

# Conservation of integrals and symplectic structure in the integration of differential equations by multistep methods

T. Eirola<sup>1</sup> and J.M. Sanz-Serna<sup>2</sup>

<sup>1</sup> Institute of Mathematics, Helsinki University of Technology, 02150 Espoo 15, Finland

<sup>2</sup> Departamento de Matemática Aplicada y Computación, Facultad de Ciencias,  
Universidad de Valladolid, E-47005 Valladolid, Spain

Received January 7, 1991

**Summary.** We consider the question of whether multistep methods inherit in some sense quadratic first integrals possessed by the differential system being integrated. We also investigate whether, in the integration of Hamiltonian systems, multistep methods conserve the symplectic structure of the phase space.

*Mathematics Subject Classification (1991):* 65L05

## 1 Introduction

The construction and analysis of so-called symplectic or canonical numerical integrators for Hamiltonian systems of differential equations has received much attention in recent years [3, 6–15, 17]. By definition, a numerical integrator is said to be canonical if it preserves the symplectic structure of the phase space (see Sect. 4 below). Most of the work on canonical integrators has dealt with one-step formulae, either within the standard classes of Runge-Kutta or Runge-Kutta-Nyström methods [8–11, 17] or within classes of special methods derived via generating functions [3, 6]. The study of canonical multistep methods has been restricted to the explicit midpoint (leap-frog) rule [12, 14, 15], a scheme which is of interest in the time-integration of non-dissipative partial differential equations. The main purpose of the present paper is to investigate under which conditions a linear multistep method (LMM) or the related one-leg method (OLM) are canonical when applied to Hamiltonian systems of differential equations. We also consider the question of whether quadratic first integrals conserved by the differential system being integrated are in some sense inherited by LMMs or OLMs. For this second question the system is not assumed to have Hamiltonian form.

An overview of the paper is as follows. In Sect. 2 we consider the second question mentioned above, i.e. conservation of quadratic first integrals. We prove that symmetric OLM inherit, in some sense, the quadratic first integrals of the differential system. In answering this second question, we associate with

each symmetric  $k$ -step method a  $k \times k$  square matrix  $A$ , whose properties are investigated in Sect. 3. In Sect. 4 we show that a OLM is canonical if it is symmetric. In the final Sect. 5, we prove that the symmetry of the method is actually necessary both for the conservation of the quadratic quantities and for the conservation of the symplectic structure. We also show that symmetric LMMs do not share the conservation properties of their one-leg counterparts.

We shall use the following notations. We consider real systems of differential equations of the general form

$$(1.1) \quad dy/dt = f(y),$$

where  $f$  is defined and smooth in an open domain  $\Omega \subset \mathbb{R}^d$ . Each multistep method is specified by its (real) characteristic polynomials

$$(1.2) \quad \rho(Z) = \sum_{j=0}^k \alpha_j Z^j, \quad \alpha_k \neq 0, \quad \sigma(Z) = \sum_{j=0}^k \beta_j Z^j,$$

where we always assume the normalization

$$(1.3) \quad \sigma(1) = 1.$$

Several formulae to come are easier to write if we introduce the convention

$$(1.4) \quad \alpha_i = \beta_i = 0, \quad \text{for } i > k \quad \text{or} \quad i < 0.$$

We shall consider both the standard LM version

$$(1.5) \quad \rho(E)y_n = h\sigma(E)f(y_n)$$

and the one-leg version

$$(1.6) \quad \rho(E)y_n = hf(\sigma(E)y_n),$$

where  $E$  denotes the standard shift operator  $Ey_n = y_{n+1}$ .

The methods (1.5)–(1.6) are said to be *symmetric* if

$$(1.7) \quad \alpha_j = -\alpha_{k-j}, \quad \beta_j = \beta_{k-j}, \quad j=0(1)k,$$

i.e.

$$(1.8) \quad \rho(Z) \equiv -Z^k \rho(1/Z), \quad \sigma(Z) \equiv Z^k \sigma(1/Z).$$

This is equivalent to the following reversibility requirement for the numerical solutions: whenever the vectors  $y_n, \dots, y_{n+k}$  satisfy the relation (1.5) (respectively (1.6)) the vectors  $y_{n+k}, \dots, y_n$  satisfy (1.5) (respectively (1.6)) with  $h$  replaced by  $-h$ . It is perhaps worth noticing that the equivalence between the reversibility of the numerical solution and (1.7)–(1.8) holds true because we assume (1.3), which rules out the (totally uninteresting) case  $\sigma(1) = 0$ . If  $\sigma(1) = 0$  were allowed, then it would be possible to consider in (1.5) the situation with

$$\alpha_j = \alpha_{k-j}, \quad \beta_j = -\beta_{k-j}, \quad j=0(1)k$$

and the LMM would also be time-reversible. Of course a method with  $\sigma(1) = 0$  cannot be convergent: it is either inconsistent or unstable.

Finally (1.5)–(1.6) are said to be *irreducible* if the polynomials  $\rho$  and  $\sigma$  have no common root.

### 2 Quadratic first integrals

In this section we assume that there exists a symmetric  $d \times d$  matrix  $S, S \neq 0$ , such that the corresponding quadratic form

$$(2.1) \quad Q_S(y) = y^T S y$$

is a first integral or invariant quantity of the system (1.1), i.e. for any solution  $y(t)$  of (1.1)  $Q_S(y(t))$  is time-independent. For this to be true, it is of course necessary and sufficient that, for all  $y$  in the domain  $\Omega$  of  $f$ ,

$$(2.2) \quad y^T S f(y) = 0.$$

If (1.1) is numerically integrated with a one-step method it is natural to ask whether for the numerical solution  $y_n$  it is true that  $Q_S(y_n)$  is also independent of the time-level  $n$ . For Runge-Kutta methods this issue was considered in [16]. For multistep formulae the situation is more complex, as, for a  $k$ -step formula, the information carried at each step is in fact a  $kd$ -dimensional vector

$$(2.3) \quad Y_n = [y_n^T, \dots, y_{n+k-1}^T]^T,$$

so that the relevant question is whether, for numerical solutions,  $Q_\Sigma(Y_n)$  is  $n$ -independent for some suitable  $kd \times kd$  symmetric matrix  $\Sigma$  ( $\Sigma \neq 0$ ). It is natural to demand that  $\Sigma = A \otimes S$ , with  $A$  a  $k \times k$  symmetric matrix depending on the numerical method but not on the specific system (1.1) being integrated or on the specific quadratic form  $Q_S$  (a given system may of course possess several quadratic first integrals (2.1)). Note that in the case  $k=1$  the conservation of  $Q_{A \otimes S}, A \neq 0$  is equivalent to the conservation of  $Q_S$ .

In view of the preceding discussion, we consider the following question: under which condition on the method coefficients, is there a  $k \times k$  symmetric matrix  $A = \{\lambda_{ij}\} (A \neq 0)$  such that, for solutions of (1.6), (2.2)–(2.3) imply

$$(2.4) \quad Q_{A \otimes S}(Y_{n+1}) - Q_{A \otimes S}(Y_n) = 0,$$

that is

$$(2.5) \quad \sum_{i,j=1}^k \lambda_{ij} y_{n+i}^T S y_{n+j} - \sum_{i,j=1}^k \lambda_{ij} y_{n-1+i}^T S y_{n-1+j} = 0.$$

To answer this question we begin by taking the inner product of (1.6) and  $\sigma(E)y_n$  to obtain, in view of (2.2),

$$\sum_{i,j=0}^k (\alpha_i \beta_j + \alpha_j \beta_i) y_{n+i}^T S y_{n+j} = 0.$$

It is then clear that (2.5) would hold true if for arbitrary real  $x_0, \dots, x_k, z_0, \dots, z_k$

$$\sum_{i,j=1}^k \lambda_{ij} x_i x_j - \sum_{i,j=1}^k \lambda_{ij} x_{i-1} z_{j-1} = \sum_{i,j=0}^k (\alpha_i \beta_j + \alpha_j \beta_i) x_i z_j,$$

a condition that in terms of generating functions can be rewritten as

$$(2.6) \quad (XZ - 1) \sum_{i,j=1}^k \lambda_{ij} X^{i-1} Z^{j-1} = \rho(X) \sigma(Z) + \rho(Z) \sigma(X).$$

On noticing the symmetric roles played by  $i$  and  $j$ , (2.6) gives  $(k + 1)(k + 2)/2$  independent linear equations for the  $k(k + 1)/2$  undetermined coefficients  $\lambda_{ij}$ . Therefore for  $A$  to exist, the coefficients  $\alpha_i$  and  $\beta_j$  should satisfy  $k + 1 = [(k + 1)(k + 2) - k(k + 1)]/2$  compatibility conditions. These conditions are easily found in terms of the characteristic polynomials: it is clear that (2.6) implies that  $\rho(X) \sigma(Z) + \rho(Z) \sigma(X)$  vanishes when  $X = 1/Z$ , i.e.

$$\frac{\rho(Z)}{\sigma(Z)} \equiv - \frac{\rho\left(\frac{1}{Z}\right)}{\sigma\left(\frac{1}{Z}\right)},$$

a condition which is equivalent to the symmetry requirement (1.8). (Note that in (1.7) there are effectively  $k + 1$  independent conditions, as required.)

Since it has not been proved that (2.6) is necessary for (2.5) to hold, the argument just outlined does not prove that the symmetry of the method is necessary for conservation. This necessity will be proved in Sect. 5 below. However the argument is helpful in that it focuses the attention on the class of symmetric methods. Assume then that (1.6) is symmetric. Then the right hand side of (2.6) vanishes on the hyperbola  $X = 1/Z$  and, by well-known results from algebraic geometry, this right hand side must be a multiple of  $XZ - 1$  so that  $A$  exists uniquely. In order to explicitly determine  $A$ , we equate in (2.6) coefficients of like powers of  $X$  and  $Z$ . Taking the powers  $X^i Z^j$  in *descending* order readily leads to the solution

$$(2.7) \quad \lambda_{ij} = \sum_{m \geq 0} (\alpha_{i+m} \beta_{j+m} + \alpha_{j+m} \beta_{i+m}), \quad 0 \leq i, j \leq k.$$

(Recall we are using (1.4).) It is also possible to equate powers in *ascending* order to find

$$(2.8) \quad \lambda_{ij} = - \sum_{m < 0} (\alpha_{i+m} \beta_{j+m} + \alpha_{j+m} \beta_{i+m}), \quad 0 \leq i, j \leq k.$$

It is a simple matter to check, using (1.7), that (2.7) and (2.8) are in fact equivalent.

To sum up, we have proved the following result.

**Theorem 2.1.** *Assume that the one-leg  $k$ -step method (1.6) is symmetric. Then, the conservation law (2.4) holds, with  $A$  given by (2.7)–(2.8), whenever (2.2) is satisfied, i.e. whenever (2.1) is a conserved quantity of the system (1.1) being integrated.*

*Remark.* In (2.4) it is tacitly assumed that, for the value of  $h$  under consideration and for the given  $Y_n$ , the Eq. (1.6) for  $y_{n+k}$  possess a solution, so that  $Y_{n+1}$  makes sense.

It is also possible to look at the case where in (2.2) we replace  $=$  by  $\leq$ , so that the quadratic form (2.1) *decreases* along solutions of (1.1). By arguing as above, it is easy to show that, for symmetric one-leg methods, (2.4) holds with  $=$  replaced by  $\leq$ . ( $A$  is still given by (2.7)–(2.8).)

Before closing this section we would like to emphasize that there is a close connection between the material in this section and the issue of  $G$ -stability [2, 4, 5]. In particular the technique of proof we have used has been borrowed from [2]. (In a first draft of the present article, we employed an alternative, more cumbersome technique, based on companion matrices as in Sect. 5.)

### 3 Properties of the $A$ matrix

In this section we investigate some properties of the  $A$  matrix that has been associated with each symmetric OLM. We begin by noticing that  $A$  is not only symmetric in the usual sense (i.e. with respect to its main diagonal) but also with respect to the diagonal that joins the right upper corner with the left lower corner.

**Theorem 3.1.** *Let the method (1.6) be symmetric, then its  $A$  matrix defined in (2.7)–(2.8) satisfies*

$$(3.1) \quad \lambda_{ij} = \lambda_{k-j+1, k-i+1}, \quad 1 \leq i, j \leq k.$$

*Proof.* It is sufficient to write the right hand side of (3.1) using (2.7) and to write the corresponding left hand side using (2.8).  $\square$

Our next result is as follows.

**Theorem 3.2.** *Let the method (1.6) be symmetric, then its  $A$  matrix (2.7)–(2.8) is singular if and only if the method is reducible.*

*Proof.* It is well known from classical algebra that  $\rho$  and  $\sigma$  possess a common factor if and only if the determinant (*resolvent*) of the  $2k \times 2k$  matrix

$$M(\rho, \sigma) = \begin{bmatrix} \alpha_0 & \alpha_1 & \alpha_2 & \dots & \alpha_{k-1} & \alpha_k & 0 & 0 & \dots & 0 \\ 0 & \alpha_0 & \alpha_1 & \dots & \alpha_{k-2} & \alpha_{k-1} & \alpha_k & 0 & \dots & 0 \\ 0 & 0 & \alpha_0 & \dots & \alpha_{k-3} & \alpha_{k-2} & \alpha_{k-1} & \alpha_k & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & \alpha_0 & \alpha_1 & \alpha_2 & \alpha_3 & \dots & \alpha_k \\ \beta_0 & \beta_1 & \beta_2 & \dots & \beta_{k-1} & \beta_k & 0 & 0 & \dots & 0 \\ 0 & \beta_0 & \beta_1 & \dots & \beta_{k-2} & \beta_{k-1} & \beta_k & 0 & \dots & 0 \\ 0 & 0 & \beta_0 & \dots & \beta_{k-3} & \beta_{k-2} & \beta_{k-1} & \beta_k & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & \beta_0 & \beta_1 & \beta_2 & \beta_3 & \dots & \beta_k \end{bmatrix}$$

equals 0. The key point is to observe that this implies that the method is reducible if and only if the product  $M(\sigma, \rho)^T M(\rho, \sigma)$  is a singular matrix. Now matrix multiplication using (1.7), (2.7), (2.8) reveals that

$$M(\sigma, \rho)^T M(\rho, \sigma) = \begin{bmatrix} -A & 0 \\ 0 & A \end{bmatrix}$$

and this concludes the proof.  $\square$

We now turn our attention to the stability polynomial

$$(3.2) \quad \pi_\mu(Z) = \rho(Z) - \mu \sigma(Z).$$

If we assume irreducibility, it is a simple matter to prove that, for symmetric methods,  $\pi_\mu$  cannot have zeros with  $|Z|=1$  if  $\mu$  is not purely imaginary. Therefore, for a symmetric irreducible method and  $\mu$  in the left half plane  $\Re(\mu) < 0$ , the number  $r$  of roots of  $\pi_\mu$  that lie in the unit disk  $|Z| < 1$  is an integer independent of the particular choice of  $\mu$ . Of course  $r = k$  corresponds to A-stable methods.

**Theorem 3.3.** *Let the method (1.6) be symmetric and irreducible. Then:*

- (i) *The method is A-stable if and only if  $A$  is positive definite.*
- (ii) *More generally, the following statements are equivalent.*
  - (a) *For  $\mu$  in the left half plane  $\Re(\mu) < 0$ , the stability polynomial (3.2) has  $r$  roots inside the unit disk  $|Z| < 1$  and  $k - r$  roots outside the unit disk.*
  - (b) *The matrix  $A$  has  $r$  positive eigenvalues and  $k - r$  negative eigenvalues.*

*Proof.* It is clearly enough to prove (ii). We argue as in [2]. Choose  $\mu$  real and negative so that the roots  $Z_1, Z_2, \dots, Z_k$  of (3.2) are simple (the number of values of  $\mu$  for which the stability polynomial has multiple roots is finite due to the irreducibility). Assume that for  $1 \leq i \leq r$ ,  $|Z_i| < 1$ , while, for  $r < i \leq k$ ,  $|Z_i| > 1$  and let  $V$  be the  $k \times r$  complex matrix with entries  $Z_j^{i-1}$ . Then for any  $r$ -dimensional complex vector  $b$ , the equalities (2.6) and (3.2) imply that

$$b^H V^H A V b = \sum_{\ell, m, i, j} \bar{b}_\ell \bar{Z}_\ell^{i-1} \lambda_{i,j} Z_m^{j-1} b_m = 2|\mu| \sum_{\ell, m} \bar{b}_\ell \sigma(\bar{Z}_\ell) (1 - \bar{Z}_\ell Z_m)^{-1} \sigma(Z_m) b_m.$$

We now expand  $(1 - \bar{Z}_\ell Z_m)^{-1}$  to obtain

$$b^H V^H A V b = 2|\mu| \sum_{v=0}^\infty \sum_{\ell, m} \bar{b}_\ell \bar{Z}_\ell^v \sigma(\bar{Z}_\ell) \sigma(Z_m) Z_m^v b_m = 2|\mu| \sum_{v=0}^\infty \left| \sum_m \sigma(Z_m) Z_m^v b_m \right|^2 \geq 0.$$

We conclude that the restriction of  $A$  to the column space of  $V$  is positive semidefinite and hence  $A$  has, at least,  $r$  eigenvalues  $\geq 0$ . For the roots outside the unit disk one can proceed in an analogous way, but now the expansion is

$$(1 - \bar{Z}_\ell Z_m)^{-1} = - \sum_{v=0}^\infty (\bar{Z}_\ell Z_m)^{-(v+1)},$$

so that we find, at least,  $k - r$  eigenvalues  $\leq 0$ . Since 0 eigenvalues are excluded by Theorem 3.2, the proof is concluded.  $\square$

### 4 Symplectic multistep methods

We now examine the case where the system (1.1) being integrated is of Hamiltonian form [1], i.e. the corresponding vector field  $f$  is given by

$$(4.1) \quad f(y) = \Theta^{-1} \text{grad } H(y),$$

where  $H$  is a smooth real function (the Hamiltonian function) and  $\Theta$  is a nonsingular skew-symmetric matrix. If the dimension  $d$  of the space is odd, it is not possible to have nonsingular skew-symmetric matrices and hence  $d$  must be of the form  $d=2g$ , where the integer  $g$  is known in mechanics as the number of degrees of freedom. Usually,  $\Theta$  is the so-called standard symplectic matrix

$$\Theta = \begin{bmatrix} 0 & I_g \\ -I_g & 0 \end{bmatrix},$$

so that when  $y$  is partitioned as  $y = [p^T, q^T]^T$ , with  $p, q$  in  $\mathbb{R}^g$ , (1.1) takes the familiar form

$$dp/dt = -\partial H(p, q)/\partial q, \quad dq/dt = \partial H(p, q)/\partial p.$$

A smooth transformation  $y \mapsto T(y)$  in  $y$ -space is said to be symplectic (with respect to  $\Theta$ ) if the Jacobian  $\partial T/\partial y$  satisfies

$$(4.2) \quad \frac{\partial T^T}{\partial y} \Theta \frac{\partial T}{\partial y} \equiv \Theta.$$

This relation can also be expressed by saying that the transformation  $T$  preserves the differential form (subindices in brackets denote components)

$$\omega_\Theta = \sum_{\ell, m=1}^d \theta_{\ell m} dy_{[\ell]} \wedge dy_{[m]}.$$

The phase flow of (1.1)–(4.1) (i.e. the solution of the system of ODEs, at any fixed time, seen as a function of the initial values) is a symplectic transformation. All qualitative properties of solutions of Hamiltonian systems can be derived from the symplectic character of the corresponding flows. In fact, if the domain  $\Omega$  of definition of  $H$  is simply connected, the property of having a symplectic flow completely characterizes the Hamiltonian systems [1, 12]. It is therefore of interest [3, 6, 9, 11, 12] to construct numerical integrators that are symplectic. For multistep methods this means that the mapping  $Y_n \mapsto Y_{n+1}$  must be symplectic with respect to some nonsingular skew-symmetric  $kd \times kd$  matrix to be determined. We are going to show that for symmetric, irreducible OLMs the matrix  $A \otimes \Theta$  does the trick. Note that according to Theorem 3.2 this matrix is in fact nonsingular.

**Theorem 4.1.** *Assume that the one-leg method (1.6) is symmetric and irreducible. Then the corresponding mapping  $Y_n \mapsto Y_{n+1}$  is symplectic with respect to the matrix  $A \otimes \Theta$ .*

*Remark.* A caveat similar to that in the remark after Theorem 2.1 should be made here. It is assumed that the attention is focused on a bounded domain of the phase space, and that  $h$  has been chosen sufficiently small for the mapping  $Y_n \mapsto Y_{n+1}$  to be well defined there.

*Proof.* It is possible to work either in terms of Jacobian matrices, as in (4.2), or in terms of differential forms. The latter technique leads to cleaner algebra. We have to show that

$$\sum_{i,j=1}^k \lambda_{ij} \sum_{\ell,m=1}^d \theta_{\ell m} dy_{n+i, [\ell]} \wedge dy_{n+j, [m]} - \sum_{i,j=1}^k \lambda_{ij} \sum_{\ell,m=1}^d \theta_{\ell m} dy_{n+i-1, [\ell]} \wedge dy_{n+j-1, [m]} = 0,$$

or, in view of (2.6), that

$$(4.3) \quad \sum_{i,j=0}^k \alpha_i \beta_j \sum_{\ell,m=1}^d \theta_{\ell m} dy_{n+i, [\ell]} \wedge dy_{n+j, [m]} + \sum_{i,j=1}^k \alpha_j \beta_i \sum_{\ell,m=1}^d \theta_{\ell m} dy_{n+i, [\ell]} \wedge dy_{n+j, [m]} = 0.$$

We prove that the second term in the left hand side is 0 (the first term can be treated in a similar manner). Differentiate (1.6), with  $f$  given by (4.1), to obtain

$$(4.4) \quad \rho(E) dy_n = h \Theta^{-1} B \sigma(E) dy_n,$$

where  $B$  is the symmetric matrix of second derivatives of  $H$  evaluated at  $\sigma(E)y_n$ . On taking (4.4) to the second term in the left hand side of (4.3), we find

$$\sum_{\ell,m=1}^d h b_{\ell,m} \left( \sum_{i=0}^k \beta_i dy_{n+i, [\ell]} \right) \wedge \left( \sum_{j=0}^k \beta_j dy_{n+j, [m]} \right),$$

an expression which is 0 because  $b_{\ell,m}$  is symmetric in the indices  $\ell, m$  while in the wedge product those indices play a skew-symmetric role.  $\square$

### 5 Necessity of the hypotheses: discussion

In the previous sections we have shown that symmetric OLM inherit, via the corresponding  $A$  matrix, both the quadratic conserved quantities of the differential system and, if the system is Hamiltonian, the symplectic character of the flow. We begin this section by proving that the symmetry of the method is also necessary for the conservation properties to hold.

Assume that the harmonic oscillator equations

$$dy/dt = Ay, \quad A = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix},$$

with the quadratic conserved quantity  $\|y\|_2^2$ , are integrated with an irreducible OLM. (Note that then  $y_{n+k}$  is uniquely defined for any choice of  $h \neq 0$ .) We



know that, if the method is symmetric, then there is a full-rank quadratic form being conserved by the vectors  $Y_n$ . Let us suppose that, conversely, for some regular matrix  $M$  and for any choice of  $h$ ,

$$(5.1) \quad Y_{n+1}^T M Y_{n+1} \equiv Y_n^T M Y_n.$$

Then for all  $h$

$$(5.2) \quad N^T(-hA) M N(hA) = M,$$

where  $N(z)$  stands for the companion matrix

$$N(z) = \begin{bmatrix} 0 & 1 & 0 & \dots & 0 & 0 \\ 0 & 0 & 1 & \dots & 0 & 0 \\ 0 & 0 & 0 & \dots & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & \dots & 0 & 1 \\ \hline \frac{\alpha_0 - z \beta_0}{\alpha_k - z \beta_k} & \frac{\alpha_1 - z \beta_1}{\alpha_k - z \beta_k} & \frac{\alpha_2 - z \beta_2}{\alpha_k - z \beta_k} & \dots & \frac{\alpha_{k-2} - z \beta_{k-2}}{\alpha_k - z \beta_k} & \frac{\alpha_{k-1} - z \beta_{k-1}}{\alpha_k - z \beta_k} \end{bmatrix}.$$

The relation (5.2) reveals that the eigenvalues of  $N(hA)^{-1}$  equal those of  $N^T(-hA)$  and hence those of  $N(-hA)$ . Since the spectrum of  $A$  is purely imaginary, we see that, for  $\Re(z)=0$ ,  $N(-z)$  and  $N(z)^{-1}$  have the same eigenvalues. Clearly this must also be true for all complex  $z$ . Now the characteristic polynomials of  $N(-z)$  and  $N(z)^{-1}$  are the same, a fact that implies that the method must be symmetric. (Notice that the argument holds true if one only asks (5.1) for  $h$  sufficiently small or even only for infinitely many values of  $h$ .)

That symmetry is also necessary to have some sort of canonicity in the integration of the harmonic oscillator is easily shown along the lines of the proof just given. Perhaps it is appropriate to mention here that it is possible to construct symplectic RK methods that are *not* symmetric (in the sense that a step of length  $h$  followed by a step of length  $-h$  does not put the solution back at the initial condition).

On the other hand we have been assuming so far that we are dealing with the OLM rather than with the classical LMM counterpart. Actually it is easy to prove that LMMs, even if assumed symmetric, do not *in general* possess good conservation properties. (The words *in general* are needed here: there are of course LMMs which are also OLMs.) Just consider the familiar trapezoidal rule: by seeing it as a RK method it is trivial to check that it does not satisfy the necessary condition [8] for a method to be symplectic. However it is possible to establish some *ad hoc* form of conservation properties for symmetric LMM, by using the known relation [4] between solutions of the LM and OL methods with the same characteristic polynomials.

The fact that multistep methods have to be symmetric if they are to be symplectic is bad news, because, of course, symmetric methods are only marginally 0-stable if  $k > 1$ . This is not necessarily fatal if one limits oneself to integrate Hamiltonian systems: the growth induced by the parasitic roots is not worse than growth-rates already present in the underlying differential system. After

all, the explicit midpoint rule is successfully used in the time-integration of non-dissipative partial differential equations (and this practical success can be theoretically accounted for by using the symplectic property to derive boundedness results even in nonlinear situations [12, 14, 15]). However if the system being integrated is a dissipative perturbation of a Hamiltonian system, the presence of the parasitic roots on the unit disk will be harmful, as now the true solution will be decreasing exponentially. This should be compared with the situation for Runge-Kutta methods [8, 10, 11, 17], where B-stable symplectic algorithms exist of arbitrarily high order, since the  $s$ -stage Gauß-Legendre method of order  $2s$  is symplectic.

Finally note that with the standard definition of local truncation error [18] a symmetric OLM has order of consistency exactly 2. However it is also possible to define the local truncation error in such a way that an OLM and the associated LMM have the same order [18]; with this alternative definition there are symmetric OLM methods of arbitrarily high orders.

*Acknowledgements.* This research started during a visit of J.M.S. to Helsinki, supported by the Rolf Nevanlinna Institute. The work has also been supported by the Academy of Finland and by "Junta de Castilla y León" under project 1031-89.

## References

1. Arnold, V.I. (1989): *Mathematical methods of classical mechanics*, 2nd ed. Springer, Berlin Heidelberg New York
2. Baiocchi, C., Crouzeix, M. (1989): On the equivalence of A-stability and G-stability. *Appl. Numer. Math.* **5**, 19–22
3. Channell, P.J., Scovel, C. (1990): Symplectic integration of Hamiltonian systems. *Nonlinearity* **3**, 231–259
4. Dahlquist, G. (1976): Error analysis for a class of methods for stiff nonlinear initial value problems. In: G.A. Watson, ed., Springer, Berlin Heidelberg New York, pp. 60–72
5. Dahlquist, G. (1978): G-stability is equivalent to A-stability. *BIT* **18**, 384–401
6. Feng, K. (1986): Difference schemes for Hamiltonian formalism and symplectic geometry. *J. Comput. Math.* **4**, 279–289
7. Frutos, J. de, Ortega, T., Sanz-Serna, J.M. (1990): A Hamiltonian explicit algorithm with spectral accuracy for the 'good' Boussinesq system. *Comput. Methods Appl. Mech. Engrg.* **80**, 417–423
8. Lasagni, F.M. (1988): Canonical Runge-Kutta methods. *Z. Angew. Math. Phys.* **39**, 952–953
9. Ruth, R. (1984): A canonical integration technique. *IEEE Trans. Nucl. Sci.* **30**, 269–271
10. Sanz-Serna, J.M. (1988): Runge-Kutta schemes for Hamiltonian systems. *BIT* **28**, 877–883
11. Sanz-Serna, J.M. (1991): The numerical integration of Hamiltonian systems. *Proceedings of the Conference on Computational Differential Equations*, Imperial College London, 3rd–7th July 1989 (to appear)
12. Sanz-Serna, J.M. (1991): Two topics in nonlinear stability. In: W. Light, ed., *Advances in Numerical Analysis*, Vol. 1. Clarendon Press, Oxford, pp. 147–174
13. Sanz-Serna, J.M., Abia, L. (1991): Order conditions for canonical Runge-Kutta schemes. *SIAM J. Numer. Anal.* **28**, 1081–1096
14. Sanz-Serna, J.M., Vadillo, F. (1986): Nonlinear instability, the dynamic approach. In: D.F. Griffiths, G.A. Watson, eds., *Numerical Analysis*. Longman, London, pp. 187–199
15. Sanz-Serna, J.M., Vadillo, F. (1987): Studies in nonlinear instability III: augmented hamiltonian systems. *SIAM J. Appl. Math.* **47**, 92–108
16. Sanz-Serna, J.M., Verwer, J.G. (1986): Conservative and nonconservative schemes for the solution of the nonlinear Schrödinger equation. *IMA J. Numer. Anal.* **6**, 25–42
17. Suris, Y.B. (1987): Canonical transformations generated by methods of Runge-Kutta type for the numerical integration of the system  $x'' = -\partial U/\partial x$ . *Zh. Vychisl. Mat. i Mat. Fiz.* **29**, 202–211 [in Russian]
18. Dahlquist, G. (1983): On one-leg multistep methods. *SIAM J. Numer. Anal.* **20**, 1130–1138