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State-dependent symplecticity and area preserving numerical methods☆

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Abstract

We introduce the definition of *state-dependent symplecticity* as a useful tool of investigation to discover nearby symplecticity in symmetric non-symplectic one-step methods applied to two-dimensional Hamiltonian systems. We first relate this property to Poisson systems and to the trapezoidal method, and then investigate Runge–Kutta and discrete gradient symmetric methods.

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1. Introduction

It is well known that, apart from the exact map defined by the continuous problem, a Hamiltonian integration method cannot preserve both the symplectic structure and the energy function [9,14]. While there is enough experimental and theoretical evidence that symmetric methods share good stability properties (such as almost energy conservation) for long times when applied to several classes of Hamiltonian systems [1,2,5,6,13], much less work has been done to show that they also may exhibit a behavior similar to symplecticity. The definition of *state-dependent symplecticity* (sd-symplecticity) has been introduced as an extension of the classical symplecticity property of Hamiltonian systems to give an account for this similarity. For simplicity, we will confine our investigation to one-step symmetric methods and to two-dimensional Hamiltonian problems (for generalization to higher dimensions see [8]). As is well known, symplecticity in two dimensions is equivalent to the conservation of areas of regions in the phase plane, under the action of the map representing the method. As is the case for the energy, in many interesting situations, it happens that the sequence of the areas of the images of a given region of the phase plane under the action of a symmetric non-symplectic method, undergoes bounded oscillations. This nearly conservation of the areas suggests that these methods can share a property that is close to symplecticity: although we have not yet carried out an exhaustive study for this question, we show that sd-symplecticity may play a key role to account for such behavior.

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The paper is organized as follows. In the next section we introduce the definition of sd-symplectic maps as a generalization of Poisson maps. In Section 3 we show that the trapezoidal method is the only sd-symplectic method in the class of linear one-step methods. Actually, in the simplest case of the trapezoidal method, sd-symplecticity reduces to the definition of a Poisson map and the almost preservation of areas may be also understood in terms of conjugate symplecticity. This is no longer the case for more general symmetric one-step methods as those presented in Sections 4 and 5, where such feature is investigated for the class of symmetric Runge–Kutta (RK) and discrete gradient methods, respectively. Sections 3–4 also contain some numerical experiments.

2. Sd-symplecticity of one-step methods

According to the original definition introduced after Hamilton (see [4, p. 209]), a general-type planar system

$$\begin{cases} \dot{x} = g_1(x, y), \\ \dot{y} = g_2(x, y) \end{cases} \tag{1}$$

is called Hamiltonian if one can find a factor $\eta(x, y)$ (*integrating factor*) and a scalar function $H(x, y)$ such that

$$\frac{\partial H}{\partial y} = -\eta g_1 \quad \text{and} \quad \frac{\partial H}{\partial x} = \eta g_2. \tag{2}$$

System (1) is then recast as

$$\begin{pmatrix} \dot{x} \\ \dot{y} \end{pmatrix} = \frac{1}{\eta(x, y)} J \nabla H(x, y) \quad \text{with } J = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}. \tag{3}$$

Systems (3) and $(\dot{x}, \dot{y})^{\mathrm{T}} = J\nabla H(x, y)$ share the same curves as trajectories in the phase plane, but the velocity in one is a scalar multiple of the velocity in the other. If, in addition, $\eta(x, y)$ never vanishes, the two systems also share the same equilibrium points. Whenever required we will assume that both H and η are sufficiently regular functions on an open subset $\Omega \subset \mathbb{R}^2$.

In the current literature systems of the form (3) are more appropriately referred to as Poisson systems.[1] With Hamiltonian systems ($\eta = 1$), Poisson systems share the property of possessing the Hamiltonian function H as first integral. This is easily checked by evaluating the derivative of H along a solution curve $z(t) = (x(t), y(t))$ of (3):

$$\dot{H}(t) = \nabla^{\mathrm{T}} H(z(t))\dot{z}(t) = \frac{1}{\eta(z(t))} \nabla^{\mathrm{T}} H(z(t)) J \nabla H(z(t)) = 0.$$

Conversely, it has been shown that any dynamical system possessing a first integral may be recast as a Poisson system (see [11] and references therein).

On the other hand, a difference is that Poisson systems fail to be symplectic, since the Jacobian matrix Φ_t' of their flow $\Phi_t = z_0 \mapsto z(t)$ satisfies the condition $(\Phi_t')^{\mathrm{T}} J (\Phi_t') = J$ for any time t only if $\eta = 1$ (Hamiltonian case). As is well known, the geometric interpretation of symplecticity in two dimensions is that symplectic maps are area preserving: if S is any compact subset of $\mathbb{R}^2$ then $\iint_S \mathrm{d}x\,\mathrm{d}y = \iint_{\Phi_t(S)} \mathrm{d}x\,\mathrm{d}y$. This follows from the transformation formula for integrals and the property $\det \Phi_t' = 1$ for any t (one easily verifies that this property fully characterizes symplectic transformations in the two-dimensional case). Nonetheless, the Jacobian matrix associated to the flow of Poisson systems (3) exhibits a similar property, namely a preservation of a different (non-Euclidean) measure. To account for this the definition of Poisson maps was introduced as transformations that, for two-dimensional flows, satisfy

$$\mu(p_1, q_1)(\Phi'(p_0, q_0))^{\mathrm{T}} J \Phi'(p_0, q_0) = \mu(p_0, q_0) J, \tag{4}$$

where $\mu(p, q)$ is a scalar function of the state vector referred to as *multiplier*. The flow $\Phi_t(z)$ associated to the Poisson system (3) satisfies (4) with multiplier $\mu(x, y) = \eta(x, y)$ for any time t.

[1] When the degree of freedom is more than one, the factor ηJ is replaced by any skew-symmetric matrix $B(z)$, that makes the associated Poisson bracket $\nabla F(z)^{\mathrm{T}} B(z) \nabla G(z)$ of two smooth functions $F(z)$ and $G(z)$, satisfy the Jacobi identity.

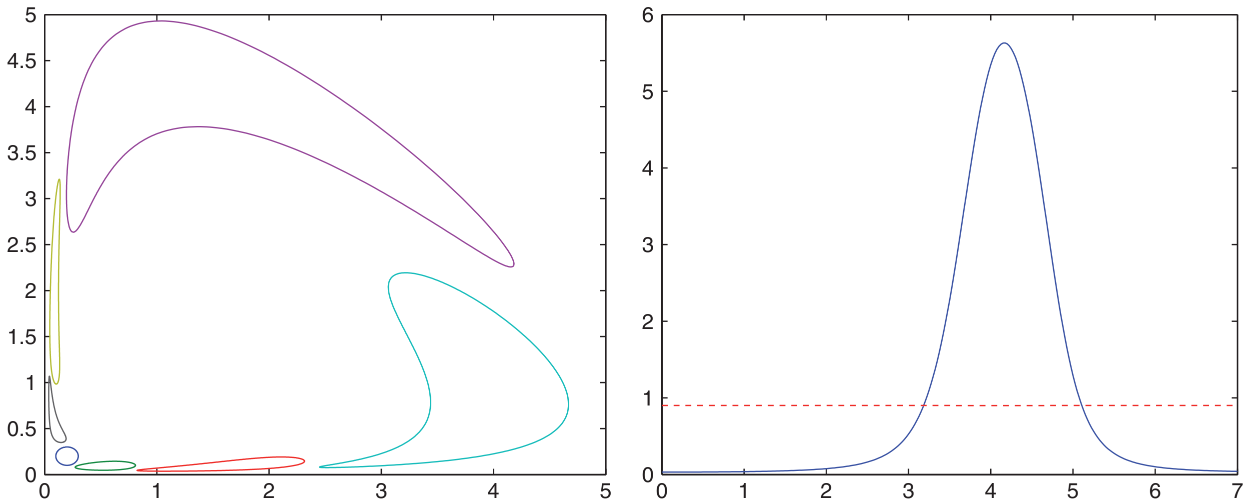

Fig. 1. Left picture: a small disk with centre (0.2, 0.2) and radius 0.1 and its images under the action of the flow of (5). Right picture: the related sequence of areas (solid line) and scaled areas (dashed line) in the time interval [0, 7].

The two eigenvalues of $\Phi'(p_0, q_0)$ are in the form λ, $(\mu(p_0, q_0)/\mu(p_1, q_1))1/\lambda$ and therefore $\det(\Phi'(p_0, q_0)) = \mu(p_0, q_0)/\mu(p_1, q_1)$. To a Poisson map we may associate the measure $\mathcal{M}(S) = \iint_S |\mu(p, q)|\,\mathrm{d}p\,\mathrm{d}q$, where $S \subset \Omega$ is any bounded open measurable subset of Ω (we assume that μ is a smooth function on Ω). It is easily checked that a Poisson map $(p_1, q_1) = \Phi(p_0, q_0)$ satisfies $\mathcal{M}(\Phi(S)) = \mathcal{M}(S)$ for any bounded measurable domain in Ω.

Example 1. The Lotka–Volterra model

$$\begin{cases} \dot{x} = ax(1-y) \\ \dot{y} = -by(1-x) \end{cases} \quad \text{with } a, b > 0 \tag{5}$$

is set in the form (3) via the integrating factor $\eta(x, y) = -1/(xy)$, and has $H(x, y) = b(\log x - x) + a(\log y - y)$ as first integral. Its flow Φ_t is therefore a Poisson map in any region Ω contained in the first sector of the phase plane (observe that $\mu(x, y) = \eta(x, y)$ is not defined at the equilibrium point $(0, 0)$). The left picture in Fig. 1 reports the action of the flow Φ_t over a small disk S close to the origin at evenly spaced times covering approximately a period around the equilibrium point $(1, 1)$. The regions $\Phi_{t_i}(S)$ widen out as long as they depart from the origin and shrink when they approach the origin again after a period. This is due to the conservation of the measure $\iint_{\Phi_t} |\eta(x, y)|\,\mathrm{d}x\,\mathrm{d}y$ and the fact that the weight function $|\eta(z)|$ has a pole at the origin while it rapidly decreases as $\|z\| \to \infty$. The left picture plots the Euclidean and scaled measures of $\Phi_t(S)$ in the period of observation $t \in [0, 7]$.

It is well known that the system (5) of the previous example is conjugate to a Hamiltonian system for example via the change of variables $p = \log x$ and $q = \log y$. This means that the portrait of the Lotka–Volterra problem in the phase plane is topologically equivalent to that of the associated Hamiltonian system. Change of variables that preserve the Hamiltonian form of a given Hamiltonian system are called *canonical* and they are characterized by the fact that the associated Jacobian matrix is symplectic (see for example [12]). On the other hand, a non-canonical change of coordinates performed on a Hamiltonian system will lead to a Poisson system.

In order to inspect the behavior of symmetric methods, we further weaken property (4), by introducing the definition of state-dependent symplecticity. In the following we assume that the map:

$$y_1 = \Phi_h(y_0), \qquad \Phi_h : \Omega \to \mathbb{R}^2, \tag{6}$$

with Ω an open subset of $\mathbb{R}^2$, represents a one-step method of order p and stepsize $h > 0$ (the following definition applies as well in the case where (6) is a generic family of maps depending on a parameter h).

Definition 2. The one-step method (6) is called sd-symplectic if its Jacobian $\Phi'_h = \partial y_1/\partial y_0$ satisfies

$$\mu_{-h}(y_1)\left(\frac{\partial y_1}{\partial y_0}\right)^{\mathrm{T}} J \frac{\partial y_1}{\partial y_0} = \mu_h(y_0)J, \tag{7}$$

for some scalar function $\mu_\gamma(y)$ and $\forall y_0 = (p_0, q_0)$, $y_1 = (p_1, q_1) \in \Omega$, and $h \in [0, \bar{h})$.

Due to the presence of the stepsize h, we see that, in general, a one-step method satisfying (7) fails to be a Poisson map. The implications of such weakening will be better elucidated in Sections 4 and 5, while for the simpler class of one-step linear methods the two definitions coincide, as shown in the next section.

3. Linear one-step methods and the role of symmetry

Even if for some methods (like non-partitioned R–K methods) symmetry and symplecticity are two equivalent properties when referred to quadratic Hamiltonians, for general nonlinear systems such concepts are no longer linked with each other, it being possible to find symplectic, non-symmetric methods as well as symmetric, non-symplectic methods. The trapezoidal rule belongs to this latter class, because it fails to be symplectic. Despite this, at least when implemented to the class of problems defined above, the trapezoidal method exhibits a behavior very close to that shown by symplectic methods.

Example 3. With relation to the nonlinear pendulum system $H(p, q) = 1/2p^2 + 1 - \cos q$, we consider, in the phase space, a disk with center (0.3, 0) and radius 0.2 and its images obtained as the iterations of the trapezoidal method, with stepsize $h = \pi/2$. The left picture of Fig. 2 reports the initial disk, and its image after 3000 iterations: it appears spiral-shaped since the velocity of rotations around the origin of the points of the original disk is greater for those points that are closer to the origin. The right picture clearly shows that the sequence of the areas of these images does not diverge and neither does it go to zero; it rather oscillates around a constant value located in the interval [0.1265, 0.127] (the area of the initial disk is $\simeq 0.1256$).

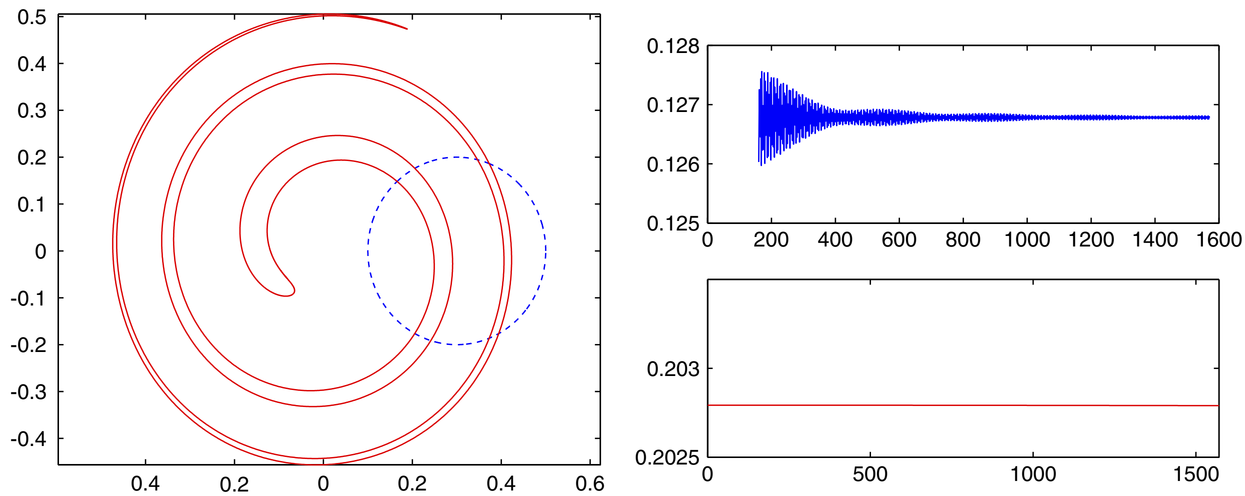

Fig. 2. Left picture: a disk (dash line) and its image in the phase plane after 3000 iteration performed by the trapezoidal method with $h = \pi/2$. Right picture: the related sequence of areas (top) and scaled areas (bottom) in the time interval $[0, 3000h]$.

For the sake of clarity, we first consider the simpler class of linear one-step formulae. The family of maps arising from the application of a consistent linear one-step method to a two-dimensional Hamiltonian system reads

$$y_1 = y_0 + hJ(\beta\nabla H(y_0) + (1-\beta)\nabla H(y_1)). \tag{8}$$

The only symmetric method belonging to (8) is of course the trapezoidal rule which, as well, turns out to be the only sd-symplectic consistent method.

Theorem 4. *The trapezoidal method is the only sd-symplectic one-step method in the class* (8).

Proof. By differentiating y_1 with respect to y_0, we see that the Jacobian matrix of the map defined by the one-step method (8) satisfies

$$(I - h(1-\beta)J\nabla^2 H(y_1))\frac{\partial y_1}{\partial y_0} = (I + h\beta J\nabla^2 H(y_0)). \tag{9}$$

Given a symmetric matrix S and any real γ, a direct computation shows that

(i) $(I-\gamma JS)^{-1} = (1/(1+\gamma^2 \det S))(I+\gamma JS)$,
(ii) $(I+\gamma JS)^{\mathrm{T}} J(I+\gamma JS) = (1+\gamma^2 \det S)J$,

From (i) we retrieve the expression of $\partial y_1/\partial y_0$, while we use twice (ii) to prove that

$$\left(\frac{\partial y_1}{\partial y_0}\right)^{\mathrm{T}} J \frac{\partial y_1}{\partial y_0} = \frac{1+h^2\beta^2 \det \nabla^2 H(y_0)}{1+h^2(1-\beta)^2 \det \nabla^2 H(y_1)} J.$$

We get sd-symplecticity by imposing $\beta^2 = (1-\beta)^2$, which yields $\beta = \frac{1}{2}$. Therefore, for the trapezoidal method we get $\mu_h(y) = 1 + h^2/4 \det \nabla^2 H(y)$ and, since $\mu_{-h} = \mu_h$, we see that this method is indeed a Poisson map (this obviously is also understood by considering that the trapezoidal method is conjugate to the implicit midpoint method, which is symplectic). □

Symmetry and sd-symplecticity are then equivalent in the class of methods in the form (8). Sd-symplecticity of a numerical method gives interesting information about the way the method fails the symplecticity condition. For the trapezoidal method we have

$$\left(\frac{\partial y_n}{\partial y_0}\right)^{\mathrm{T}} J \frac{\partial y_n}{\partial y_0} = \frac{\mu(y_0)}{\mu(y_n)} J = \left(1 + \frac{h^2}{4} R(y_0, y_n)\right) J,$$

with

$$R(y_0, y_n) = \frac{\det \nabla^2 H(y_0) - \det \nabla^2 H(y_n)}{1 + (h^2/4)\det \nabla^2 H(y_n)}.$$

If we assume boundedness of $R(y_0, y_n)$ with respect to the time-step n, we get

$$\left(\frac{\partial y_n}{\partial y_0}\right)^{\mathrm{T}} J \frac{\partial y_n}{\partial y_0} = J + \mathrm{O}(h^2)J, \tag{10}$$

which means symplecticity up to a term of order 2 (and independent of n). We see that boundedness of $R(y_0, y_n)$ is guaranteed in case of a bounded solution y_n, or a bounded term $\det \nabla^2 H(y_n)$, provided the stepsize $h < h_0$ is such that $1 + (h^2/4)\det \nabla^2 H(y_n) > \varepsilon > 0$. For some problems, such as the pendulum equation, one has always $\det \nabla^2 H(y)$ bounded and positive (at least in a neighborhood of the equilibrium point) and therefore no restrictions on h must be imposed in order to have the denominator of $R(y_0, y_n)$ bounded away from zero.

4. Symmetric Runge–Kutta methods

Due to the presence of internal stages, the question of sd-symplecticity of higher order schemes is more delicate. We consider a symmetric s-stage RK method applied to a Hamiltonian system $y' = J\nabla H(y)$ in the form

$$y_1 = y_0 + hJ(b^{\mathrm{T}} \otimes I)\nabla H(K), \quad K = e \otimes y_0 + h(A \otimes J)\nabla H(K),$$

where $K = [K_1^{\mathrm{T}}, \dots, K_s^{\mathrm{T}}]^{\mathrm{T}}$ is the block vector of the internal stages and $\nabla H(K) \equiv [\nabla^{\mathrm{T}} H(K_1), \dots, \nabla^{\mathrm{T}} H(K_s)]^{\mathrm{T}}$. Symmetry leads to the following relation involving the Butcher array A and the weights b_i:

$$A + PAP = eb^{\mathrm{T}}, \quad P = \begin{pmatrix} & & 1 \\ & \cdot^{\cdot^{\cdot}} & \\ 1 & & \end{pmatrix}_{s \times s}, \quad e = (1, \dots, 1)^{\mathrm{T}}.$$

By inserting this relation in the nonlinear system defining the stages, we can express $\widehat{K} \equiv (P \otimes I)K$ as a function of y_1 by simply exchanging, in the original system, y_0 with y_1, and by reversing the sign of the stepsize h: $\widehat{K} = e \otimes y_1 - h(A \otimes J)\nabla H(\widehat{K})$. This dual representation allows us to construct a relation similar to (9). Considering that $b = Pb$, we can split $(b^{\mathrm{T}} \otimes I)\nabla H(K)$ in two (symmetric) terms depending uniquely on y_0 and y_1, respectively, thus obtaining

$$y_1 = y_0 + \frac{h}{2} J(b^{\mathrm{T}} \otimes I)(\nabla H(K^+(y_0)) + \nabla H(K^-(y_1))), \tag{11}$$

where

$$K^{\pm}(y) = e \otimes y \pm h(A \otimes J)\nabla H(K^{\pm}(y)). \tag{12}$$

Differentiation of (11) with respect to y_0 yields

$$\left(I - \frac{h}{2} JF_{-h}(y_1)\right)\frac{\partial y_1}{\partial y_0} = \left(I + \frac{h}{2} JF_h(y_0)\right), \tag{13}$$

where, denoting by I_{2s} the identity matrix of dimension $2s$, and defining $\nabla^2 H(K^{\pm}(y)) \equiv \text{block-diag}(\nabla^2 H(K_1^{\pm}), \dots, \nabla^2 H(K_s^{\pm}))$,

$$\begin{aligned} F_{\pm h}(y) &\equiv (b^{\mathrm{T}} \otimes I)\nabla^2 H(K^{\pm}(y))\frac{\partial K^{\pm}(y)}{\partial y} \\ &= (b^{\mathrm{T}} \otimes I)\nabla^2 H(K^{\pm}(y))(I_{2s} \mp h(A \otimes J)\nabla^2 H(K^{\pm}(y)))^{-1}(e \otimes I). \end{aligned} \tag{14}$$

Formula (14) comes from differentiation of (12). Because of symmetry, we have $K^+(y_0) = (P \otimes I)K^-(y_1)$, and hence $\nabla^2 H(K^+(y_0)) = (P \otimes I)\nabla^2 H(K^-(y_1))(P \otimes I)$. By setting

$$\mu_\gamma(y) = \det\left(I + \frac{\gamma}{2} JF_\gamma(y)\right),$$

we finally arrive at (7).

From (7) we get $\iint_{S_0} \mu_h(y_0)\,\mathrm{d}y_0 = \iint_{S_1} \mu_{-h}(y_1)\,\mathrm{d}y_1$. Since in general $\mu_h(y) \neq \mu_{-h}(y)$, it is no longer possible to apply a transitivity argument to extend this conservation property from a region S_0 to a region S_n. By applying (7) repeatedly for n steps we obtain

$$\left(\frac{\partial y_n}{\partial y_0}\right)^{\mathrm{T}} J \frac{\partial y_n}{\partial y_0} = \varphi_n(h)J, \quad \varphi_n(h) = \frac{\mu_h(y_0)\mu_h(y_1), \dots, \mu_h(y_{n-1})}{\mu_{-h}(y_1), \dots, \mu_{-h}(y_{n-1})\mu_{-h}(y_n)}. \tag{15}$$

For the trapezoidal rule μ_h is an even function of h, so that the ratios $\mu_h(y_k)/\mu_{-h}(y_k)$ in (15) cancel out. For higher order scheme this property is lost because, in general, $F_{-h}(y) \neq F_h(y)$.

Example 5. We consider the Lobatto IIIA formula of order 4 (three stages), the separable regular Hamiltonian function $H(p,q)=1/2p^2+U(q)$ and look for an asymptotic bound for $\varphi_n(h)$. For such method, at step k, we have $K_1=y_k$, $K_3=y_{k+1}$ and we denote by $(p_{k,k+1},q_{k,k+1})\equiv K_2$ the approximation of the solution at the intermediate time $t_k+h/2$. From (15) the function $\psi_n(h)\equiv\log(\varphi_n(h))$ reads

$$\psi_n(h)=\sum_{k=0}^{n-1}(\log(\mu_h(p_k,q_k))-\log(\mu_{-h}(p_{k+1},q_{k+1}))).$$

In particular, for our method and Hamiltonian function, a direct computation shows that

$$\mu_h(p_k,q_k)=1+\frac{h^2}{12}g(q_{k,k+1})+\frac{h^4}{12^2}g(q_{k,k+1})g(q_k),$$

$$\mu_{-h}(p_{k+1},q_{k+1})=1+\frac{h^2}{12}g(q_{k,k+1})+\frac{h^4}{12^2}g(q_{k,k+1})g(q_{k+1}),$$

where $g(q)\equiv U''(q)$. The expansion $\log(1+u)\simeq u-1/2u^2+1/3u^3$, for small values of u, yields

$$\begin{aligned}\log(\mu_h(p_k,q_k))-\log(\mu_{-h}(p_{k+1},q_{k+1}))&=\frac{h^4}{12^2}g(q_{k,k+1})(g(q_k)-g(q_{k+1}))\\&\quad-\frac{h^6}{12^3}g^2(q_{k,k+1})(g(q_k)-g(q_{k+1}))+\mathrm{O}(h^8).\end{aligned}\tag{16}$$

From (12) we obtain

$$q_{k,k+1}=q_k+h(a_{21}p_k+a_{22}p_{k,k+1}+a_{23}p_{k+1}),$$

$$q_{k,k+1}=q_{k+1}-h(a_{21}p_{k+1}+a_{22}p_{k,k+1}+a_{23}p_k),$$

and hence

$$g(q_{k,k+1})=g(q_k)+hg'(q_k)(a_{21}p_k+a_{22}p_{k,k+1}+a_{23}p_{k+1})+\mathrm{O}(h^2),$$

$$g(q_{k,k+1})=g(q_{k+1})-hg'(q_{k+1})(a_{21}p_{k+1}+a_{22}p_{k,k+1}+a_{23}p_k)+\mathrm{O}(h^2).$$

Considering that $g'(q_k)(a_{21}p_k+a_{22}p_{k,k+1}+a_{23}p_{k+1})-g'(q_{k+1})(a_{21}p_{k+1}+a_{22}p_{k,k+1}+a_{23}p_k)=\mathrm{O}(h)$, summing up the last two equations gives

$$g(q_{k,k+1})=\tfrac{1}{2}(g(q_k)+g(q_{k+1}))+h^2R_k,$$

where h^2R_k stands for the Lagrange residual term. By inserting this expression in (16), we arrive at

$$\psi_n(h)=\frac{1}{2}\frac{h^4}{12^2}\sum_{k=0}^{n-1}(g^2(q_k)-g^2(q_{k+1}))+\frac{h^6}{12^2}\sum_{k=0}^{n-1}(g(q_k)-g(q_{k+1}))E_k,$$

with $E_k=(R_k-\frac{1}{12}g^2(q_{k,k+1}))$. Considering that the first sum is of telescopic type and that $g(q_k)-g(q_{k+1})=\mathrm{O}(h)$, and assuming that $g(q_k)$ remains uniformly bounded[2] with respect to n for $0<h<\bar{h}$, we finally obtain

$$\varphi_n(h)=1+\mathrm{O}(h^4+th^6),\qquad t=nh.\tag{17}$$

[2] For example, this would be true in the cases where g is bounded or the solution lies in a compact set.

This result is intimately related to the one presented in [3] and pertaining to the error in the Hamiltonian function of the Lobatto IIIA method. The authors list a number of problems where the $O(th^6)$ term explicitly appears as a drift in the numerical Hamiltonian: for those counterexamples we can likewise experience a $O(th^6)$ drift in the error $\|(\partial y_n/\partial y_0)^{\mathrm{T}} J(\partial y_n/\partial y_0) - J\|$ as stated by formula (17).

Nonetheless, for several kinds of systems, the symmetry of the method seems not to destroy the essential symplecticity property already revealed in (10) by the trapezoidal method; on the contrary, the deviation from symplecticity becomes $O(h^p)$, p being the order of the underlying method, provided $\varphi_n(h)$ remains bounded away from infinity and zero with respect to n, namely there exists $\bar{h} > 0$ such that, for all $h \in [0, \bar{h}]$:

$$M(h) \equiv \sup_{n\in\mathbb{N}} |\varphi_n(h)| = \sup_{n\in\mathbb{N}} \prod_{k=0}^{n-1} \left| \frac{\mu_h(y_k)}{\mu_{-h}(y_{k+1})} \right| < +\infty, \tag{18}$$

$$N(h) \equiv \inf_{n\in\mathbb{N}} |\varphi_n(h)| = \inf_{n\in\mathbb{N}} \prod_{k=0}^{n-1} \left| \frac{\mu_h(y_k)}{\mu_{-h}(y_{k+1})} \right| > 0. \tag{19}$$

Under the assumptions (18)–(19), it follows that $M(h) \leqslant 1 + O(h^p)$ and $N(h) \geqslant 1 + O(h^p)$, and therefore $\varphi_n(h) = 1 + O(h^p)$, where the $O(h^p)$ term is uniformly bounded with respect to n. In fact, the matrix $\partial y_n/\partial y_0$ is the numerical solution at time step n of the RK method applied to the continuous variational equation $(\partial y(t)/\partial y_0)' = J\nabla^2 H(y(t))(\partial y(t)/\partial y_0)$ augmented by the original system $y' = J\nabla H(y)$. From the order condition we get $\partial y_n/\partial y_0 = \partial y(nh)/\partial y_0 + O(th^p)$, with $t = nh$. Symplecticity of $\partial y(nh)/\partial y_0$ implies that $\det(\partial y(nh)/\partial y_0) = 1$ and hence $\det(\partial y_n/\partial y_0) = \varphi_n(h) = 1 + O(th^p)$. But the $O(t)$ term will be indeed missing since (18)–(19) hold uniformly with respect to h.

Remark 6. Considering that $(b^{\mathrm{T}} \otimes I)(e \otimes I) = I$, from the definitions of $\mu_{\pm h}(y)$ and $F_{\pm h}(y)$, it follows that

$$\frac{\mu_h(y_0)}{\mu_{-h}(y_1)} = \frac{\det((b^{\mathrm{T}} \otimes I)[I_{2s} + (h/2)\widetilde{J}\nabla^2 H(K^+(y_0))(I_{2s} - h(A \otimes I)\widetilde{J}\nabla^2 H(K^+(y_0)))^{-1}](e \otimes I))}{\det((b^{\mathrm{T}} \otimes I)[I_{2s} - (h/2)\widetilde{J}\nabla^2 H(K^-(y_1))(I_{2s} + h(A \otimes I)\widetilde{J}\nabla^2 H(K^-(y_1)))^{-1}](e \otimes I))},$$

where $\widetilde{J} = I \otimes J$. For linear problems $y' = JSy$ the matrices that form the arguments of the determinants at numerator and denominator reduce to the rational stability function $R_{\pm h}$ evaluated at *JS*. For example if S is positive definite, all the eigenvalues of *JS* lie on the imaginary axis and, because of symmetry, they are mapped by R to (complex-conjugate) points on the boundary of the unit circle thus giving stability (indeed in the linear case one knows that the RK method becomes a symplectic integrator). For nonlinear problems it happens that the block diagonal matrices have no longer constant block entries and boundedness of the product appearing in (15) requires the study of a scalar linear but non-autonomous system.

There are many interesting situations where $\varphi_n(h)$ remains bounded with respect to n. Hereafter we consider a couple of examples (see [8] for further examples regarding problems with higher degrees of freedom): for both of them the dynamics takes place along a closed curve embracing the origin and possessing some symmetries.

In the case of separable Hamiltonian functions $\nabla H(p, q) = [f_1(p), f_2(q)]^{\mathrm{T}}$, the matrix $\nabla^2 H(K^{\pm}(y))$ is diagonal and the following result provides a useful tool to state conditions (18)–(19) under special situations (see Example 8).

Lemma 7. *Let y and z such that $\nabla^2 H(K^+(y)) = \nabla^2 H(K^-(z)) \equiv D$, with D diagonal. Then $\mu_h(y) = \mu_{-h}(z)$.*

Proof. Let

$$T = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \widetilde{T} = I_s \otimes T.$$

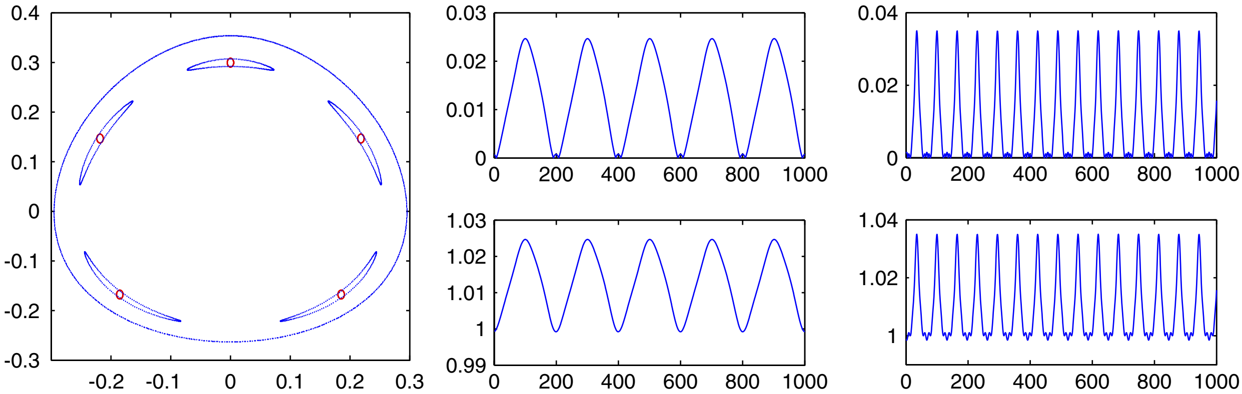

Fig. 3. Behavior of the Lobatto IIIB method applied to the separate Hamiltonian systems of Example 8, with stepsize $h \simeq 1.317$. We chose the time interval $[0, 5000h]$ but, in order to make the visualization clearer, the central and right pictures contain plots at times $5nh$, $n=0,1,\ldots,1000$ (hence the central plot displays the behavior of one island).

We observe that $\widetilde{T}\widetilde{J}D = -\widetilde{J}\widetilde{T}D$ and $T^{-1} = T$. Therefore,

$$
\begin{aligned}
\mu_h(y) &= \det\left(T(b^{\mathrm{T}} \otimes I)\left[I_{2s} + \frac{h}{2}\widetilde{J}D(I_{2s} - h(A \otimes I)\widetilde{J}D)^{-1}\right](e \otimes I)T\right) \\
&= \det\left((b^{\mathrm{T}} \otimes I)\widetilde{T}\left[I_{2s} + \frac{h}{2}\widetilde{J}D(I_{2s} - h(A \otimes I)\widetilde{J}D)^{-1}\right]\widetilde{T}(e \otimes I)\right) \\
&= \det\left((b^{\mathrm{T}} \otimes I)\left[I_{2s} - \frac{h}{2}\widetilde{J}D\widetilde{T}(I_{2s} - h(A \otimes I)\widetilde{J}D)^{-1}\widetilde{T}\right](e \otimes I)\right) \\
&= \det\left((b^{\mathrm{T}} \otimes I)\left[I_{2s} - \frac{h}{2}\widetilde{J}D(I_{2s} + h(A \otimes T^2)\widetilde{J}D)^{-1}\right](e \otimes I)\right) \\
&= \mu_{-h}(z). \qquad \square
\end{aligned}
$$

The next example shows an application of Lemma 7. To assess the general applicability of the sd-symplecticity property, we use the Lobatto IIIB formula of order $p=4$, which is symmetric but neither symplectic nor conjugate to a symplectic method (see [7, p. 206]).

Example 8. We consider the Hamiltonian system defined by

$$H(p,q) = 1/2p^2 + (1 - \cos(q))\mathrm{e}^{-q}$$

that may be interpreted as a modified pendulum equation, and solve it by means of the Lobatto IIIB formula of order $p=4$. The leftmost picture in Fig. 3 shows a cycle of period 5 (small circles) in the (p,q) phase plane, surrounded by two neighboring solutions obtained by slightly perturbing the initial conditions yielding the periodic orbit. We first consider the special situation of the cycle. Due to the symmetry of the problem, to each point $y=(p,q)$ of the orbit, there corresponds a symmetric point $z=(-p,q)$ lying on the orbit too: for two such points Lemma 7 applies; the function $\varphi_n(h)$ becomes periodic and its value is 1 after each complete period. This argument extends to any periodic orbit like the one considered (in a neighborhood of the equilibrium, one can find infinitely many periodic orbits by suitably tuning the stepsize h). A slight perturbation of the initial conditions results in an almost periodic orbit made up of small islands surrounding each point of the cycle. Increasing the perturbation causes the islands to crash, giving birth to an orbit that densely covers a closed curve around the equilibrium. Almost periodicity means that for any neighborhood $B(y,\varepsilon)$ of any point y on the orbit, an integer $N_\varepsilon > 0$ exists such that $\{y_k, y_{k+1}, \ldots, y_{k+N_\varepsilon}\} \cap B(y,\varepsilon) \neq \emptyset$, $\forall k \in \mathbb{Z}$. Assuming that the limit curve shares the same symmetry as for the periodic case, we deduce that if $y=(p,q)$ is on the orbit, the same does not hold for $z=(-p,q)$, however any ball $B(z,\varepsilon)$ will contain infinitely many points of the orbit.

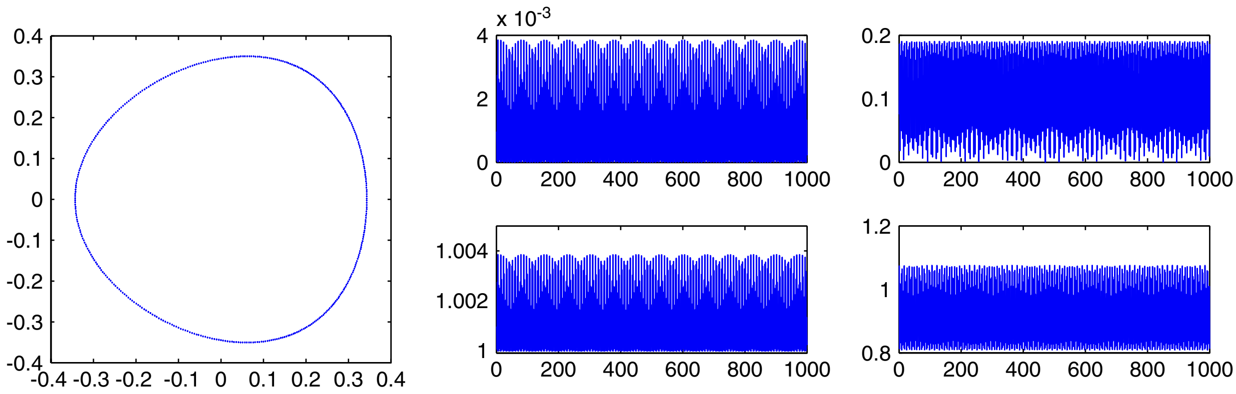

Fig. 4. Behavior of Lobatto IIIB and method (25) applied to the Hamiltonian system of Example 9 in the interval is $[0, 10^4]$ (sampled times: $10nh$, $n = 0, \dots, 1000$).

Exploiting a similar argument as the one used in Lemma 7, we conclude that $\varphi_n(h)$ inherits the almost periodic nature of the orbit itself. For the two orbits under consideration, this is displayed in the middle and right pictures of Fig. 3, respectively. Each picture contains two plots: the upper plot reports $\|(\partial y_n/\partial y_0)^{\mathrm{T}} J(\partial y_n/\partial y_0) - J\|$ as an estimation of the deviation of the method from being purely symplectic, while the lower plot reports the values of $\varphi_n(h)$.

Example 9. We now provide a numerical experiment for a non-separate Hamiltonian system that however retains some symmetries in the solution:

$$H(p, q) = 1/2p^2 \cos(q) + (1 - \cos(q))\mathrm{e}^{-p}.$$

The pictures of Fig. 4 are analogous to those in Fig. 3. The orbit in the phase plane has been obtained by Lobatto IIIB method of order 4, initial condition $y_0 = (0.3, 0.2)^{\mathrm{T}}$ and stepsize $h = 1$; the middle and right pictures report the quantities $\|(\partial y_n/\partial y_0)^{\mathrm{T}} J(\partial y_n/\partial y_0) - J\|$ and $\varphi_n(h)$ for Lobatto IIIB and the discrete gradient method (25) (see the next section).

5. Symmetric discrete gradient methods

The aim of discrete gradient methods is that of exactly conserving the conservation/dissipation features of the continuous dynamical system they are applied to. In their first formulation (low-order schemes), when applied to Hamiltonian systems, they read

$$\frac{y_1 - y_0}{h} = J\nabla_{\mathrm{d}} H(y_0, y_1), \tag{20}$$

where $\nabla_{\mathrm{d}} H(y, z)$ is a discrete gradient operator on H satisfying, by definition, the two conditions (here again we confine our study to the two-dimensional case)

(1) $H(y) - H(z) = \nabla_{\mathrm{d}}^{\mathrm{T}} H(y, z)(y - z)$, for all $y, z \in \mathbb{R}^2$, and
(2) for any sufficiently smooth function $\zeta(t) : \mathbb{R} \to \mathbb{R}^2$, and for any $t_1, t_2 \in \mathbb{R}$, there exists $\bar{t} = \bar{t}(t_1, t_2)$ such that $\nabla_{\mathrm{d}} H(\zeta(t_1), \zeta(t_2)) = \nabla H(\zeta(\bar{t})) + \mathrm{O}(|t_1 - t_2|^p)$, where p is the order of approximation of the discrete gradient as well as of formula (20).

Under the formulation (20), only schemes of first or second order have been derived. The systematic conservation of the energy function is derived by multiplying both sides of (20) on the left by $\nabla_{\mathrm{d}}^{\mathrm{T}} H(y_0, y_1)$ and then by applying property (1):

$$0 = \nabla_{\mathrm{d}}^{\mathrm{T}} H(y_0, y_1) J \nabla_{\mathrm{d}} H(y_0, y_1) = \nabla_{\mathrm{d}}^{\mathrm{T}} H(y_0, y_1)(y_0 - y_1) = H(y_0) - H(y_1).$$

However, this favorable result also prevents these methods to be symplectic: it is therefore interesting to see whether they may instead be sd-symplectic.

One of the simplest methods is due to Itoh and Abe who just replaced the partial derivatives of $H(p,q)$ with increments along the p- and q-axes:

$$\nabla_{\mathrm{d}} H((p_0,q_0),(p_1,q_1)) = \begin{pmatrix} \dfrac{H(p_1,q_0)-H(p_0,q_0)}{p_1-p_0} \\ \dfrac{H(p_1,q_1)-H(p_1,q_0)}{q_1-q_0} \end{pmatrix}. \tag{21}$$

The corresponding method is in general first order and not symmetric. However, when confined to separate Hamiltonian systems $H(p,q)=V(p)-U(q)$, it turns out to be second order and symmetric. In such a case (20) becomes

$$\begin{cases} (p_1-p_0)(q_1-q_0) = -h(U(q_1)-U(q_0)), \\ (q_1-q_0)(p_1-p_0) = h(V(p_1)-V(p_0)). \end{cases} \tag{22}$$

Concerning the Jacobian matrix $\partial y_1/\partial y_0$ defined by the map (22), an easy computation leads to the relation

$$M_{-h}(y_1,y_0)\frac{\partial y_1}{\partial y_0} = -M_h(y_0,y_1), \tag{23}$$

with

$$M_s((p,q),(\hat p,\hat q)) = \begin{pmatrix} \hat q - q & \hat p - p - sU'(q) \\ \hat q - q - sV'(p) & \hat p - p \end{pmatrix}. \tag{24}$$

Taking the transpose in (23) yields

$$\left(\frac{\partial y_1}{\partial y_0}\right)^{\mathrm{T}} M_{-h}^{\mathrm{T}}(y_1,y_0) J M_{-h}(y_1,y_0) \left(\frac{\partial y_1}{\partial y_0}\right) = M_h^{\mathrm{T}}(y_0,y_1) J M_h(y_0,y_1).$$

A direct computation gives

$$M_s^{\mathrm{T}}((p,q),(\hat p,\hat q)) J M_s((p,q),(\hat p,\hat q)) = \hat\mu_s((p,q),(\hat p,\hat q)) J,$$

with

$$\hat\mu_s((p,q),(\hat p,\hat q)) = s(U'(q)(\hat q - q) + V'(p)(\hat p - p) - sU'(q)V'(p)).$$

Finally, we derive the expression of the factor μ for (22), by setting $\mu_s(y) \equiv \hat\mu_s(y, \Phi_s(y))$, where Φ_h denotes the considered method.

In [10], the following generalization of (21) was introduced:

$$\nabla_{\mathrm{d}} H((p_0,q_0),(p_1,q_1)) = \frac{1}{2}\begin{pmatrix} \dfrac{H(p_1,q_0)-H(p_0,q_0)}{p_1-p_0} + \dfrac{H(p_1,q_1)-H(p_0,q_1)}{p_1-p_0} \\ \dfrac{H(p_1,q_1)-H(p_1,q_0)}{q_1-q_0} + \dfrac{H(p_0,q_1)-H(p_0,q_0)}{q_1-q_0} \end{pmatrix}, \tag{25}$$

which makes (20) symmetric and second order for general problems. By repeating the above computation, we can state again sd-symplecticity, with

$$\begin{aligned} \hat\mu_s((p,q),(\hat p,\hat q)) = s\Bigg[& \frac{\partial H}{\partial q}(p,q)(q-\hat q) + \frac{\partial H}{\partial p}(p,q)(\hat p - p) \\ & +2s\left(\frac{\partial H}{\partial p}(p,q)\frac{\partial H}{\partial q}(\hat p,q) + \frac{\partial H}{\partial q}(p,q)\frac{\partial H}{\partial p}(p,\hat q)\right)\Bigg]. \end{aligned}$$

The right plot of Fig. 4 reports the behavior of this method applied to the Hamiltonian system of Example 9.

Finally, we consider the method [11] defined by the discrete gradient

$$\nabla_{\mathrm{d}} H(y_0, y_1) = \nabla H\left(\frac{y_0 + y_1}{2}\right) + R(y_0, y_1), \tag{26}$$

with $R(y, z) = g(y, z)(y - z)$ and the (nonlinear) scalar function g defined as

$$g(y, z) = \frac{H(y) - H(z) - \nabla^{\mathrm{T}} H((y + z)/2)(y - z)}{\|y - z\|_2^2}.$$

The term $R(y_0, y_1)$ in (26) acts as a correction in the implicit midpoint formula, that makes it of discrete gradient type. The method is second order and symmetric, since $g(z, y) = -g(y, z)$ implies $\nabla_{\mathrm{d}} H(y_0, y_1) = \nabla_{\mathrm{d}} H(y_1, y_0)$. To show that it is also sd-symplectic, we observe that the term $R(y, z)$ satisfies the property: $(\partial R/\partial z)(y_0, y_1) = (\partial R/\partial y)(y_1, y_0)$. Therefore, the variational equation of (20), with the choice (26), may be put in the form $M_{-h}(y_1, y_0)\partial y_1/\partial y_0 = M_h(y_0, y_1)$, with $M_s(y, z) = I + (s/2)J\nabla^2 H((y + z)/2) + sJ(\partial R/\partial y)(y, z)$, which yields sd-symplecticity.

6. Conclusions

We have introduced the definition of sd-symplecticity and exploited it to state nearby symplecticity in symmetric non-symplectic one-step methods applied to Hamiltonian systems whose solutions display some symmetries with respect to an equilibrium point. Although the presented results are not meant to be exhaustive, there are a number of interesting issues that sd-symplecticity raises. In the weaker sense expressed by (7), symmetric methods leave the Poisson structure of several Hamiltonian systems invariant by introducing, in their associated flow, an integrating factor $\mu_h = 1 + \mathrm{O}(h^p)$. Thus, sd-symplecticity sheds some lights on the fact that, for a number of important Hamiltonian systems (several test problems of higher dimensions may be found in [8]), the topological portrait in the phase space of the numerical solutions remains the same as for symplectic methods. As shown by Examples 8 and 9, this feature may not be simply retrieved by exploiting a conjugate symplecticity argument. Two open questions are whether the sd-symplecticity property fully characterizes symmetric methods and whether one can always construct a measure that is exactly preserved by the flow of symmetric methods.

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