Symmetric schemes, time reversal symmetry and conservative methods for Hamiltonian systems

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Abstract

It is important, when integrating numerically Hamiltonian problems, that the numerical methods retain some properties of the continuous problem such as the constants of motion and the time reversal symmetry. This may be a difficult task for multistep numerical methods. In the present paper we discuss the problem in the case of linear autonomous Hamiltonian systems and we show the equivalence among the symmetry of the numerical methods and the above-mentioned requirements. In particular, the analysis is carried out for the class of methods known as boundary value methods (BVMs) (Brugnano, Trigiante. Solving Differential Problems by Multistep Initial and Boundary Value Methods. Gordon and Breach Science Publishers, Amsterdam, 1998). © 1999 Elsevier Science B.V. All rights reserved.

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1. Introduction

The approximation of the solution of differential problems by means of numerical methods consists in replacing a given continuous problem with a discrete one, which can be solved on a computer.

An appropriate way to derive numerical methods (see for example [10]) requires that the discrete dynamical system, generated by a given method, retains as many properties of the continuous problem as possible. The application of this principle is, however, difficult to realize. Essentially, the main difficulties are: to maintain the same critical sets of the continuous dynamical system; to preserve the same stability properties of the critical sets; to reproduce different time scales of the solutions; to keep spurious critical sets far from the regions of interest. The application of the
above principle to the case of dissipative problems, where one has a dynamical system with an asymptotically stable solution, has led to the development of the usual linear stability analysis. The resulting appropriate methods are those which are able to reproduce the asymptotic stability of the equilibrium. This stability problem has been extensively studied starting from the fifties until the mid-seventies and has been settled in the framework of a theory whose pre-eminent contribute is due to Dahlquist [6]. Nevertheless, the previous results are not sufficient for more general dynamical systems, where other properties need to be considered. In [5,8–10] (to quote only few recent works related to the present subject) such tendency is evident.

An important recent instance is given by Hamiltonian problems, where the equilibrium solution is only marginally stable. In such a case, if the method is not appropriately chosen, the discrete dynamical system may destroy this property. The first results on this subject were obtained for the class of Runge–Kutta methods [9,11] since they are formally one-step methods. The class of multistep methods, which generate $k$th order difference equations, seemed to be useless in the same circumstance. In fact, Suris [11], Eirola and Sanz-Serna [7] and Cano and Sanz-Serna [5] have proved that no stable methods in such class exist which is suitable for Hamiltonian systems.

A more general approach to the use of multipoint methods, however, has permitted to overcome the above negative results.

As said before, multistep methods substitute to a first-order continuous equation a $k$th order difference one or, equivalently, a first-order discrete equation in an higher-dimensional space. Obviously, one is interested in a subset of such space which approximates the continuous solution. The localization of such subset may be done either by giving all the conditions at beginning of the interval of integration or, more in general, by fixing some of them at the beginning and the others at the end. In the latter case, the obtained discrete problem defines a boundary value method (BVM) [4].

In a series of papers [1–3,12] it has been shown that the solution of the discrete problem is able to maintain, at least in a subsequence of points, important qualitative properties of linear Hamiltonian problems, such as the symplecticness of the map and the conservation of quadratic forms.

The conditions for multipoint methods to be appropriate for Hamiltonian problems, derived in [4,12] by using a variational approach, will be derived here by imposing that the methods must satisfy the so-called time reversal symmetry of the solutions. Such property assumes a particular importance when the considered problem is Hamiltonian. We shall consider this topic in Section 3. In Section 4 we prove the equivalence between the time reversal symmetry and the symmetry of the scheme. In Section 5 we obtain results to be used in Section 6 to prove the equivalence among the symmetry conditions and the conservation of quadratic forms. Before that, in Section 2 we recall the main facts about the considered numerical methods, posed in matrix form as used in the following sections.

In the paper we deal only with linear autonomous Hamiltonian systems since they present the main conservative properties of more general systems and therefore are suitable for to establish in the simplest form the conditions on the methods. In other words, they play the same role of the linear test equation $\dot{y} = \lambda y$, $\text{Re} \lambda < 0$, in the classical dissipative case.

For the sake of simplicity, in order to avoid heavy notation generated by tensor products, in Sections 2–5 we shall refer to a scalar equation.
2. Numerical methods in matrix form

Consider the scalar initial value problem
\[
\frac{dy(t)}{dt} = \lambda y(t) + g(t), \quad t \in [t_0, T],
\]
where \( \eta \in \mathbb{R}, \lambda \in \mathbb{C} \) and \( g(t) \) is a suitably smooth function. The solution will be denoted by \( y(t; t_0, \eta) \).

By considering the partition
\[
t_i = t_0 + ih, \quad i = 0, \ldots, N - 1, \quad h = (T - t_0)/(N - 1)
\]
and \( d \) \( k \)-steps linear multistep methods (LMMs) of order \( p \):
\[
\sum_{j=0}^{k} \left( (\zeta_j^{(\xi)} - h\lambda\beta_{j}^{(\xi)})y_{n+j} - h\beta_{j}^{(\xi)}g_{n+j} \right) = 0, \quad \zeta = 1, \ldots, d,
\]
we can discretize the continuous Eq. (1) at \( d \) consecutive grid points. In matrix form the discrete equation becomes
\[
(Ad - hBd)y - hBg = 0,
\]
where the entries of the vector
\[
y = (y_0, \ldots, y_{N-1})^T
\]
are the approximate values of the solutions, while the vector \( g \) is defined by \( g = (g_0, \ldots, g_{N-1})^T \). The matrices \( A_d \) and \( B_d \), both of dimension \( d \times N \), have the \( \xi \)th row made up with the coefficients \( \zeta_j^{(\xi)} \) and \( \beta_{j}^{(\xi)} \), respectively. Since the methods are \( k \)-steps, the nonzero entries on each row are at most \( k + 1 \) and
\[
|\zeta_j^{(\xi)}| + |\beta_{0}^{(\xi)}| > 0, \quad |\zeta_j^{(\xi)}| + |\beta_{k}^{(\xi)}| > 0, \quad \zeta = 1, \ldots, d.
\]
Moreover, we require that the matrices \( A_d \) and \( B_d \) have maximum rank. When \( d = N - k \), in order to select a particular solution of Eq. (3), we must add a set of \( k \)-independent conditions. We shall consider these topics later.

Let each method be consistent and irreducible. Such requirements imply \( \sum_{j=0}^{k} \zeta_j^{(\xi)} = 0, \sum_{j=0}^{k} j\zeta_j^{(\xi)} = \sum_{j=0}^{k} \beta_{j}^{(\xi)} \) and \( \sum_{j=0}^{k} \beta_{j}^{(\xi)} = 1 \). In matrix form they become
\[
A_d e_N = 0,
A_d u = B_d e_N = e_d,
\]
where \( u = (0, 1, \ldots, N - 1)^T \) and, hereafter, for every integer \( \gamma \), \( e_\gamma = (1, \ldots, 1)^T \) is a vector in \( \mathbb{R}^\gamma \). Further order requirements essentially consist in asking that the methods are exact for polynomial problems, i.e. when \( \lambda = 0 \) and \( g(t) = t, i = 1, \ldots, p - 1 \). All together, the order conditions can be
also posed in matrix form by introducing the matrices

\[
H_s = \begin{pmatrix}
0 & & & & \\
1 & & & & \\
& & & & \\
& & & & \\
\gamma & 0 & & & \\
\end{pmatrix}
\]

(7)

and

\[
Q_s^{(\gamma)} = (q_s^{(0)}, \ldots, q_s^{(\gamma)})_{m \times (\gamma + 1)},
\]

(8)

where

\[
q_s^{(j)} = ((-s)^j, (1 - s)^j, (2 - s)^j, \ldots, (m - s - 1)^j)^T, \quad j = 0, \ldots, \gamma
\]

with \( s \) any integer number. One verifies that method (3) has order \( p \) provided that the following conditions are satisfied, with \( m = N \) in (8):

\[
A_d Q_s^{(p+1)} - B_d Q_s^{(p+1)} H^T_{p+1} = W,
\]

(9)

where the matrix \( W \equiv [O|c] \) has the first \( (p + 1) \) columns null. The entries of the vector \( c \) are the error constants of the methods.

Let \( \Psi_s^{(p+1)} \) be the matrix whose columns are the discrete solutions of the polynomial problems. It is clear that

\[
\Psi_s^{(p+1)} = Q_s^{(p+1)} + E,
\]

(10)

where \( E = [O|w] \) is the error matrix. Since

\[
A_d \Psi_s^{(p+1)} - B_d Q_s^{(p+1)} H^T_{p+1} = O
\]

from (9) and (10) it follows that

\[
W = -A_d E.
\]

(11)

3. Time reversal symmetry (TRS)

Let \( \tau = t_0 + T - t \). Problem (1) can be written as

\[
\frac{dz(\tau)}{d\tau} = -\lambda z(\tau) - s(\tau), \quad \tau \in [t_0, T],
\]

\[
z(T) = \eta,
\]

(12)

where \( z(\tau) \equiv y(t_0 + T - \tau) \) and \( s(\tau) \equiv g(t_0 + T - \tau) \). One realizes that

\[
z(\tau; T, \eta) \equiv y(t; t_0, \eta), \quad t, \tau \in [t_0, T].
\]

On the discrete points \( \{t_i\} \) defined in (2) and on the corresponding mesh \( \{\tau_i\}, \tau_i = t_0 + T - t_i \), we define the two vectors

\[
Y = \begin{pmatrix}
\eta \\
y(t_1) \\
\vdots \\
y(T)
\end{pmatrix}, \quad Z = \begin{pmatrix}
z(\tau_{N-1}) \\
z(\tau_{N-2}) \\
\vdots \\
\eta
\end{pmatrix}.
\]
It is easy to check that
\[ Z = P_N Y, \]  
where, in general,
\[ P_\gamma = \begin{pmatrix} \mathbf{1} \\ \vdots \\ \mathbf{1} \end{pmatrix}_{N \times \gamma}. \]  
(14)

By applying the same numerical method to problems (1) and (12), we obtain, respectively,
\[ \begin{pmatrix} e^{t/N}T \\ A_d - h\lambda B_d \end{pmatrix} y = \begin{pmatrix} \eta \\ hB_d g \end{pmatrix} \]  
(15)
and
\[ \begin{pmatrix} A_d + h\lambda B_d \\ e^{N/T} \end{pmatrix} z = \begin{pmatrix} -hB_d P_N g \\ \eta \end{pmatrix}. \]  
(16)
Here \( e^{t/N} \), \( i = 1, N \), is the \( i \)th unit vector in \( \mathbb{R}^N \); \( y \) is defined in (4), \( z = (z_{N-1}, \ldots, z_0)^T \) contains the approximate values of the solutions \( z(\tau; T, \eta) \) and \( P_N g = s = (s_{N-1}, \ldots, s_0)^T, s_i = s(\tau_i) \). Note that when \( d < N - 1 \) (15) and (16) have not a unique solution because they need additional conditions. It is not obvious that a discrete analogous to (13) holds for the numerical solutions \( y \) and \( z \). When it happen, i.e. when
\[ z = P_N y, \]  
(17)
we say that the numerical method satisfies the time reversal symmetry (TRS).

**Remark 3.1.** Condition (13) is a tautology for the continuous solution evaluated at the discrete points. Condition (17) is an effective one because a generic numerical method works differently according to the time direction.

In order to clarify the above statement, let, for example, approximate the constant \( 1 = e^{h/2}e^{-h/2} \), \( \lambda \in \mathbb{R} \), by using the approximation to the exponential derived from the explicit Euler method. We have \( (1 + \frac{h}{2})(1 - \frac{h}{2}) = 1 - \frac{h^2}{2} \lambda^2 \neq 1 \). The same does not occur, for example, when we use the trapezoidal rule. The above consideration, which seems almost obvious for one-step methods, needs to be generalized to multistep methods and this will be done below, by using TRS. Before that, let us stress that the use of methods having the above property is important, for example, when the continuous problem is time isotropic (Hamiltonian problems are in this class). In the simplest case (i.e. the harmonic oscillator \( y'' + \omega^2 y = 0, y(0) = y_0, y'(0) = 0 \) the time isotropy of the solution \( y(t) \) means \( y(t) = y(-t) \). Often such solution is the sum of two elementary solutions generated by eigenvalues of opposite sign, such as, for example, \( e^{it} + e^{-it} \). If the method used does not satisfy (17), \( e^{it} \) and \( e^{-it} \) are approximated inappropriately and the discrete solution will not maintain the time isotropy property of the continuous one. Therefore, our time reversal symmetry is a necessary condition for a numerical method to maintain the time isotropy.
In order to obtain from (17) conditions on the coefficients \( \alpha_j \) and \( \beta_j \) of the methods, we also need to impose the order conditions by using polynomials in the new variable \( \tau \). We obtain (see (9))

\[
A_d \tilde{Q}_s^{(p+1)} + B_d \tilde{Q}_s^{(p+1)} H_{p+1}^T = \tilde{W},
\]

where \( \tilde{W} = (-1)^{p+1} [O|\tilde{c}] \) and \( \tilde{Q}_s^{(p+1)} = P_N Q_s^{(p+1)} \) are the analogous of \( W \) and \( Q_s^{(p+1)} \) in (9) on the new mesh \( \{\tau_i\} \). We proceed as done at the end of the previous section by defining the corresponding matrices

\[
\tilde{Q}_s^{(p+1)} = Q_s^{(p+1)} + \tilde{E}
\]

with \( \tilde{E} = [O|\tilde{w}] \). With similar arguments one obtains the analogous of (11), i.e.

\[
\tilde{W} = -A_d \tilde{E}.
\]

**Theorem 3.1.** If TRS holds true, then

\[
\tilde{E} = P_N E.
\]

**Proof.** Since TRS is satisfied, \( \tilde{Q}_s^{(p+1)} = P_N \Psi_s^{(p+1)} \), or, equivalently (see (9) and (10)), \( \tilde{Q}_s^{(p+1)} + \tilde{E} = P_N Q_s^{(p+1)} + P_N E \). □

Let us now particularize \( A_d \) and \( B_d \) by considering the more usual case when the same LMM (main method), \( \sum_{j=0}^k ((x_j - h \lambda \beta_j) y_{n+j} - h \beta_{n+j}) = 0 \), is applied at each grid point. In this case \( A_d \) and \( B_d \) are Toeplitz matrices which in the sequel will be denoted by \( A \) and \( B \), respectively. Consequently, Eq. (3) becomes

\[
(A - h \lambda B)y - hBg = 0
\]

and (see (9) and (18)) \( c = \tilde{c} = ce_d \), where \( c \) is the error constant of the method. Moreover, we need the following result. Consider the polynomial \( p(v) = \sum_{j=0}^k (x_j + x_{k-j}) v^j \), whose roots \( \{v_i\} \), for simplicity, are supposed to be simple.

**Lemma 3.1.** Let \( d = N - k > k \) and \( w \in \mathcal{N}(A + P_N - k A P_N) \). Then

\[
w = \sum_{i=1}^k a_i \begin{pmatrix} v_i \\ \vdots \\ v_i^{N-1} \end{pmatrix},
\]

where \( v_i \) is a root of the polynomial \( p(v) \). One of such roots is 1.

**Proof.** Trivial considering that \( A + P_N - k A P_N \) is a Toeplitz matrix whose symbol is \( p(v) \). Moreover, from the consistence conditions \( \sum_{j=0}^k (x_j + x_{k-j}) = 0 \) and then \( p(1) = 0 \). □

**Theorem 3.2.** Suppose that the main method, used to define the matrices \( A \) and \( B \), is of order \( p \geq k \) and irreducible and TRS holds true. Then,
(i) the matrices $A$ and $B$ satisfy the symmetry conditions

\begin{align}
    P_{N-k}AP_N &= -A, \quad P_{N-k}BP_N = B, \tag{22}
\end{align}

(ii) $p$ is even.

**Proof.** By considering that the TRS holds true, from (11), (20) and Theorem 3.1 we obtain

\begin{align}
    Aw &= -ce_{N-k}, \tag{23}
    -AP_Nw &= (-1)^{p+1}ce_{N-k}. \tag{24}
\end{align}

We consider first the case of $p$ even, i.e.

\begin{align}
    AP_Nw &= ce_{N-k}. \tag{25}
\end{align}

By adding to (23) the last equation multiplied on the left by $P_{N-k}$ and by observing that, for every integer $\gamma$, $P_{N-k}e_{x} = e_{x}$, we have

\begin{align}
    (A + P_{N-k}AP_N)w &= 0. \tag{26}
\end{align}

We claim that a vector $w$ cannot exist which satisfies both (23) and (25). In fact, since $w \in N(A + P_{N-k}AP_N)$, from Lemma 3.1 one obtains

\begin{align}
    Aw &= A \sum_{i=1}^{k} a_i \left( \begin{array}{c}
        1 \\
        v_i \\
        \vdots \\
        v_i^{N-1}
    \end{array} \right) = \sum_{i=1}^{k} a_i \rho(v_i) \left( \begin{array}{c}
        1 \\
        v_i \\
        \vdots \\
        v_i^{N-k-1}
    \end{array} \right),
\end{align}

where $\rho(v_i) = \sum_{j=0}^{k} z_j v_i^j$. Moreover, by considering that $\rho(v_1) \equiv \rho(1) = 0$, the previous equation and (23) give the system

\begin{align}
    ce_{N-k} + \sum_{i=2}^{k} a_i \rho(v_i) \left( \begin{array}{c}
        1 \\
        v_i \\
        \vdots \\
        v_i^{N-k-1}
    \end{array} \right) &= 0,
\end{align}

which does not have a solution. One then concludes that (23) and (25) can be simultaneously satisfied only when $A + P_{N-k}AP_N = O$. In order to prove the second equality in (22), we add Eq. (18), multiplied on the left by $P_{N-k}$, to (9). By using the first equality in (22) just proved, we then obtain $(P_{N-k}BP_N - B)Q_{p+1}^{p+1} H_{p+1} = O$. By multiplying on the left by $e^{(1)\top}$, the transpose of the relation obtained is

\begin{align}
    H_{p+1}Q_{p+1}^{p+1} \left( \begin{array}{c}
        \beta_k - \beta_0 \\
        \vdots \\
        \beta_0 - \beta_k \\
        0 \\
        \vdots \\
        0
    \end{array} \right) &= 0.
\end{align}
Since the matrix $H_{p+1}Q^{(p+1)T}$ has rank $p + 1 \geq k + 1$, the only solution is $\beta_{k-j} - \beta_j = 0$, $j = 0, \ldots, k$, from which the second of (22) follows.

When $p$ is odd, (24) becomes

$$-AP_Nw = ce_{N-k}. $$

Arguments similar to those used in the previous case lead, instead of (22), to

$$A = P_{N-k}AP_N, \quad B = -P_{N-k}BP_N.$$ 

The second of the above relations together with the irreducibility condition (see (6)) leads to $e_{N-k} = -e_{N-k}$ which is impossible. 
\[ \Box \]

4. Boundary value methods

In this section we consider the additional conditions for (21) to get a unique solution. Assume $d = N - k$. Then $k$-independent additional conditions are needed. The continuous problem only provides one of them (i.e. the initial condition). The classical use of LMMs consists in fixing the remaining $k - 1$ at the initial points. For Hamiltonian problems this choice is not appropriate because, as pointed out in [5,7,11], the methods satisfying the conservation properties turn out to be unstable. On the contrary, if one imposes part of conditions, say $k_1$, at beginning and the remaining $k_2 = k - k_1$ at the end of the interval, this difficulty may be overcome (see [3,4]). In the latter case, continuous problem (1) is approximated by means of a discrete boundary value problem. This defines a boundary value method with $(k_1, k_2)$-boundary conditions. Instead of fixing the $k_1 - 1$ initial additional values, an equal number of additional initial methods, whose coefficients define the matrices $A^{(I)}$ and $B^{(I)}$, are introduced. Similarly, we introduce $k_2$ additional final methods, whose coefficients define the matrices $A^{(F)}$ and $B^{(F)}$. In order to get a global error of order $p$, all the methods used later to define $(A^{(I)}, B^{(I)})$ $(A^{(F)}, B^{(F)})$ cannot be of order less then $p - 1$ (see [4]). The resulting discrete equation can then be written as

$$(\tilde{A} - h\tilde{B})y = h\tilde{B}g,$$

where

$$\tilde{A} = \begin{pmatrix} (A^{(I)} O) \\ A \\ (O A^{(F)}) \end{pmatrix}_{(N-1)\times N}, \quad \tilde{B} = \begin{pmatrix} (B^{(I)} O) \\ B \\ (O B^{(F)}) \end{pmatrix}_{(N-1)\times N},$$

$$A^{(I)} = \begin{pmatrix} \varphi^{(1)}_0 & \ldots & \ldots & \varphi^{(1)}_{k_1} \\ \vdots & \ddots & \ddots & \vdots \\ \varphi^{(1)}_0 & \ldots & \ldots & \varphi^{(1)}_{k_1} \end{pmatrix}_{(k_1-1)\times (r+1)},$$

$$B^{(I)} = \begin{pmatrix} \beta^{(1)}_0 & \ldots & \ldots & \beta^{(1)}_r \\ \vdots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \vdots \\ \beta^{(k_1-1)}_0 & \ldots & \ldots & \beta^{(k_1-1)}_r \end{pmatrix}_{(k_1-1)\times (r+1)}.$$
where \( l_1 = r - k_1 + 2 \) and

\[
A^{(F)} = \begin{pmatrix}
\alpha_0^{(N)} & \cdots & \cdots & \alpha_{l_1}^{(N)} \\
\vdots & \ddots & \ddots & \vdots \\
\alpha_0^{(N)} & \cdots & \cdots & \alpha_{l_1}^{(N)}
\end{pmatrix}_{k_2 \times (r+1)},
\]

\[
B^{(F)} = \begin{pmatrix}
p_0^{(N-k_2+1)} & \cdots & \cdots & p_r^{(N-k_2+1)} \\
\vdots & \ddots & \ddots & \vdots \\
p_0^{(N)} & \cdots & \cdots & p_r^{(N)}
\end{pmatrix}_{k_2 \times (r+1)},
\]

where \( l_1 = r - k_2 + 1 \). The Toeplitz form of \( A^{(I)} \) and \( A^{(F)} \) has been chosen for convenience. It is possible to obtain similar results by fixing the Toeplitz form for the matrices \( B^{(I)} \) and \( B^{(F)} \). In (28)–(29) we have assumed that the additional methods have the same number of steps, \( r \geq k \), appropriately chosen. Moreover, they must satisfy order conditions (9) and must be taken such that both \( \tilde{A}, \tilde{B} \) have maximum rank.

In the sequel we shall refer to Eq. (26) as the complete method. In particular, when the matrices \( \tilde{A}, \tilde{B} \) verify the symmetry conditions

\[
P_{N-1}\tilde{A}P_N = -\tilde{A}, \quad P_{N-1}\tilde{B}P_N = \tilde{B},
\]

the complete method is also called a symmetric scheme.

**Lemma 4.1.** Suppose that (30) holds true for method (26). Then the matrices \( A \) and \( B \) in (27) satisfy the analogous symmetry relations (22).

**Proof.** The matrices \( A^{(I)}, B^{(I)}, A^{(F)}, B^{(F)} \) in (28) and (29) have \( (k_1 - 1) \) and \( k_2 \) rows, respectively. Suppose that \( k_1 - 1 = k_2 \equiv v - 1 \). From (30) one has then

\[
\begin{pmatrix}
(A^{(I)} & O) \\
A \\
(O & A^{(F)})
\end{pmatrix} = \begin{pmatrix}
(-P_{v-1}A^{(F)}P_{r+1} & O) \\
-P_{N-k}AP_N \\
(O & -P_{v-1}A^{(I)}P_{r+1})
\end{pmatrix}
\]

and

\[
\begin{pmatrix}
(B^{(I)} & O) \\
B \\
(O & B^{(F)})
\end{pmatrix} = \begin{pmatrix}
(P_{v-1}B^{(F)}P_{r+1} & O) \\
P_{N-k}BP_N \\
(O & P_{v-1}B^{(I)}P_{r+1})
\end{pmatrix}
\]

from which (22) follows.

Suppose now that \( k_1 - 1 \neq k_2 \). In particular, we consider the case \( k_1 - 1 > k_2 \). Condition (30) then gives that \( \alpha_0 \) is the entry \((k_1, 1)\) of \( \tilde{A} \), while 0 is the corresponding entry of \( -P_{N-1}\tilde{A}P_N \). Similarly, \( \beta_0 \) is the entry \((k_1, 1)\) of \( \tilde{B} \), while 0 is the corresponding entry of \( P_{N-1}\tilde{B}P_N \). Consequently, one has \( \alpha_0 = \beta_0 = 0 \), which contradicts the first inequality in (5). Similarly, when \( k_1 - 1 < k_2 \) the symmetry
conditions (30) imply that \( \alpha_k = \beta_k = 0 \), which contradicts the second inequality in (5). One then concludes that \( k_1 - 1 = k_2 \) and then (22) holds true. \( \square \)

**Corollary 4.1.** For a symmetric scheme \( k \) must be odd, say \( 2v - 1 \).

**Corollary 4.2.** For a symmetric scheme the matrices \( A^{(1)}, B^{(1)} \) and \( A^{(F)}, B^{(F)} \) (see (28)–(29)) satisfy the following symmetry conditions:

\[
P_{r-1}A^{(1)}P_r + 1 = -A^{(F)}, \quad P_{r-1}B^{(1)}P_r + 1 = B^{(F)}.
\]

(31)

We now generalize Theorem 3.2 to the complete method.

**Theorem 4.1.** Suppose that each method (i.e. initial, main and final methods) is of order \( p \geq k \) and irreducible. Then, TRS holds true if and only if

(i) the matrices \( \tilde{A} \) and \( \tilde{B} \) satisfy (30); (ii) \( p \) is even.

**Proof.** The if implication can be proved by using arguments similar to those used in Theorem 3.2. For brevity we shall omit to repeat them.

We now prove that (30) implies TRS. By observing that, for any integer \( \gamma \), \( P^2_\gamma = I_\gamma \), where \( I_\gamma \) is the identity matrix of dimension \( \gamma \), from (26) one obtains

\[
P_{N-1}(\tilde{A} - h\tilde{B})P_N^2y = hP_{N-1}\tilde{B}P_N^2g,
\]

that is

\[
(P_{N-1}\tilde{A}P_N - h\tilde{B}P_N)(P_N^2y) = h(P_{N-1}\tilde{B}P_N)y = h(P_{N-1}\tilde{B}P_N)P_Ny.
\]

From (30) it follows that \( (\tilde{A} + h\tilde{B})P_Ny = -h\tilde{B}P_Ng \), which implies TRS (see (16) and (17)). \( \square \)

5. A property of symmetric schemes

In [4] it was proved that symmetry conditions (22) imply that the matrix \( K = A^T B + B^T A \) is centro-skew-symmetric, that is

\[
K = -P_NKP_N.
\]

(32)

Here we derive and generalize the previous result by showing that the converse implication is also true.

**Theorem 5.1.** Suppose that the main method is consistent and irreducible. Then, symmetry conditions (22) are satisfied if and only if \( K \) verifies (32).

**Proof.** Suppose that (22) holds true. One has

\[
K = (-P_N A^T P_{N-k})(P_{N-k} B P_N) + (P_N B^T P_{N-k})(-P_{N-k} A P_N)
\]

and then (32) follows.
Conversely, suppose that (32) holds true. From (6) we then obtain
\[ 0 = (K + P_NK)e_N = ((A^TB + B^TA) + P_N(A^TB + B^TA)P_N)e_N = (A^T + P_NA^T)e_{N-k}. \]

Considering that
\[
A^T + P_NA^T = \begin{pmatrix}
\alpha_0 & 0 & \cdots & 0 \\
\vdots & \ddots & \vdots & \vdots \\
\vdots & \ddots & \ddots & \vdots \\
\vdots & \ddots & 0 & \alpha_k \\
0 & \cdots & \cdots & \alpha_k \\
0 & \cdots & \cdots & 0 \\
\end{pmatrix}
\]

it follows that \( \alpha_j + \alpha_{k-j} = 0, j = 0, \ldots, k, \) which is equivalent to the first equality in (22). In order to prove the second equality in (22), we observe that from (32), by posing \( F = A^T(B - P_{N-k}BP_N), \) one also obtains
\[ F + F^T = 0. \] (33)

Namely, the matrix
\[
F = \begin{pmatrix}
\alpha_0 & \cdots & 0 \\
\vdots & \ddots & \vdots \\
\vdots & \ddots & 0 \\
0 & \cdots & \alpha_k \\
0 & \cdots & \alpha_k \\
\end{pmatrix}
\]
is skew-symmetric. Let \( \alpha_i \) be the first nonzero coefficient of the method, i.e. \( \alpha_0 = \cdots = \alpha_{i-1} = 0, \alpha_i \neq 0. \) The \((i+1)\)-st row in (33) then gives \( \alpha_i(\beta_j - \beta_{k-j}) = 0, j = 0, \ldots, k, \) from which the second equality in (22) readily follows.

In order to generalize the above result to the complete method, the following Lemma will be useful.

**Lemma 5.1.** Let \( D_j = \text{diag}(1, -1, 1, -1, \ldots, (-1)^\gamma) \in \mathbb{R}^{(\gamma+1)\times(\gamma+1)}. \) Then the matrices \( Q^{(\gamma)}_s \) and \( H^{(\gamma)}_s \) defined in (8) and (7), respectively, satisfy the following properties:

- P1 \( P_mQ^{(\gamma)}_{s}D_{\gamma} = Q^{(\gamma)}_{s-m-1}, \)
- P2 \( D_{\gamma}H^{(\gamma)}_{s}D_{\gamma} = -H^{(\gamma)}_{s}. \)

**Proof.** We prove only P1 since P2 can be proved similarly.
\[
(P_mQ^{(\gamma)}_{s})_{h} = \sum_{b=1}^{m}(P_m)_{bh}(Q^{(\gamma)}_{s})_{bh}, \quad i = 1, \ldots, m, \quad \ell = 1, \ldots, \gamma + 1.
\]
From the definition of $P_m$ it follows that the right-hand side of the previous equality is nonzero only when $i + b = m + 1$. By considering that the entries of $(Q_s^{(s)})_{b'} = (b - 1 - s)^{i-1}$, we obtain

$$(P_m Q_s^{(s)})_{ij} = (m - i - s)^{j-1} = (i - 1 - (m - s - 1))^{j-1} = (Q_{m-s})_{ij}.$$ 

**Theorem 5.2.** Consider an irreducible complete method (26). Suppose that each method (i.e. initial, main and final methods) is of order $p > k$ and the additional methods are $r$-steps, with $k \leq r \leq p - 1$. Symmetry conditions (30) are satisfied if and only if $k$ is odd and $K = A^T B + B^T A$ is centro-skew-symmetric, that is

$$K + P N \tilde{K} P N = O.$$ (34)

**Proof.** Suppose that (30) holds true. Then

$$\tilde{K} = (-P N A^T P_{N-1})(P_{N-1} B P N) + (P N B^T P_{N-1})(-P_{N-1} A P N),$$

from which (34) follows. Moreover, by Corollary 4.1 one has that $k$ is odd. Conversely, if (34) is satisfied one has

$$O = \tilde{K} + P N \tilde{K} P N = (K + P N K P N)

+ \begin{pmatrix} (A^{(1)T} B^{(1)} + B^{(1)T} A^{(1)} + P_{r+1} A^{(F)T} B^{(F)} P_{r+1} + P_{r+1} B^{(F)T} A^{(F)} P_{r+1}) & O \\
O & (A^{(F)T} B^{(F)} + B^{(F)T} A^{(F)} + P_{r+1} A^{(I)T} B^{(I)} P_{r+1} + P_{r+1} B^{(I)T} A^{(I)} P_{r+1}) \end{pmatrix}.$$  

Since the main method is independent of the additional methods, it must be $K + P N K P N = O$. Then, from Theorem 5.1 symmetry conditions (22) hold true. We only need to verify that conditions (31) follow from the relation

$$A^{(1)T} B^{(1)} + B^{(1)T} A^{(1)} + P_{r+1} A^{(F)T} B^{(F)} P_{r+1} + P_{r+1} B^{(F)T} A^{(F)} P_{r+1} = O.$$ 

By multiplying on the right by $e_{r+1}$ and by using both consistence conditions and irreducibility (6), the above equation becomes

$$A^{(1)T} e_{k_1-1} + P_{r+1} A^{(F)T} e_{k_2} = 0.$$ (35)

Considering that $k$ is odd, it is easy to check that if $k_1 - 1 \neq k_2$ all the entries of $A^{(1)}$ and $A^{(F)}$ must be zero. We take then $k_1 - 1 = k_2 \equiv v - 1$. This implies that $l_1 = l_F \equiv l$ (see (28)–(29)). Then,
considering that

\[
A(I)^T + P_{r+1}A(F)^T = \begin{pmatrix}
\begin{array}{ccc}
0 & \cdots & 0 \\
\vdots & \ddots & \vdots \\
0 & \cdots & 0 \\
\end{array}
\end{pmatrix} + \begin{pmatrix}
\begin{array}{ccc}
0 & \cdots & 0 \\
0 & \cdots & 0 \\
\vdots & \ddots & \vdots \\
0 & \cdots & 0 \\
\end{array}
\end{pmatrix},
\]

from (35) one has

\[
0 = \alpha_0^{(1)} + \alpha_j^{(N)},
0 = \alpha_0^{(1)} + \alpha_j^{(N)} + \alpha_1^{(I)} + \alpha_{l-1}^{(N)},
\]

that is \( \alpha_j^{(1)} = -\alpha_{j-1}^{(N)} \), and then the first of (31). It remains to prove the second equality. From the order conditions (9) for the additional methods we have

\[
A(F)Q(p) = B(F)Q(p)H_T, \quad A(I)Q(p) = B(I)Q(p)H_T.
\]

By using the first equality just proved and the result of Lemma 5.1, one then obtains

\[
A(F)Q_{r-s} = P_{r-1}B(I)P_{r+1}Q_{r-s}H_T.
\]

This is verified for all integers \( r-s \). By replacing \( r-s \) by \( s \) and by subtracting the above equation from the first equation in (36), we get

\[
(B(F) - P_{r-1}B(I)P_{r+1})Q_{s}H_T = O.
\]

Since \( Q_{s}H_T \in \mathbb{R}^{(r+1)\times(p+1)} \) has rank \( p \geq r+1 \), one then concludes that

\[
B(F) - P_{r-1}B(I)P_{r+1} = O
\]

from which the thesis follows. \( \Box \)

As an example of symmetric main method not satisfying the requirements of Theorem 5.2, we quote the explicit midpoint method. In fact, for this method \( k \) is even (\( k = 2 \)).

The results obtained in the above sections can be straightforwardly generalized to the case of a system of first-order differential equations, that is when in (1) \( y(t) \) and \( g(t) \) are vectors in \( \mathbb{R}^m \) and \( \lambda \equiv L \in \mathbb{R}^{m \times m} \).
6. Conservation property for linear autonomous Hamiltonian problems

We restrict our analysis to linear autonomous Hamiltonian problems, i.e. to problems in the following form,
\[
\frac{d y(t)}{dt} = L y(t), \quad t \in [t_0, T],
\]
\[y(t_0) = \eta \in \mathbb{R}^{2m}\]
(37)
with
\[L = J_{2m} S, \quad J_{2m} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \otimes I_m, \quad S = S^T \in \mathbb{R}^{2m \times 2m}.
\]

First of all, we recall some basic facts about problem (37). It is known that for every matrix \(C\) satisfying
\[L^T C + CL = O
\]
(38)
the quadratic form
\[V(t; C) = y(t)^T C y(t)
\]
(39)
is a constant of motion. In particular, for \(C = S\) one obtains the conservation for the Hamiltonian function of the problem. One wishes to construct methods such that a conservation property similar to (39) holds true for the discrete solution. It is known that (see [3,4]) a BVM, whose matrices \(\tilde{A}\) and \(\tilde{B}\) verify the symmetry conditions (30), satisfies the following relation:
\[y_i^T C y_j + y_j^T C y_i = y_{N-i}^T C y_{N-j} + y_{N-j}^T C y_{N-i},
\]
i, j = 0, \ldots, N - 1. The above property, in the case where \(j = i\), simplifies to
\[y_i^T C y_i = y_{N-i}^T C y_{N-i},
\]
i = 0, \ldots, N - 1. In particular, when \(i = 0\) one obtains
\[y_0^T C y_0 = y_{N-1}^T C y_{N-1},
\]
namely, the constants of motion are exactly preserved in the last point of the discrete solution. When property (40) holds true, a method is said to be essentially conservative symplectic [4].

Our aim is to prove that symmetry conditions (30) are equivalent to property (40) which, in turn, is equivalent to the TRS of the method. Before that, we need to establish an additional result.

**Lemma 6.1.** Consider Hamiltonian problem (37) and let \(C\) be any matrix satisfying (38). Then, Eq. (40) implies that \(\tilde{K}\) is centro-skew-symmetric.

**Proof.** Let \(y\) be a discrete solution obtained by applying to problem (37) the numerical method defined by the matrices \(\tilde{A}\) and \(\tilde{B}\):
\[(\tilde{A} \otimes I_{2m} - h\tilde{B} \otimes L)y = 0.
\]
By multiplying the above equation on the left by \(y^T (\tilde{B}^T \otimes C)\) one has
\[y^T (\tilde{B}^T \tilde{A} \otimes C - h\tilde{B}^T \tilde{B} \otimes CL)y = 0.
\]
Similarly, by multiplying the same equation on the left by $y^T(\hat{B}^T \otimes C^T)$ we obtain

$$y^T(\hat{B}^T \hat{A} \otimes C^T - h\hat{B}^T \hat{B} \otimes C^T L)y = 0.$$ 

Finally, by adding the transpose of the latter expression to the former one,

$$0 = y^T((\hat{B}^T \hat{A} + A^T \hat{B}) \otimes C - h\hat{B}^T \hat{B} \otimes (CL + L^T C))y$$

$$= y^T((\hat{B}^T \hat{A} + A^T \hat{B}) \otimes C) = y^T(\hat{K} \otimes C)y. \quad (42)$$

By introducing the notation

$$\tilde{k}_{ij} = \begin{cases} 
2\sigma_{ij} & \text{if } i = j, \\
2\sigma_{ij} & \text{if } i + j = N - 1, \\
\sigma_{ij} & \text{otherwise}, 
\end{cases}$$

where $\tilde{k}_{ij}$, $i,j = 0,\ldots,N-1$, are the entries of the symmetric matrix $\tilde{K}$ (for simplicity, we assume $N$ to be even) and by using (40), (42) can be written as

$$\sum_{i=0}^{N-1} \sum_{j=0}^{N-1-i} (y^T_i C y_j + y^T_j C y_i)(\sigma_{ij} + \sigma_{N-1-i,N-1-i}) = 0,$$

where, obviously, the inner summation is zero when $i > N - 1 - i$. This equality must be satisfied for any continuous problem in form (37) and for all $C$ satisfying (38). One then concludes that $\sigma_{ij} + \sigma_{N-1-i,N-1-i} = 0$, that is $\tilde{K}$ is centro-skew-symmetric.

We now are able to prove the following:

**Theorem 6.1.** Consider an irreducible complete method applied to Hamiltonian problem (37). Suppose that,

(i) each method (i.e. initial, main and final methods) is of order $p \geq k$,

(ii) the additional methods are $r$-steps, $k \leq r \leq p - 1$,

(iii) $C$ is any matrix satisfying (38).

Then conservation property (40) for the discrete solution is equivalent to symmetry conditions (30).

**Proof.** The implication (30) $\Rightarrow$ (40) is already known (see [3,4]).

The converse implication follows from the Theorem 5.2 and Lemma 6.1.

7. Conclusions

In this paper we have shown that for an irreducible BVM the following diagram holds true:

- Time reversal property $\iff$ Conservation property (40)
- Symmetry conditions (30) $\iff$ $\tilde{K}$ is centro-skew-symmetric.

In order to highlight the theoretical results, we shall consider a simple example.
Example 7.1. Let the continuous Hamiltonian problem be

\[
\frac{dy}{dt} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} y, \quad t \in [0, 10], \quad y(0) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}.
\]

(43)

We approximate (43) and the corresponding time-reversed problem by using the same symmetric main method, i.e. the fourth-order Extended Trapezoidal Rule (ETR [4]), with stepsize \( h = 0.5 \). The corresponding matrices are

\[
A = \begin{pmatrix} -1 & 1 & & & \\ & -1 & 1 & & \\ & & & \ddots & 1 \\ & & & & -1 & 1 \\ & & & & & -1 & 1 \\ & & & & & & \ddots & \end{pmatrix}, \quad B = \frac{1}{24} \begin{pmatrix} -1 & 13 & 13 & -1 \\ & -1 & 13 & 13 & -1 \\ & & & \ddots & \end{pmatrix}.
\]

As additional methods we take

(i)

\[
A^{(i)} = ( -1 & 1 & 0 & 0), \quad A^{(F)} = (0 & 0 & -1 & 1),
\]

\[
B^{(i)} = ( \frac{3}{8} & \frac{19}{24} & -\frac{5}{24} & \frac{1}{24} ), \quad B^{(F)} = (\frac{1}{24} & -\frac{5}{24} & \frac{19}{24} & \frac{3}{8} ),
\]

which are symmetric, according to (31), and

(ii)

\[
A^{(i)} = ( -1 & 1 & 0 & 0 & 0), \quad A^{(F)} = (0 & 0 & 0 & -1 & 1),
\]

\[
B^{(i)} = (\frac{251}{720} & \frac{323}{360} & \frac{-11}{30} & \frac{53}{360} & \frac{-19}{720}), \quad B^{(F)} = (0 & \frac{1}{24} & -\frac{5}{24} & \frac{19}{24} & \frac{3}{8}),
\]

which are not symmetric.

The complete method turns out to be symmetric in the first case and nonsymmetric in the second case. In Fig. 1 we plot the absolute value of the difference between the first component of the discrete solution and the time-reversed one. The error is significant only in the case where the additional methods are not symmetric. On the contrary, the error is due only to round-off errors (indeed it is of the order of the machine precision) when the additional methods are symmetric.

Similar results hold true for the conservation property. We plot the values of the discrete approximation of the Hamiltonian function \( V_i = y_i^T y_i \). In Fig. 2 on the left side it is evident that the conservation property (41) (and then (40)) does not hold, as predicted. On the contrary, the conservation in the last point shows up on the right side.
Fig. 1. Difference between the discrete solution and time-reversed solution. On the left the additional methods are taken nonsymmetric. On the right they are taken symmetric.

Fig. 2. Discrete values of the Hamiltonian function obtained by the fourth-order ETR with nonsymmetric (on the left) and with symmetric (on the right) additional methods. Note that the exact value of the Hamiltonian is never obtained for $t \neq 0$ on the left and it is obtained for $t = 10$ on the right.
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