Numerical Algorithms
https://doi.org/10.1007/s11075-020-00898-6

ORIGINAL PAPER

# Symplecticness conditions of some low order partitioned methods for non-autonomous Hamiltonian systems

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Received: 8 October 2019 / Accepted: 27 January 2020 / Published online: 28 May 2020


**Abstract**
We consider the application of partitioned Runge-Kutta (PRK) methods to non-autonomous Hamiltonian systems. Necessary and sufficient conditions for the symplecticness of PRK methods are given, more particularly for two low order PRK methods: the partitioned (explicit-implicit) Euler method and the 2-stage Lobatto IIIA-B PRK method. Both methods are often the basis of composition schemes of higher order. In particular for irreducible PRK methods we show the necessity for the nodes of the two underlying PRK methods to be equal.

**Keywords** Hamiltonian systems · Non-autonomous · Partitioned Runge-Kutta methods · Symplecticness

## 1 Introduction

We consider the numerical solution of non-autonomous Hamiltonian systems

$$\dot{q} = \nabla_p H(t, q, p), \quad \dot{p} = -\nabla_q H(t, q, p) \tag{1.1}$$

with $(t, q, p) \in \mathbb{R}\times\mathbb{R}^n\times\mathbb{R}^n$ and where we assume that $H \in \mathcal{C}^2(\mathbb{R}\times\mathbb{R}^n\times\mathbb{R}^n, \mathbb{R})$. The time-dependent flow of such systems preserves the standard symplectic two-form

$$\omega = \sum_{k=1}^{n} dq_k \wedge dp_k, \tag{1.2}$$

but generally not the Hamiltonian $H$. For such problems it has been shown in several papers that preservation of $\omega$ is a desirable property for a numerical scheme [2, 5–7, 11].

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In this paper we consider necessary and sufficient conditions for symplecticness of partitioned Runge-Kutta (PRK) methods when applied to non-autonomous Hamiltonian systems (1.1). We are especially interested in some low order PRK methods. Low order methods are often used in composition schemes to obtain higher order methods [4, 9]. The low order methods considered in this paper are the *partitioned (explicit-implicit) Euler method* (also known as the symplectic Euler method) and the *2-stage Lobatto IIIA-B PRK method* (also known as the Störmer/Verlet/leapfrog method in various other contexts [9]). For autonomous systems the partitioned Euler method can be obtained as a combination of the explicit and implicit Euler methods, and the 2-stage Lobatto IIIA-B PRK method can be obtained as a combination of the trapezoidal and midpoint rules. These PRK methods are known to be symplectic for autonomous Hamiltonian systems. Using the matrix characterization of symplecticness (2.5) we show in this note that for general non-autonomous Hamiltonian systems (1.1) it is necessary for the nodes $c_j, \widehat{c}_j$ of these PRK methods to be equal in order for these methods to be symplectic. Therefore, for non-autonomous Hamiltonian systems, the partitioned Euler method, respectively the 2-stage Lobatto IIIA-B PRK method, cannot be obtained as a straightforward combination of the explicit and implicit Euler methods, respectively of the trapezoidal and midpoint rules. Special care must be taken in treating the independent time variable $t$. In particular for symplecticness the famous simplifying assumption $C(1)$ (i.e., $\sum_{j=1}^{s} a_{ij} = c_i$ for $i = 1, \ldots, s$), cannot hold for the two underlying methods of these low order PRK methods. We also show the necessity of the conditions $\widehat{c}_j = c_j$ for $j = 1, \ldots, s$ for general irreducible PRK methods satisfying $\widehat{b}_j = b_j \neq 0$ for $j = 1, \ldots, s$ though the only methods of interest which a priori may not satisfy the conditions $\widehat{c}_j = c_j$ for $j = 1, \ldots, s$ are the partitioned Euler method and possibly the 2-stage Lobatto IIIA-B PRK method (e.g., when considered as a combination of the trapezoidal rule and of the midpoint rule), and composition schemes based on these methods.

## 2 Partitioned Runge-Kutta methods

To ease the presentation hereafter we consider partitioned systems of ODEs

$$\dot{q} = f(t, q, p), \qquad \dot{p} = g(t, q, p) \tag{2.1}$$

with $(t, q, p) \in \mathbb{R} \times \mathbb{R}^m \times \mathbb{R}^n$ and $f \in \mathcal{C}^1(\mathbb{R} \times \mathbb{R}^m \times \mathbb{R}^n, \mathbb{R}^m)$, $g \in \mathcal{C}^1(\mathbb{R} \times \mathbb{R}^m \times \mathbb{R}^n, \mathbb{R}^n)$. Non-autonomous Hamiltonian systems (1.1) simply correspond to $m = n$ and

$$f(t, q, p) = \nabla_p H(t, q, p), \qquad g(t, q, p) = -\nabla_q H(t, q, p).$$

Hamiltonians of the form

$$H(t, q, p) = T(t, p) + U(t, q) \tag{2.2}$$

are called *separable*. Hence, when $f(t, q, p) = f(t, p)$ and $g(t, q, p) = g(t, q)$ we will call the system of ODEs $\dot{q} = f(t, p)$, $\dot{p} = g(t, q)$ *separable* as well.

General partitioned Runge-Kutta methods applied to (2.1) are defined as follows, see, e.g., [13]:

**Definition 2.1** An *s-stage partitioned Runge-Kutta (PRK) method* with coefficients $b_j, c_j, a_{ij}, \widehat{b}_j, \widehat{c}_j, \widehat{a}_{ij}$ for $i, j = 1, \ldots, s$ applied to (1.1) with initial conditions $q(t_0) = q_0$, $p(t_0) = p_0$, stepsize $h$ is given by the system of equations

$$\begin{aligned} Q_i &= q_0 + h \sum_{j=1}^{s} a_{ij} f(T_j, Q_j, P_j), \quad P_i = p_0 + h \sum_{j=1}^{s} \widehat{a}_{ij} g(S_j, Q_j, P_j) \quad (2.3a)\\ &\text{for } i = 1, \ldots, s,\\ q_1 &= q_0 + h \sum_{j=1}^{s} b_j f(T_j, Q_j, P_j), \quad p_1 = p_0 + h \sum_{j=1}^{s} \widehat{b}_j g(S_j, Q_j, P_j) \quad (2.3b) \end{aligned}$$

where $T_j := t_0 + c_j h$ and $S_j := t_0 + \widehat{c}_j h$ for $j = 1, \ldots, s$. The coefficients of PRK methods can be expressed with two Butcher tableaux

$$\begin{array}{c|ccc} c_1 & a_{11} & \cdots & a_{1s} \\ \vdots & \vdots & \ddots & \vdots \\ c_s & a_{s1} & \cdots & a_{ss} \\ \hline & b_1 & \cdots & b_s \end{array} \qquad \begin{array}{c|ccc} \widehat{c}_1 & \widehat{a}_{11} & \cdots & \widehat{a}_{1s} \\ \vdots & \vdots & \ddots & \vdots \\ \widehat{c}_s & \widehat{a}_{s1} & \cdots & \widehat{a}_{ss} \\ \hline & \widehat{b}_1 & \cdots & \widehat{b}_s \end{array}.$$

Notice that when the (2.1) are disconnected, i.e., $\dot{q} = f(t, q)$ and $\dot{p} = g(t, p)$, we obtain two disconnected Runge-Kutta methods applied to these two distinct systems of ODEs.

In this paper we will use the notation

$$J_n := \begin{bmatrix} O & I_n \\ -I_n & O \end{bmatrix} \in \mathbb{R}^{2n \times 2n}$$

for the standard symplectic matrix. First we state sufficient conditions for a PRK method (2.3) to be a symplectic transformation of $\mathbb{R}^n \times \mathbb{R}^n$ [13, Theorem 2.6]:

**Theorem 2.1** *Consider the non-autonomous Hamiltonian system* (1.1) *and a PRK method* (2.3). *Suppose that the PRK coefficients satisfy*

$$\begin{aligned} \widehat{b}_j &= b_j \quad \textit{for } j = 1, \ldots, s, && (2.4a)\\ \widehat{c}_j &= c_j \quad \textit{for } j = 1, \ldots, s, && (2.4b)\\ \widehat{b}_i a_{ij} + b_j \widehat{a}_{ji} - \widehat{b}_i b_j &= 0 \quad \textit{for } i, j = 1, \ldots, s. && (2.4c) \end{aligned}$$

*Then the map* $\Phi_{t_0+h,t_0}(q_0, p_0) := (q_1, p_1)$ *is a symplectic transformation of* $(\mathbb{R}^n \times \mathbb{R}^n, \omega)$ *into* $(\mathbb{R}^n \times \mathbb{R}^n, \omega)$ *for the constant differential 2-form* $\omega := \sum_{k=1}^{n} dq_k \wedge dp_k$, *i.e., $\omega$ is preserved by the mapping* $\Phi_{t_0+h,t_0}$, *i.e.,*

$$\sum_{k=1}^{n} dq_{1k} \wedge dp_{1k} = \sum_{k=1}^{n} dq_{0k} \wedge dp_{0k}.$$

*In matrix form we obtain equivalently*

$$\begin{bmatrix} \frac{\partial q_1}{\partial q_0} & \frac{\partial q_1}{\partial p_0} \\ \frac{\partial p_1}{\partial q_0} & \frac{\partial p_1}{\partial p_0} \end{bmatrix}^T J_n \begin{bmatrix} \frac{\partial q_1}{\partial q_0} & \frac{\partial q_1}{\partial p_0} \\ \frac{\partial p_1}{\partial q_0} & \frac{\partial p_1}{\partial p_0} \end{bmatrix} = J_n. \tag{2.5}$$

Various proofs can be obtained by simple extensions of the proofs given for autonomous Hamiltonian systems for example in [4, 9, 12, 14]. Here, we give a short argument based on an explicit generating function.

*Proof* For $|h|$ sufficiently small the map $(q_0, p_0) \mapsto (q_1, p_1)$ satisfies

$$p_0 - \nabla_{q_0} S_2^h(t_0, q_0, p_1) = 0, \qquad q_1 - \nabla_{p_1} S_2^h(t_0, q_0, p_1) = 0$$

where $S_2^h(t_0, q_0, p_1)$ is a globally defined generating function of type II given by

$$\begin{aligned} S_2^h(t_0, q_0, p_1) := q_0^T p_1 + h \sum_{i=1}^{s} b_i H(T_i, Q_i, P_i) \\ -h^2 \sum_{i=1}^{s} \sum_{j=1}^{s} b_i a_{ij} \nabla_q H(T_i, Q_i, P_i)^T \nabla_p H(T_j, Q_j, P_j). \end{aligned}$$

□

*Remark 2.1* For autonomous Hamiltonian systems, it has been shown in [8] and [9, Theorem VI.7.10, p. 222] that the conditions (2.4a) and (2.4c) are also necessary for irreducible PRK methods (i.e., for PRK methods without equivalent stages, which is equivalent to a certain matrix $\Phi_{PRK} \in \mathbb{R}^{s\times\infty}$ indexed by the stages and by certain elementary differentials/trees to be of full rank $s$, see details in [9, VI.7.3]). The necessity of (2.4c) was first proved in [1] for separable autonomous Hamiltonians.

*Remark 2.2* The main importance in preserving symplecticness resides in the backward error analysis of symplectic PRK methods: for constant stepsizes $h$ the numerical solution of such methods is formally equal to the exact solution of a non-autonomous Hamiltonian system with a global perturbed Hamiltonian $\widetilde{H}_h(t, q, p)$ depending on the stepsize $h$. Precise backward error analysis statements with explicit error bounds are outside the scope of this paper. This type of results has been proved for autonomous Hamiltonian systems [4, 9, 14].

In this paper we are particularly interested by the necessity of the conditions (2.4b) for the partitioned Euler PRK method and the 2-stage Lobatto IIIA-B PRK method for non-autonomous Hamiltonian systems. These two methods are important since they can form the basis of higher order composition schemes. The combination of the explicit Euler and of the implicit Euler method forms a PRK method with Butcher-tableaux

$$\begin{array}{c|c} 0 & 0 \\ \hline & 1 \end{array} \qquad\qquad \begin{array}{c|c} 1 & 1 \\ \hline & 1 \end{array} \tag{2.6}$$

and is known in the literature usually under the name of *symplectic Euler method*. Clearly this irreducible PRK method does not satisfy $c_1 = \widehat{c}_1$ and is thus not symplectic for general non-autonomous Hamiltonian systems according to Theorem 2.2

and Theorem 3.1 hereafter. The 2-stage Lobatto IIIA-IIIB method is sometimes presented in the literature, e.g., in [9, Table II.2.1, p. 39] and [4, p. 49], as a combination of the trapezoidal rule with the midpoint rule, hence having Butcher-tableaux

$$\begin{array}{c|cc} 0 & 0 & 0 \\ 1 & 1/2 & 1/2 \\ \hline & 1/2 & 1/2 \end{array} \qquad \begin{array}{c|cc} 1/2 & 1/2 & 0 \\ 1/2 & 1/2 & 0 \\ \hline & 1/2 & 1/2 \end{array}. \tag{2.7}$$

Clearly this irreducible PRK method satisfies neither $c_1 = \widehat{c}_1$, nor $c_2 = \widehat{c}_2$ and is thus not symplectic for general non-autonomous Hamiltonian systems according to Theorem 2.2 and Theorem 4.1 hereafter. Using the matrix characterization of symplecticness (2.5), we show that the conditions (2.4b) are necessary for the symplecticness of the partitioned Euler method and the 2-stage Lobatto IIIA-B PRK method. We also give the main lines of a proof of the necessity of (2.4b) for irreducible PRK methods satisfying $\widehat{b}_j = b_j \neq 0$ for $j = 1, \ldots, s$. This proof is much more technical and appeals to the results given in [9, VI.7] and [9, Theorem VI.7.10, p. 222]. However, since very few PRK methods of interest may not satisfy the conditions (2.4b), the proofs using the matrix characterization of symplecticness (2.5) for the partitioned Euler methods and the 2-stage Lobatto IIIA-B PRK method are less technical and easier to understand since they are only based on some matrix relations. Note that the 2-stage Lobatto IIIA-B PRK method can also be obtained as a composition of the partitioned Euler methods, see Section 4.

One may argue that the only PRK methods of interest which may not satisfy (2.4b) are the symplectic Euler method and possibly the 2-stage Lobatto IIIA-B PRK method, and any composition scheme based on those low order methods. Nevertheless, for completeness we state a general result of the necessity of conditions (2.4b):

**Theorem 2.2** *Consider the non-autonomous Hamiltonian system* (1.1) *and an irreducible PRK method* (2.3) *with coefficients* $b_j, \widehat{b}_j$ *for* $j = 1, \ldots$ *satisfying*

$$b_j \neq 0, \quad \widehat{b}_j \neq 0 \quad \textit{for } j = 1, \ldots, s. \tag{2.8}$$

*Suppose that the map* $\Phi_{t_0+h,t_0}(q_0, p_0) := (q_1, p_1)$ *is a symplectic transformation for the 2-form* $\omega := \sum_{k=1}^n dq_k \wedge dp_k$ *for any Hamiltonian* $H(t, q, p) \in \mathcal{C}^2(\mathbb{R} \times \mathbb{R}^n \times \mathbb{R}^n, \mathbb{R})$ *for* $|h|$ *sufficiently small. Then the conditions* (2.4b) *are necessary. When* $H(t, q, p) = H(q, p)$ *or for separable Hamiltonians* (2.2) *there is no necessary condition on* $c_j, \widehat{c}_j$ *for* $j = 1, \ldots, s$.

The main lines of a proof are given in Appendix. This Theorem 2.2 which discusses only the necessity of the conditions (2.4b) for irreducible PRK methods is an extension to non-autonomous Hamiltonian systems of [9, Theorem VI.7.10, p. 222] which discusses the sufficiency and necessity of the conditions (2.4a) and (2.4c) of irreducible PRK methods applied to autonomous Hamiltonian systems. As stated before the main consequence of Theorem 2.2 is the non-symplecticness of the symplectic Euler method and of the 2-stage Lobatto IIIA-IIIB method when the nodes are chosen for example as in (2.6) and (2.7). However, simpler direct proofs of Theorem 2.2 are given for these two methods in Sections 3 and 4 respectively.

## 3 The partitioned Euler methods I and II

The Butcher tableaux of the explicit Euler method and of the implicit Euler method are given in (2.6). The two PRK methods based directly on these two methods will not satisfy the relation (2.4b) since these methods have distinct node coefficients $c_1 = 0$ for the explicit Euler method and $\widehat{c}_1 = 1$ for the implicit Euler method (or vice-versa $c_1 = 1$ and $\widehat{c}_1 = 0$). Nevertheless, we can consider more general PRK methods by not setting a priori the values of the nodes $c_1$ and $\widehat{c}_1$. We consider 2 families of partitioned Euler methods applied to (2.1) for various values of the parameters $\alpha, \beta \in \mathbb{R}$ (though it makes little sense to consider values $\alpha, \beta$ outside of the interval $[0, 1]$) as follows: the *partitioned Euler method I (PEI)*

$$\text{PEI}: \quad q_1 = q_0 + hf(t_0 + \alpha h, q_0, p_1), \quad p_1 = p_0 + hg(t_0 + \beta h, q_0, p_1) \tag{3.1}$$

corresponding to the Butcher-tableaux

$$\begin{array}{c|c} c_1 = \alpha & 0 \\ \hline & 1 \end{array} \qquad \begin{array}{c|c} \widehat{c}_1 = \beta & 1 \\ \hline & 1 \end{array}$$

and the *partitioned Euler method II (PEII)*

$$\text{PEII}: \quad q_1 = q_0 + hf(t_0 + \beta h, q_1, p_0), \quad p_1 = p_0 + hg(t_0 + \alpha h, q_1, p_0) \tag{3.2}$$

corresponding to the Butcher-tableaux

$$\begin{array}{c|c} c_1 = \beta & 1 \\ \hline & 1 \end{array} \qquad \begin{array}{c|c} \widehat{c}_1 = \alpha & 0 \\ \hline & 1 \end{array}.$$

Notice that PEII is simply PEI where the roles of $q$ and $p$, respectively, $f$ and $g$, are exchanged. We observe that PEI can be interpreted as an approximate splitting scheme of the type described in [2–5] where the time $t$ is first 'frozen' in $\dot{q} = f(t_0 + \alpha h, q, p)$, $\dot{p} = 0$ before the explicit Euler method is applied and then frozen in $\dot{q} = 0$, $\dot{p} = g(t_0 + \beta h, q, p)$ before the implicit Euler method is applied. An analogous remark holds for PEII. The standard choice for the partitioned Euler methods I and II is $\alpha = 0$, $\beta = 1$, see (2.6). However, we will see in the context of non-autonomous non-separable Hamiltonian systems that the condition $\alpha = \beta$ is essential to preserve symplecticness. For separable ODEs $\dot{q} = f(t, p)$, $\dot{p} = g(t, q)$ we obtain two explicit methodsS

$$\begin{aligned} \text{PEI}: &\quad p_1 = p_0 + hg(t_0 + \beta h, q_0), \quad q_1 = q_0 + hf(t_0 + \alpha h, p_1), \\ \text{PEII}: &\quad q_1 = q_0 + hf(t_0 + \beta h, p_0), \quad p_1 = p_0 + hg(t_0 + \alpha h, q_1). \end{aligned}$$

**Theorem 3.1** *Consider the non-autonomous Hamiltonian system* (1.1) *and the partitioned Euler methods I and II*

$$\text{PEI}: q_1 = q_0 + h\nabla_p H(t_0 + \alpha h, q_0, p_1), \; p_1 = p_0 - h\nabla_q H(t_0 + \beta h, q_0, p_1) \tag{3.3}$$

$$\text{PEII}: q_1 = q_0 + h\nabla_p H(t_0 + \beta h, q_1, p_0), \; p_1 = p_0 - h\nabla_q H(t_0 + \alpha h, q_1, p_0). \tag{3.4}$$

*Then the map* $\Phi_{t_0+h,t_0}(q_0, p_0) := (q_1, p_1)$ *of the partitioned Euler method I (or II) is a symplectic transformation for the 2-form* $\omega := \sum_{k=1}^{n} dq_k \wedge dp_k$ *for any Hamiltonian* $H(t, q, p) \in \mathcal{C}^2(\mathbb{R} \times \mathbb{R}^n \times \mathbb{R}^n, \mathbb{R})$ *for* $|h|$ *sufficiently small if and only* *if $\alpha = \beta$. When $H(t, q, p) = H(q, p)$ or for separable Hamiltonians (2.2) both methods are symplectic without any condition on $\alpha$, $\beta$.*

*Proof* We cannot apply Theorem 2.1 when $\alpha \neq \beta$ since the partitioned Euler methods I and II do not satisfy (2.4b). Let us consider the partitioned Euler method I (3.3). We have

$$\begin{bmatrix} \frac{\partial q_1}{\partial q_0} & \frac{\partial q_1}{\partial p_0} \\ \frac{\partial p_1}{\partial q_0} & \frac{\partial p_1}{\partial p_0} \end{bmatrix} = \begin{bmatrix} I_n + h(\partial_q \nabla_p H)(t_0 + \alpha h, q_0, p_1) & O \\ -h(\partial_q \nabla_q H)(t_0 + \beta h, q_0, p_1) & I_n \end{bmatrix}$$
$$+ \begin{bmatrix} O & h(\partial_p \nabla_p H)(t_0 + \alpha h, q_0, p_1) \\ O & -h(\partial_p \nabla_q H)(t_0 + \beta h, q_0, p_1) \end{bmatrix} \begin{bmatrix} \frac{\partial q_1}{\partial q_0} & \frac{\partial q_1}{\partial p_0} \\ \frac{\partial p_1}{\partial q_0} & \frac{\partial p_1}{\partial p_0} \end{bmatrix}$$

which can be reexpressed as

$$A \begin{bmatrix} \frac{\partial q_1}{\partial q_0} & \frac{\partial q_1}{\partial p_0} \\ \frac{\partial p_1}{\partial q_0} & \frac{\partial p_1}{\partial p_0} \end{bmatrix} = B$$

where

$$A := \begin{bmatrix} I_n & -h(\partial_p \nabla_p H)(t_0 + \alpha h, q_0, p_1) \\ O & I_n + h(\partial_p \nabla_q H)(t_0 + \beta h, q_0, p_1) \end{bmatrix},$$
$$B := \begin{bmatrix} I_n + h(\partial_q \nabla_p H)(t_0 + \alpha h, q_0, p_1) & O \\ -h(\partial_q \nabla_q H)(t_0 + \beta h, q_0, p_1) & I_n \end{bmatrix}.$$

For the symplecticness conditions we have

$$\begin{bmatrix} \frac{\partial q_1}{\partial q_0} & \frac{\partial q_1}{\partial p_0} \\ \frac{\partial p_1}{\partial q_0} & \frac{\partial p_1}{\partial p_0} \end{bmatrix}^T J_n \begin{bmatrix} \frac{\partial q_1}{\partial q_0} & \frac{\partial q_1}{\partial p_0} \\ \frac{\partial p_1}{\partial q_0} & \frac{\partial p_1}{\partial p_0} \end{bmatrix} = J_n \iff (A^{-1}B)^T J_n A^{-1} B = J_n$$
$$\iff A^{-T} J_n A^{-1} = B^{-T} J_n B^{-1}.$$

By inverting the last relation and from $J_n^{-1} = -J_n$ we obtain $A J_n A^T = B J_n B^T$. We easily get

$$A J_n A^T = \begin{bmatrix} O & I_n + h(\partial_q \nabla_p H)(t_0 + \beta h, q_0, p_1) \\ -I_n - h(\partial_p \nabla_q H)(t_0 + \beta h, q_0, p_1) & O \end{bmatrix},$$

$$B J_n B^T = \begin{bmatrix} O & I_n + h(\partial_q \nabla_p H)(t_0 + \alpha h, q_0, p_1) \\ -I_n - h(\partial_p \nabla_q H)(t_0 + \alpha h, q_0, p_1) & O \end{bmatrix}.$$

Hence, the condition $A J_n A^T = B J_n B^T$ is clearly satisfied for any Hamiltonian $H(t, q, p)$ if and only if $\alpha = \beta$. When $H(t, q, p) \equiv H(q, p)$ or $(\partial_p \nabla_q H)(t, q, p) \equiv 0$ we always have $A J_n A^T = B J_n B^T$ without any condition on $\alpha$, $\beta$. The proof for the partitioned Euler method II (3.4) can be obtained in a similar fashion. □

For a general non-autonomous Hamiltonian system we propose the choice $c_1 = \widehat{c}_1 = 1/2$ which together with $b_1 = \widehat{b}_1 = 1$ corresponds to the quadrature formula given by the midpoint rule. Even for ODEs $\dot{y} = f(t, y)$ the version of the explicit Euler method with $c_1 = 1/2$ has the advantage of integrating polynomials $p(t)$ of degree at most one exactly whereas with $c_1 = 0$ only constants are integrated exactly. A similar remark holds for the implicit Euler method. The Butcher-tableaux of these modified explicit and implicit Euler methods read as follows

$$\begin{array}{c|c} 1/2 & 0 \\ \hline & 1 \end{array} \qquad \begin{array}{c|c} 1/2 & 1 \\ \hline & 1 \end{array}.$$

We actually recommend using both the explicit Euler method and the implicit Euler method with a node equal to 1/2 even for general non-autonomous systems of ODEs. We are not aware of such a recommendation for these two methods elsewhere in the literature. Our analysis has thus shed a new light on these two basic methods.

## 4 The 2-stage Lobatto IIIA-B PRK method

The Butcher-tableaux of coefficients of the $s = 2$-stage Lobatto IIIA-B PRK method of order 2 are given by

$$\begin{array}{c|cc} 0 & 0 & 0 \\ 1 & 1/2 & 1/2 \\ \hline A & 1/2 & 1/2 \end{array} \qquad \begin{array}{c|cc} 0 & 1/2 & 0 \\ 1 & 1/2 & 0 \\ \hline B & 1/2 & 1/2 \end{array}. \tag{4.1}$$

The coefficients of the 2-stage Lobatto IIIA and IIIB methods are based on the quadrature formula given by the trapezoidal rule and are defined through some so-called simplifying assumptions, see [10, Chapter IV.5].

The coefficients of this method are easily shown to satisfy the sufficient conditions (2.4) for symplecticness of Theorem 2.1. This method applied to (2.1) reads as follows:

$$\begin{aligned}
Q_1 &= q_0, \\
Q_2 &= q_0 + h\left(\frac{1}{2}f(T_1, Q_1, P_1) + \frac{1}{2}f(T_2, Q_2, P_2)\right), \\
P_1 &= p_0 + h\frac{1}{2}g(T_1, Q_1, P_1), \\
P_2 &= p_0 + h\frac{1}{2}g(T_1, Q_1, P_1), \\
q_1 &= q_0 + h\left(\frac{1}{2}f(T_1, Q_1, P_1) + \frac{1}{2}f(T_2, Q_2, P_2)\right), \\
p_1 &= p_0 + h\left(\frac{1}{2}g(T_1, Q_1, P_1) + \frac{1}{2}g(T_2, Q_2, P_2)\right),
\end{aligned}$$

where

$$T_1 := t_0, \quad T_2 := t_0 + h, \quad t_1 := t_0 + h.$$

From $T_1 = t_0$, $Q_1 = q_0$, $T_2 = t_1$, $Q_2 = q_1$, $P_2 = P_1$, and denoting $p_{1/2} := P_1 = P_2$ this method can be simplified to

$$p_{1/2} = p_0 + h\frac{1}{2}g(t_0, q_0, p_{1/2}), \tag{4.2a}$$

$$q_1 = q_0 + h\left(\frac{1}{2}f(t_0, q_0, p_{1/2}) + \frac{1}{2}f(t_1, q_1, p_{1/2})\right), \tag{4.2b}$$

$$p_1 = p_{1/2} + h\frac{1}{2}g(t_1, q_1, p_{1/2}). \tag{4.2c}$$

The equations for $p_{1/2}$ and $q_1$ are implicit. This method is also known under the names of *Störmer/Verlet/leapfrog method* depending on the context. Of course one can exchange the roles of $q$ and $p$, respectively $f$ and $g$, to obtain another nonequivalent version of the Störmer/Verlet/leapfrog method

$$q_{1/2} = q_0 + h\frac{1}{2}f(t_0, q_{1/2}, p_0), \tag{4.3a}$$

$$p_1 = p_0 + h\left(\frac{1}{2}g(t_0, q_{1/2}, p_0) + \frac{1}{2}g(t_1, q_{1/2}, p_1)\right), \tag{4.3b}$$

$$q_1 = q_{1/2} + h\frac{1}{2}f(t_1, q_{1/2}, p_1) \tag{4.3c}$$

which could be named as the Störmer/Verlet/leapfrog method II and which formally corresponds to a 2-stage Lobatto IIIA-B PRK method applied to (2.1) where the roles of $q$ and $p$, respectively, $f$ and $g$, are exchanged. We will not explicitly consider this method (4.3) hereafter, completely similar results to the ones presented below for (4.2) hold for the method (4.3) as well.

The method (4.2) (denoted $\rho_h$) can also be interpreted as the composition of the partitioned Euler method I (3.1) with stepsize $h/2$ and $\alpha_I = \beta_I = 0$ (denoted $\Phi_{h/2}$) and of the partitioned Euler method II (3.2) with stepsize $h/2$ and $\beta_{II} = \alpha_{II} = 1$ (denoted $\widetilde{\Phi}_{h/2}$), i.e., $\rho_h = \widetilde{\Phi}_{h/2} \circ \Phi_{h/2}$ since we get for $\rho_h$

$$\begin{aligned}
q_{1/2} &= q_0 + \frac{h}{2}f(t_0, q_0, p_{1/2}),\\
p_{1/2} &= p_0 + \frac{h}{2}g(t_0, q_0, p_{1/2}),\\
q_1 &= q_{1/2} + \frac{h}{2}f(t_{1/2} + h/2, q_1, p_{1/2}) = q_0 + \frac{h}{2}f(t_0, q_0, p_{1/2}) + \frac{h}{2}f(t_1, q_1, p_{1/2}),\\
p_1 &= p_{1/2} + \frac{h}{2}g(t_{1/2} + h/2, q_1, p_{1/2}) = p_{1/2} + \frac{h}{2}g(t_1, q_1, p_{1/2}),
\end{aligned}$$

leading to (4.2). This gives an alternative proof to its symplecticness for non-autonomous Hamiltonian systems (1.1), see Theorem 3.1, since the partitioned Euler methods I and II have their node coefficients satisfy $\alpha_I = \beta_I$ and $\beta_{II} = \alpha_{II}$ here. For separable Hamiltonians (2.2) we obtain an explicit method

$$\begin{aligned} p_{1/2} &= p_0 - h\frac{1}{2}\nabla_q U(t_0, q_0), \\ q_1 &= q_0 + h\left(\frac{1}{2}\nabla_p T(t_0, p_{1/2}) + \frac{1}{2}\nabla_p T(t_1, p_{1/2})\right), \\ p_1 &= p_{1/2} - h\frac{1}{2}\nabla_q U(t_1, q_1). \end{aligned}$$

It has the advantage to require one evaluation of the function $\nabla_q U(t, q)$ per step since the value $\nabla_q U(t_1, q_1)$ can be reused for the next step. For general nonautonomous Hamiltonian systems we have the following result:

**Theorem 4.1** *Consider non-autonomous Hamiltonian systems* (1.1) *and the modified 2-stage Lobatto IIIA-B PRK method*

$$p_{1/2} = p_0 - h\frac{1}{2}\nabla_q H(t_0 + \widehat{c}_1 h, q_0, p_{1/2}), \tag{4.4a}$$

$$q_1 = q_0 + h\left(\frac{1}{2}\nabla_p H(t_0 + c_1 h, q_0, p_{1/2}) + \frac{1}{2}\nabla_p H(t_0 + c_2 h, q_1, p_{1/2})\right), \tag{4.4b}$$

$$p_1 = p_{1/2} - h\frac{1}{2}\nabla_q H(t_0 + \widehat{c}_2 h, q_1, p_{1/2}), \tag{4.4c}$$

*corresponding to a modified 2-stage Lobatto IIIA-B PRK method with coefficients*

$$\begin{array}{c|cc} c_1 & 0 & 0 \\ c_2 & 1/2 & 1/2 \\ \hline & 1/2 & 1/2 \end{array} \qquad \begin{array}{c|cc} \widehat{c}_1 & 1/2 & 0 \\ \widehat{c}_2 & 1/2 & 0 \\ \hline & 1/2 & 1/2 \end{array} \tag{4.5}$$

*where the nodes $c_1, c_2, \widehat{c}_1, \widehat{c}_2$ are free. Then the map $\Phi_{t_0+h,t_0}(q_0, p_0) := (q_1, p_1)$ is a symplectic transformation for the 2-form $\omega := \sum_{k=1}^{n} dq_k \wedge dp_k$ for any Hamiltonian $H(t, q, p) \in \mathcal{C}^2(\mathbb{R} \times \mathbb{R}^n \times \mathbb{R}^n, \mathbb{R})$ for $|h|$ sufficiently small if and only if $\widehat{c}_1 = c_1$ and $\widehat{c}_2 = c_2$. When $H(t, q, p) = H(q, p)$ or for separable Hamiltonians* (2.2) *there is no condition on $c_1, c_2, \widehat{c}_1, \widehat{c}_2$ for symplecticness.*

*Proof* One can interpret the method (4.4) as the composition of the partitioned Euler method I (3.3) with stepsize $h/2$ and $\alpha_I = 2c_1, \beta_I = 2\widehat{c}_1$ and of the partitioned

Euler method II (3.4) with stepsize $h/2$ and $\beta_{II} = 2c_2 - 1$, $\alpha_{II} = 2\widehat{c}_2 - 1$. Denoting $t_{1/2} := t_0 + h/2$, we have

$$\begin{aligned} q_{1/2} &= q_0 + \frac{h}{2}\nabla_p H(t_0 + \alpha_I h/2, q_0, p_{1/2}),\\ p_{1/2} &= p_0 - \frac{h}{2}\nabla_q H(t_0 + \beta_I h/2, q_0, p_{1/2}),\\ q_1 &= q_{1/2} + \frac{h}{2}\nabla_p H(t_{1/2} + \beta_{II} h/2 q_1, p_{1/2}),\\ p_1 &= p_{1/2} - \frac{h}{2}\nabla_q H(t_{1/2} + \alpha_{II} h/2, q_1, p_{1/2}) \end{aligned}$$

which corresponds to the PRK method with Butcher-tableaux (4.5) and nodes

$$c_1 = \frac{\alpha_I}{2}, \quad c_2 = \frac{1+\beta_{II}}{2}, \quad \widehat{c}_1 = \frac{\beta_I}{2}, \quad \widehat{c}_2 = \frac{1+\alpha_{II}}{2}.$$

We have

$$\left(\frac{\partial(q_1, p_1)}{\partial(q_0, p_0)}\right) = \left(\frac{\partial(q_1, p_1)}{\partial(q_{1/2}, p_{1/2})}\right)\left(\frac{\partial(q_{1/2}, p_{1/2})}{\partial(q_0, p_0)}\right)$$

and

$$A_1\left(\frac{\partial(q_{1/2}, p_{1/2})}{\partial(q_0, p_0)}\right) = B_1, \qquad A_2\left(\frac{\partial(q_1, p_1)}{\partial(q_{1/2}, p_{1/2})}\right) = B_2$$

where

$$\begin{aligned} A_1 &:= \begin{bmatrix} I_n & -\frac{h}{2}(\partial_p \nabla_p H)(t_0 + \alpha_I h/2, q_0, p_{1/2}) \\ O & I_n + \frac{h}{2}(\partial_p \nabla_q H)(t_0 + \beta_I h/2, q_0, p_{1/2}) \end{bmatrix},\\ B_1 &:= \begin{bmatrix} I_n + \frac{h}{2}(\partial_q \nabla_p H)(t_0 + \alpha_I h/2, q_0, p_{1/2}) & O \\ -\frac{h}{2}(\partial_q \nabla_q H)(t_0 + \beta_I h/2, q_0, p_{1/2}) & I_n \end{bmatrix},\\ A_2 &:= \begin{bmatrix} I_n - \frac{h}{2}(\partial_q \nabla_p H)(t_{1/2} + \beta_{II} h/2, q_1, p_{1/2}) & O \\ \frac{h}{2}(\partial_q \nabla_q H)(t_{1/2} + \alpha_{II} h/2, q_1, p_{1/2}) & I_n \end{bmatrix},\\ B_2 &:= \begin{bmatrix} I_n & \frac{h}{2}(\partial_p \nabla_p H)(t_{1/2} + \beta_{II} h/2, q_1, p_{1/2}) \\ O & I_n - \frac{h}{2}(\partial_p \nabla_q H)(t_{1/2} + \alpha_{II} h/2, q_1, p_{1/2}) \end{bmatrix}. \end{aligned}$$

For symplecticness we have the equivalent conditions

$$\begin{aligned} \left(\frac{\partial(q_1, p_1)}{\partial(q_0, p_0)}\right)^T J_n \left(\frac{\partial(q_1, p_1)}{\partial(q_0, p_0)}\right) = J_n \quad &\Longleftrightarrow \\ (A_1^{-1}B_1)^T (A_2^{-1}B_2)^T J_n (A_2^{-1}B_2)(A_1^{-1}B_1) = J_n \quad &\Longleftrightarrow \\ A_1^{-1}B_1 J_n B_1^T A_1^{-T} = B_2^{-1}A_2 J_n A_2^T B_2^{-T}. & \end{aligned} \tag{4.6}$$

When $\alpha_I = \beta_I$ and $\beta_{II} = \alpha_{II}$ we have

$$A_1^{-1}B_1 J_n B_1^T A_1^{-T} = J_n = B_2^{-1}A_2 J_n A_2^T B_2^{-T},$$

see the proof of Theorem 3.1. This also holds without any condition on $\alpha_I$, $\beta_I$, $\beta_{II}$, $\alpha_{II}$ when $H(t, q, p) = H(q, p)$ or for separable Hamiltonians (2.2). When $\alpha_I \neq \beta_I$ the value of

$$A_1^{-1}B_1 J_n B_1^T A_1^{-T}$$

generally depends in particular on the values of $(\partial_q \nabla_p H)(t_0 + \alpha_I h/2, q_0, p_{1/2})$ and of $(\partial_q \nabla_p H)(t_0 + \beta_I h/2, q_0, p_{1/2})$ whereas when $\beta_{II} \neq \alpha_{II}$ the value of

$$B_2^{-1} A_2 J_n A_2^T B_2^{-T}$$

generally depends in particular on the values of $(\partial_q \nabla_p H)(t_{1/2} + \beta_{II} h/2, q_1, p_{1/2})$ and of $(\partial_q \nabla_p H)(t_{1/2} + \alpha_{II} h/2, q_1, p_{1/2})$. Hence, it is intuitively clear that we cannot have the equality (4.6) in general for non-separable non-autonomous Hamiltonians $H(t, q, p)$. We can obtain a simple counterexample by considering the Hamiltonian $H(t, q, p) := 2tqp$ for $(t, q, p) \in \mathbb{R} \times \mathbb{R} \times \mathbb{R}$ and we get

$$A_1^{-1} B_1 J_n B_1^T A_1^{-T} = \begin{bmatrix} 0 & \frac{1+h(t_0+\alpha_I h/2)}{1+h(t_0+\beta_I h/2)} \\ -\frac{1+h(t_0+\alpha_I h/2)}{1+h(t_0+\beta_I h/2)} & \end{bmatrix},$$

$$B_2^{-1} A_2 J_n A_2^T B_2^{-T} = \begin{bmatrix} 0 & \frac{1-h(t_0+(1+\beta_{II})h/2)}{1-h(t_0+(1+\alpha_{II})h/2)} \\ -\frac{1-h(t_0+(1+\beta_{II})h/2)}{1-h(t_0+(1+\alpha_{II})h/2)} & 0 \end{bmatrix}.$$

The rational functions

$$\frac{1 + h\,(t_0 + \alpha_I h/2)}{1 + h\,(t_0 + \beta_I h/2)}, \qquad \frac{1 - h\,(t_0 + (1 + \beta_{II})h/2)}{1 - h\,(t_0 + (1 + \alpha_{II})h/2)}$$

are not equal for arbitrary values of $t_0$ and $h$ when $\alpha_I \neq \beta_I$ or $\beta_{II} \neq \alpha_{II}$. Therefore the conditions $\alpha_I = \beta_I$ and $\beta_{II} = \alpha_{II}$ are also necessary for symplecticness, leading to the necessity of the relations $\widehat{c}_1 = c_1$ and $\widehat{c}_2 = c_2$. □

*Remark 4.1* An analogous theorem holds for a similar modification of the Störmer/Verlet/leapfrog method II (4.3).

From Theorem 4.1 we see that there exists a symplectic extension of the 2-stage Lobatto IIIA-B method for non-autonomous Hamiltonian systems satisfying $\widehat{c}_1 = 1/2, \widehat{c}_2 = 1/2$, it must satisfy $c_1 = \widehat{c}_1 = 1/2$, $c_2 = \widehat{c}_2 = 1/2$ and corresponds to the following Butcher-tableaux of coefficients

$$\begin{array}{c|cc} 1/2 & 0 & 0 \\ 1/2 & 1/2 & 1/2 \\ \hline & 1/2 & 1/2 \end{array} \qquad \begin{array}{c|cc} 1/2 & 1/2 & 0 \\ 1/2 & 1/2 & 0 \\ \hline & 1/2 & 1/2 \end{array} \tag{4.7}$$

the second method being equivalent to the midpoint rule. This method applied to (2.1) reads

$$p_{1/2} = p_0 + h\frac{1}{2}g(t_{1/2}, q_0, p_{1/2}), \tag{4.8a}$$

$$q_1 = q_0 + h\left(\frac{1}{2}f(t_{1/2}, q_0, p_{1/2}) + \frac{1}{2}f(t_{1/2}, q_1, p_{1/2})\right), \tag{4.8b}$$

$$p_1 = p_{1/2} + h\frac{1}{2}g(t_{1/2}, q_1, p_{1/2}), \tag{4.8c}$$

and for separable problems we obtain

$$
\begin{aligned}
p_{1/2} &= p_0 + h\frac{1}{2}g(t_{1/2}, q_0),\\
q_1 &= q_0 + hf(t_{1/2}, p_{1/2}),\\
p_1 &= p_{1/2} + h\frac{1}{2}g(t_{1/2}, q_1).
\end{aligned}
$$

It has the disadvantage that it requires two evaluations of the function $g(t, q)$ per step since the value $g(t_{1/2}, q_1)$ cannot be reused for the next step. Notice that the coefficients of the 2-stage Lobatto IIIA-B method given in [9, Table II.2.1, p. 39] and [4, p. 49], see (2.7), satisfy $c_1 = 0, c_2 = 1$ and $\widehat{c}_1 = 1/2, \widehat{c}_2 = 1/2$, hence according to Theorem 4.1 the corresponding method is not symplectic for general non-autonomous Hamiltonian $H(t, q, p)$. Notice that any choice of $c_1, c_2, \widehat{c}_1, \widehat{c}_2$ in (4.5) satisfying $c_2 = 1 - c_1, \widehat{c}_2 = 1 - \widehat{c}_1$ gives a symmetric method of order 2. Any other choice of those coefficients leads to a method of order 1.

## 5 Extended autonomous Hamiltonian systems

By introducing two additional variables $u$ and $s$, the non-autonomous Hamiltonian system (1.1) can be expressed as an extended autonomous Hamiltonian system for the augmented variables $(q, u)$, $(p, s)$ with extended autonomous Hamiltonian

$$
\mathcal{H}(q, u, p, s) := H(s, q, p) - u, \tag{5.1}
$$

giving

$$
\begin{aligned}
\dot{q} &= \nabla_p \mathcal{H}(q, u, p, s) = \nabla_p H(s, q, p), &\text{(5.2a)}\\
\dot{u} &= \mathcal{H}_s(q, u, p, s) = H_t(s, q, p), &\text{(5.2b)}\\
\dot{p} &= -\nabla_q \mathcal{H}(q, u, p, s) = -\nabla_q H(s, q, p), &\text{(5.2c)}\\
\dot{s} &= -\mathcal{H}_u(q, u, p, s) \equiv 1. &\text{(5.2d)}
\end{aligned}
$$

The extended Hamiltonian $\mathcal{H}(q, u, p, s)$ (5.1) is a first integral of the extended autonomous Hamiltonian system (5.2) and thus remains constant along trajectories. The flow of the extended Hamiltonian system (5.2) preserves the extended symplectic two-form

$$
\eta := \sum_{k=1}^{n} dq_k \wedge dp_k + du \wedge ds. \tag{5.3}
$$

The variable $u$ is independent from the rest of the equations and has thus no influence on the other variables. We have $u(t) = H(s(t), q(t), p(t)) + Const$ along solutions of (5.2). Given initial conditions $(q_0, u_0, p_0, s_0)$ at $t_0$ we have $\mathcal{H}(q(t), u(t), p(t), s(t)) \equiv \mathcal{H}(q_0, u_0, p_0, s_0)$ along the corresponding solution.

Moreover, for $u_0 := H(s_0, q_0, p_0)$ we obtain $\mathcal{H}(q(t), u(t), p(t), s(t)) \equiv 0$ along the solution. To have $s(t) \equiv t$ we must choose $s_0 := t_0$. The two-form

$$\sum_{k=1}^{n} dq_k \wedge dp_k + dH(t, q, p) \wedge dt \tag{5.4}$$

is thus preserved in $\mathbb{R} \times \mathbb{R}^n \times \mathbb{R}^n$ by the non-autonomous flow of (1.1). From Stokes' Theorem this corresponds to the preservation of the Poincaré-Cartan integral invariant

$$\int_\gamma \sum_{k=1}^{n} p_k dq_k - H(t, q, p)dt$$

along closed curves $\gamma \in \mathbb{R} \times \mathbb{R}^n \times \mathbb{R}^n$.

We consider the extended autonomous Hamiltonian (5.1) with initial conditions $(q_0, u_0, p_0, s_0)$ at $t_0$. Applied to the corresponding extended autonomous Hamiltonian system (5.2) with these initial conditions, we consider PRK methods given by

$$Q_i = q_0 + h \sum_{j=1}^{s} a_{ij} \nabla_p H(T_j, Q_j, P_j), \; P_i = p_0 - h \sum_{j=1}^{s} \widehat{a}_{ij} \nabla_q H(S_j, Q_j, P_j), \tag{5.5a}$$

$$T_i = s_0 + c_i h, \quad S_i = s_0 + \widehat{c}_i h \qquad \text{for } i = 1, \ldots, s, \tag{5.5b}$$

$$q_1 = q_0 + h \sum_{j=1}^{s} b_j \nabla_p H(T_j, Q_j, P_j), \quad p_1 = p_0 - h \sum_{j=1}^{s} \widehat{b}_j \nabla_q H(S_j, Q_j, P_j), \tag{5.5c}$$

$$u_1 = u_0 + \sum_{j=1}^{s} b_j H_t(T_j, Q_j, P_j), \quad s_1 = s_0 + h, \tag{5.5d}$$

where the variable $s$ is treated like the independent time variable $t$ in (2.3). For $s_0 = t_0$ PRK methods (5.5) satisfying

$$\sum_{j=1}^{s} \widehat{a}_{ij} = \widehat{c}_i = c_i \qquad \text{for } i = 1, \ldots, s, \tag{5.6}$$

are equivalent to PRK methods (2.3) applied to the non-autonomous Hamiltonian system (1.1) with the additional equation for $u_1$. By Theorem 2.1 PRK methods (5.5) satisfying the conditions (2.4) and (5.6) are thus symplectic for the extended Hamiltonian system (5.2), i.e., they preserve the extended two-form (5.3).

However, for PRK methods that do not satisfy (5.6) but (2.4b) such as the partitioned Euler methods I (3.1) and II (3.2) with $\widehat{c}_1 = c_1 \neq 1$, and the modified 2-stage Lobatto IIIA-B PRK method (4.4)–(4.5) with $\widehat{c}_1 = c_1 \neq 1/2$ and $\widehat{c}_2 = c_2 \neq 1/2$, we cannot conclude directly under the assumptions (2.4) that the extended two-form (5.3) is preserved. This is the subject of the following theorem:

**Theorem 5.1** *Consider the extended autonomous Hamiltonian system (5.2) and PRK methods (5.5a) satisfying the assumptions (2.4). Then the map* $\Psi_h(q_0, u_0, p_0, s_0) := (q_1, u_1, p_1, s_1)$ *is a symplectic transformation of* $(\mathbb{R}^{n+1} \times \mathbb{R}^{n+1}, \eta)$ *into* $(\mathbb{R}^{n+1} \times \mathbb{R}^{n+1}, \eta)$ *for the constant two-form* $\eta$ *(5.3), i.e.,* $\eta$ *is preserved by the mapping* $\Psi_h$.

*Proof* The proof given here is analogous to the one given for Theorem 2.1. For $|h|$ sufficiently small the map $(q_0, u_0, p_0, s_0) \mapsto (q_1, u_1, p_1, s_1)$ satisfies

$$p_0 - \nabla_{q_0} S_2^h(q_0, u_0, p_1, s_1) = 0, \qquad s_0 - \partial_{u_0} S_2^h(q_0, u_0, p_1, s_1) = 0,$$
$$q_1 - \nabla_{p_1} S_2^h(q_0, u_0, p_1, s_1) = 0, \qquad u_1 - \partial_{s_1} S_2^h(q_0, u_0, p_1, s_1) = 0$$

where $S_2^h(q_0, u_0, p_1, s_1)$ is a globally defined generating function of type II given by

$$\begin{aligned} S_2^h(q_0, u_0, p_1, s_1) := q_0^T p_1 + u_0 s_1 + h \sum_{i=1}^{s} b_i (H(S_i, Q_i, P_i) - U_i) \\ -h^2 \sum_{i=1}^{s} \sum_{j=1}^{s} b_i a_{ij} (\nabla_q H(S_i, Q_i, P_i)^T \nabla_p H(S_j, Q_j, P_j) \\ -\partial_t H(S_j, Q_j, P_j)) \end{aligned}$$

and where to (5.5) we add

$$U_i = u_0 + \sum_{j=1}^{s} a_{ij} H_t(T_j, Q_j, P_j) \quad \text{for } i = 1, \ldots, s.$$

□

As another possibility, by introducing the additional variables $r, w$, the non-autonomous Hamiltonian system (1.1) can be expressed equivalently as another extended autonomous Hamiltonian system for the augmented variables $(q, r)$, $(p, w)$ with extended autonomous Hamiltonian

$$\widetilde{\mathcal{H}}(q, r, p, w) := \mathcal{H}(q, -w, p, r) = H(r, q, p) + w \tag{5.7}$$

giving

$$\dot{q} = \nabla_p \widetilde{\mathcal{H}}(q, r, p, w) = \nabla_p H(r, q, p), \tag{5.8a}$$
$$\dot{r} = \widetilde{\mathcal{H}}_w(q, r, p, w) \equiv 1, \tag{5.8b}$$
$$\dot{p} = -\nabla_q \widetilde{\mathcal{H}}(q, r, p, w) = -\nabla_q H(r, q, p), \tag{5.8c}$$
$$\dot{w} = -\widetilde{\mathcal{H}}_r(q, r, p, w) = H_t(r, q, p). \tag{5.8d}$$

The extended Hamiltonian $\widetilde{\mathcal{H}}(q, r, p, w)$ (5.7) is a first integral of the extended Hamiltonian system (5.8) and thus remains constant along trajectories. The flow of the extended Hamiltonian system (5.8) preserves the extended symplectic two-form

$$\sum_{k=1}^{n} dq_k \wedge dp_k + dr \wedge dw.$$

The variable $w$ is independent from the rest of the equations and has thus no influence on the other variables. We have $w(t) = -H(r(t), q(t), p(t)) + Const$ along solutions. Given initial conditions $(q_0, r_0, p_0, w_0)$ at $t_0$ we have $\widetilde{\mathcal{H}}(q(t), r(t), p(t), w(t)) \equiv \widetilde{\mathcal{H}}(q_0, r_0, p_0, w_0)$ along the corresponding solution. Moreover, for $w_0 := -H(r_0, q_0, p_0)$ we obtain $\widetilde{\mathcal{H}}(q(t), r(t), p(t), w(t)) \equiv 0$ along the solution. To have $r(t) \equiv t$ we must choose $r_0 := t_0$.

## 6 Numerical experiments

For PRK methods satisfying (2.4a) and (2.4c), the condition (2.4b) only matters for non-autonomous non-separable Hamiltonians. Hence, to illustrate the relevance of (2.4b) we will consider non-separable Hamiltonians. Starting from an autonomous Hamiltonian system

$$\dot{q} = \nabla_p H(q, p), \quad \dot{p} = -\nabla_q H(q, p), \tag{6.1}$$

we consider differential equations for the differences $Q(t) := q(t) - b(t)$, $P(t) := p(t) - a(t)$ for some functions $(b(t), a(t)) \in \mathbb{R}^n \times \mathbb{R}^n$

$$\dot{Q} = \nabla_p H(Q+b(t), P+a(t)) - \dot{b}(t), \;\; \dot{P} = -\nabla_q H(Q+b(t), P+a(t)) - \dot{a}(t). \tag{6.2}$$

This forms a non-autonomous Hamiltonian system for $(Q, P)$ with Hamiltonian

$$K(t, Q, P) := H(Q + b(t), P + a(t)) + Q^T \dot{a}(t) - P^T \dot{b}(t) \tag{6.3}$$

as can be directly verified. The quantity

$$I(t, Q, P) := H(Q + b(t), P + a(t)) = K(t, Q, P) - Q^T \dot{a}(t) + P^T \dot{b}(t) \tag{6.4}$$

is a first integral of this non-autonomous Hamiltonian system since its Lie derivative vanishes

$$\begin{aligned} & \partial_t I(t, Q, P) + \partial_Q I(t, Q, P) \nabla_P K(t, Q, P) + \partial_P I(t, Q, P)(-\nabla_Q K(t, Q, P)) \\ = \; & \nabla_q H(Q + b(t), P + a(t))^T \dot{b}(t) + \nabla_p H(Q + b(t), P + a(t))^T \dot{a}(t) \\ & + \nabla_q H(Q + b(t), P + a(t))^T (\nabla_p H(Q + b(t), P + a(t)) - \dot{b}(t)) \\ & + \nabla_p H(Q + b(t), P + a(t))^T (-\nabla_q H(Q + b(t), P + a(t)) - \dot{a}(t)) \\ \equiv \; & 0, \end{aligned}$$

i.e., the quantity $H(Q(t) + b(t), P(t) + a(t))$ remains constant along any solution $(t, Q(t), P(t))$. Applying various methods to non-autonomous Hamiltonian systems with Hamiltonian $K(t, Q, P)$ as in (6.3) constitutes a simple test to show the relevance of the necessity of conditions (2.4b) when the Hamiltonian $H(q, p)$ is non-separable. We consider the non-autonomous Hamiltonian system (6.2) corresponding to a non-autonomous Hamiltonian $K(t, Q, P)$ (6.3) based on the non-separable Hamiltonian

$$H(q_1, p_1) = \frac{1}{2} p_1^2 - \cos(q_1) + \frac{1}{5} \sin(2q_1) \left(1 + \frac{1}{4} p_1\right) \tag{6.5}$$

and the functions $(b_1(t), a_1(t)) := (\cos(t), \sin(t))$. This Hamiltonian is a simple non-separable perturbation $\sin(2q_1)p_1/20$ of the separable Hamiltonian given in [9, p. 379]. We consider the initial conditions $(Q_1(0), P_1(0)) := (-1, 2.5)$.

Using a constant stepsize $h = 0.005$ on the interval $[0, 500]$ we have applied 100000 steps of the partitioned Euler method PEI (3.3) for various choice of the coefficients $c_1 = \alpha$ and $\widehat{c}_1 = \beta$: $\alpha = \beta = 1/2$, $\alpha = \beta = 1$, $\alpha = \beta = 0.2$, and $\alpha = 0 \neq \beta = 1$ (the standard partitioned Euler method (2.6)). In Fig. 1 we have plotted the errors in the invariant $I(t) := H(Q(t) + b(t), P(t) + a(t))$ for all four methods. We observe that the error in this invariant oscillates around zero for the first three symplectic methods satisfying $\widehat{c}_1 = c_1$, but that there is a drift in the error for the fourth non-symplectic one (the standard partitioned Euler method (2.6)) satisfying $\widehat{c}_1 \neq c_1$.

We now turn our interest to the modified 2-stage Lobatto IIIA-B method (4.4) for a few choices of the coefficients $c_1, c_2, \widehat{c}_1, \widehat{c}_2$, all satisfying the symmetry conditions $c_2 = 1 - c_1$, $\widehat{c}_2 = 1 - \widehat{c}_1$. When $c_1 = \widehat{c}_1$ and $c_2 = \widehat{c}_2$ the method is symplectic for both the standard symplectic two-form $\omega$ (1.2) and the extended symplectic two-form $\eta$ (5.3). Otherwise the method is in general not symplectic for $\omega$ and certainly also not for $\eta$. Using a constant stepsize $h = 0.05$ on the interval $[0, 5000]$ we have applied 100000 steps of the standard 2-stage Lobatto IIIA-B method (4.1), i.e., (4.4) with $c_1 = \widehat{c}_1 = 0$, $c_2 = \widehat{c}_2 = 1$, the modified 2-stage Lobatto IIIA-B method (4.7) i.e., (4.4) with $c_1 = \widehat{c}_1 = 1/2$, $c_2 = \widehat{c}_2 = 1/2$, the modified 2-stage Lobatto IIIA-B method (4.4) with $c_1 = \widehat{c}_1 = 0.2$, $c_2 = \widehat{c}_2 = 0.8$, and the modified 2-stage Lobatto IIIA-B method (4.4) with $c_1 = 0$, $c_2 = 1$ and $\widehat{c}_1 = 1/2 \neq c_1$, $\widehat{c}_2 = 1/2 \neq c_2$. In Fig. 2 we have plotted the errors in the invariant $I(t) := H(Q(t)+b(t), P(t)+a(t))$ for all four methods. We observe that the error in this invariant oscillates around zero for the first three symplectic methods satisfying $\widehat{c}_1 = c_1$, $\widehat{c}_2 = c_2$, but that there is a drift in the error for the fourth non-symplectic method satisfying $\widehat{c}_1 \neq c_1$, $\widehat{c}_2 \neq c_2$.

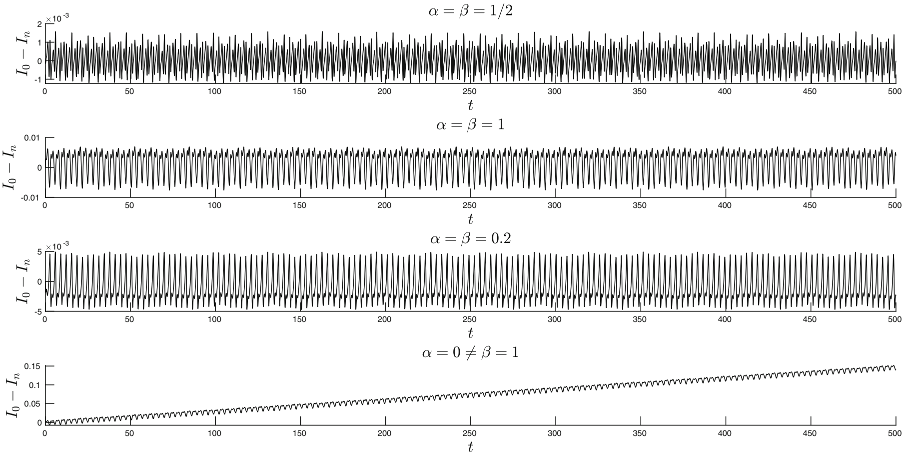


**Fig. 1** Error in the invariant $I(t) := H(Q(t) + b(t), P(t) + a(t))$ for partitioned Euler methods PEI (3.3) applied to (6.2) with $H$ of (6.5)

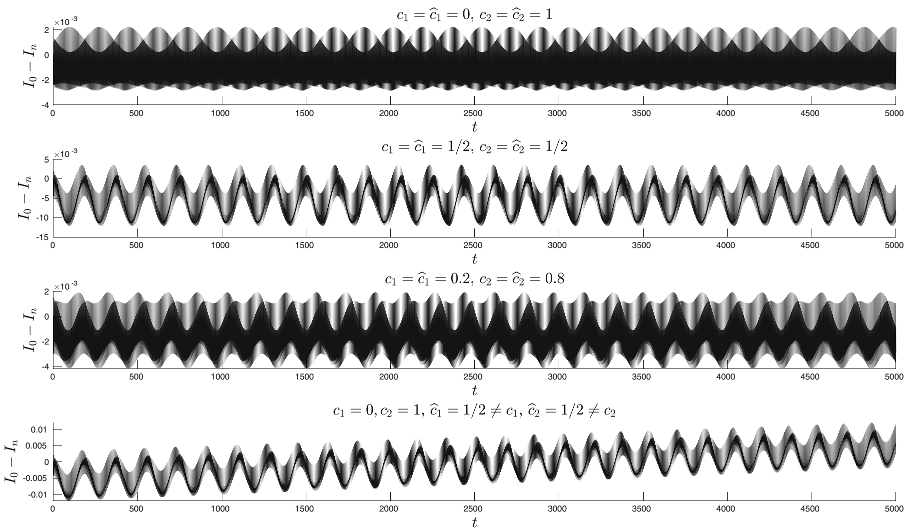


**Fig. 2** Error in the invariant $I(t) := H(Q(t) + b(t), P(t) + a(t))$ for modified Lobatto IIIA-B methods (4.4) applied to (6.2) with $H$ of (6.5)

## 7 Conclusion

We have shown the necessity for the nodes $c_i, \widehat{c_i}$ of symplectic irreducible PRK methods to satisfy the conditions $\widehat{c_i} = c_i$ for $i = 1, \ldots, s$ when applied to non-autonomous non-separable Hamiltonian systems. These conditions are especially relevant to the partitioned Euler method and the 2-stage Lobatto IIIA-B method. We have illustrated numerically the relevance of these conditions on a simple Hamiltonian system.

**Acknowledgements** The author would like to thank the anonymous referees for their constructive criticisms which helped improve the clarity of the paper.

## Appendix: Main lines of a proof of Theorem 2.2

To prove the necessity of conditions (2.4b) we have assumed that the PRK method is irreducible in the sense given in [9, VI.7] and [9, Theorem VI.7.10, p. 222]. A reducible PRK method is defined as a method having equivalent stages ($Q_i = Q_j$ and $P_i = P_j$ for $i \neq j$). We have also added the condition (2.8), i.e., that no index $i$ exists where $b_i = 0$ and $\widehat{b_i} = 0$. This eliminates methods having stages that have no influence on the numerical solution $q_1, p_1$ similar to the DJ-irreducibility of RK methods [10, Definition 12.15]. This is justified as follows. We already know that the conditions (2.4a), and (2.4c) are necessary for symplecticness. Assuming that there is an index $i$ such that $b_i = 0$ or $\widehat{b_i} = 0$, supposed to be unique for now, from the necessary conditions (2.4a) and (2.4c) we then obtain $\widehat{b_i} = 0$, $b_i = 0$, $a_{ji} = 0$, and $\widehat{a}_{ji} = 0$ for $j \in \{1, \ldots, s\} \backslash \{i\}$. Hence, clearly in this situation the internal stages $Q_i, P_i$ will not influence the solution $q_1, p_1$ and the other internal stages $Q_j, P_j$ for $j \neq i$. If there is more than one index $i$ with $b_i = 0$ and $\widehat{b_i} = 0$, then one can easily show that all those internal stages can only influence each other, but they can influence neither the solution $q_1, p_1$, nor the other internal stages $Q_j, P_j$ with coefficients $b_j = \widehat{b_j} \neq 0$. With that additional assumption (2.8) one is then in position to prove the necessity of (2.4b).

*Proof* We can extend the sets of trees considered in [9, VI.7] and [9, Theorem VI.7.10, p. 222] by having an extra type of nodes, say grey nodes, standing for the value 1 of the scalar differential equation $\dot{t} = 1$. We use the notation and definitions given in [9] though we exchange the role of $q$ and $p$ and $f$ and $g$. No node is attached on top of a grey node since the partial derivatives of a constant vanish. A branch leading to a grey node stands for a partial differentiation with respect to $t$. For the order conditions of partitioned methods, grey nodes need not be indexed. When a grey node follows a black node with index $j$, then the sum in the order conditions over the index $j = 1, \ldots, s$ must contain the coefficients $c_j$. When a grey node follows a white node with index $j$, then the sum in the order conditions over the index $j = 1, \ldots, s$ must contain the coefficients $\widehat{c}_j$. Consider a $P$-series with coefficients $a(u)$

$$\begin{pmatrix} \sum_{u \in TP_q} \frac{h^{|u|}}{\sigma(u)} a(u) F(u)(t_0, q_0, p_0) \\ \sum_{u \in TP_p} \frac{h^{|u|}}{\sigma(u)} a(u) F(u)(t_0, q_0, p_0) \end{pmatrix}$$

For a $P$-series to be symplectic one of the necessary conditions for autonomous Hamiltonian systems is to have

$$a(u) \text{ is independent of the color of the root of } u.$$

The same necessary condition holds for non-autonomous Hamiltonian systems for trees also containing grey nodes. This can be easily shown on a similar example given in the proof of [9, Theorem VI.7.4, p. 217] where the top black node of the tree $u$ is replaced by a grey node. For that tree we take

$$H(t, q, p) = q^1 p^2 p^3 q^4 + q^3 t + p^4$$

and for that Hamiltonian we get

$$F^2(u)(t, q, p) = (-1)^{\delta(u)} \sigma(u) q^1, \qquad F^1(\bar{u})(t, q, p) = (-1)^{\delta(u)} \sigma(u) p^2$$

where $\bar{u}$ is the tree obtained from $u$ by replacing its black root with a white root. These elementary differentials are the only contribution to

$$\left(\frac{\partial(q_1, p_1)}{\partial q_0^1}\right)^T J_n \left(\frac{\partial(q_1, p_1)}{\partial p_0^2}\right)$$

and we get

$$0 = \left(\frac{\partial(q_1, p_1)}{\partial q_0^1}\right)^T J_n \left(\frac{\partial(q_1, p_1)}{\partial p_0^2}\right) = (-1)^{\delta(u)} h^{|u|} (a(u) - a(\bar{u})).$$

Now to prove our statement we can consider the same PRK matrix $\Phi_{PRK}$ as given in [9, VI.7] and [9, Theorem VI.7.10, p. 222], we do not even need to consider trees with grey nodes in that matrix. We define the vector $d \in \mathbb{R}^s$ with elements $d_i := b_i c_i - \widehat{b_i}\widehat{c_i}$ for $i = 1, \dots, s$. For irreducible PRK methods we already know that the condition $\widehat{b_i} = b_i$ for $i = 1, \dots, s$ is necessary for symplecticness, hence we obtain $d_i = b_i(c_i - \widehat{c_i})$ for $i = 1, \dots, s$. The vector $d$ satisfies

$$d^T \Phi_{PRK} = 0$$

since $d^T \phi(u) = a(v) - a(\bar{v})$ where $v$ is obtained from $u$ by appending a grey node to its root and $a(v) = a(\bar{v})$ for $v \in TP_q$ as seen above. Since the matrix $\Phi_{PRK}$ is of maximal rank $s$ we must have $d = 0$, hence its components satisfy $d_i = b_i(c_i - \widehat{c_i}) = 0$ for $i = 1, \dots, s$. Since $b_i \neq 0$ for $i = 1, \dots, s$ we obtain (2.4b). □

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