution; (**Top-right**) error in the Hamiltonian function; (**Bottom-left**) error in the angular momentum; (**Bottom-right**) error in the first component of the Lenz vector.

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