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Error growth in the numerical integration of periodic orbits by multistep methods, with application to reversible systems

B. CANO† AND J. M. SANZ-SERNA‡

Departamento de Matemática Aplicada y Computación, Universidad de Valladolid, Valladolid, Spain

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We study the growth with time of (the coefficients of the asymptotic expansion of) the error in the numerical integration with linear multistep methods of periodic solutions of systems of ordinary differential equations. Particular attention is devoted to reversible systems. It turns out that symmetric linear multistep methods cannot be recommended in spite of the fact that they mimic the reversibility of the true flow. For reversible second-order systems, linear multistep methods without parasitic double roots are useful.

1. Introduction

This paper is devoted to the analysis of the error growth in the numerical integration by linear multistep methods (LMMs) of periodic orbits of systems of differential equations. Our motivation has been twofold. First, we devoted a previous paper (Cano & Sanz-Serna (1995)) to the investigation of the same question in the case of *one-step* methods and we wished to complete our earlier study by also treating LMMs. Furthermore we had another, deeper aim in mind. There has been much recent interest in *geometric integrators* (Sanz-Serna (1997)), i.e., in integrators that mimic some of the geometric properties in phase space of the system being solved. Since, due to the need to store past solution values, multistep methods naturally live in a phase space different from the phase space of the underlying system of differential equations, LMMs have not played an important role in geometric integration. In particular little is known about the application of multistep methods to Hamiltonian or reversible problems. As shown in Cano & Sanz-Serna (1995) (see also Calvo & Hairer (1995), Calvo & Sanz-Serna (1993), Estep & Stuart (1995), Frutos & Sanz-Serna (1997), Hairer & Stoffer (1997), Portillo & Sanz-Serna (1995), Stoffer (1995)), the use of time-reversible one-step methods for reversible systems or of symplectic one-step methods for Hamiltonian systems leads to an error growth in periodic orbits that is smaller than the one found with 'general' methods. Therefore we were interested in identifying properties of an LMM that lead to slow error growth for periodic orbits; by doing so we expected to identify LMMs suitable for 'geometric integration'.

Symmetric LMMs appear to be good candidates to integrate reversible systems; as first noted by Stoffer (1988), the time-symmetry of linear symmetric methods implies a reversible behaviour of the numerical solution. Symmetric methods have also been suggested in connection with Hamiltonian problems, see e.g. Eirola & Sanz-Serna (1991). Quinlan &

† Email: bego@cpd.uva.es

‡ Email: sanzserna@cpd.uva.es

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Tremaine (1990) have derived symmetric linear multistep methods for second-order equations (LMM2s) and found that, for Kepler's problem, the error growth is linear. In spite of the foregoing considerations, the following conclusions emerge from the present paper. (i) Symmetric LMMs cannot be recommended for the integration of reversible or Hamiltonian problems, because the parasitic roots typically lead to numerical errors that grow at a rate that is faster than the 'natural' rate at which the perturbations of the differential equation itself would grow. (ii) Symmetric LMM2s are useful for reversible problems, *provided* that the first characteristic polynomial has no double root of unit modulus $\neq 1$.

The remainder of the paper is divided into three sections, devoted respectively to strongly stable LMMs, weakly stable LMMs, and LMM2s. As distinct from Cano & Sanz-Serna (1995), for simplicity, we only consider the case of constant stepsizes and we do not study explicitly the Hamiltonian case. Of course our study of reversible problems is relevant to Hamiltonian systems because many Hamiltonian systems found in practice are also reversible.

2. Strongly stable methods

2.1 *Preliminaries*

We consider an initial value problem

$$\dot{y} = f(y), \tag{1}$$

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

where, for simplicity, we assume that f is smooth (C^∞) in the whole of R^D. All the results in this paper can be easily adapted to the case where f is only defined in the domain $\Omega \subset R^D$ and/or only of class C^k. Also for simplicity, we assume that all solutions of (1) are defined for each real t.

We study LMMs of the form

$$\sum_{l=0}^{k} \alpha_l y_{n+l} = h \sum_{l=0}^{k} \beta_l f(y_{n+l}), \qquad n = 0, 1, \ldots, \tag{3}$$

where y_n is the numerical solution at time $t_n = t_0 + nh$, $h > 0$.

Introducing the first and second characteristic polynomials

$$\rho(x) = \alpha_k x^k + \alpha_{k-1} x^{k-1} + \cdots + \alpha_0,$$
$$\sigma(x) = \beta_k x^k + \beta_{k-1} x^{k-1} + \cdots + \beta_0,$$

and the shift operator E, (3) becomes

$$\rho(E) y_n = h\sigma(E) f(y_n).$$

We assume throughout that $\alpha_k \neq 0$, and that the method is irreducible (i.e. ρ and σ have no common factors) and consistent (i.e. $\rho(1) = 0$, $\rho'(1) = \sigma(1)$). Furthermore we normalize the method coefficients so that $\sigma(1) = 1$.

For a method of order r, the truncation error

$$L(z, t, h) = \rho(E) z(t) - h\sigma(E) \dot{z}(t)$$

is $O(h^{r+1})$ as $h \to 0$ for each t and each smooth function $z = z(t)$. It follows easily that, for any integer $J \geqslant r + 1$, there is an expansion

$$L(z, t, h) = \sigma(E)\left(\sum_{l=r}^{J-1} c_l h^{l+1} z^{(l+1)}(t)\right) + O(h^{J+1}), \quad h \to 0, \tag{4}$$

for suitable constants $\{c_l\}$ depending only on ρ and σ.

We say that the formula (3) is started with a starting procedure of order $s \geqslant 1$ if

$$y_\nu - y(t_\nu) = O(h^s), \quad \nu = 0, 1, \dots, k-1,$$

as $h \to 0$, where $y(t)$ is the solution of (1)–(2). It is assumed that the starting procedure is smooth in the sense that an expansion

$$y_\nu = y(t_\nu) + \sum_{j=s}^{J} h^j s_\nu^{(j)} + O(h^{J+1}), \qquad \nu = 0, 1, \dots, k-1, \tag{5}$$

is valid for each $J \geqslant s$. All starting procedures used in practice are smooth.

In this section we consider the case where (3) is strongly stable, i.e. all roots of ρ have modulus $\leqslant 1$ and 1 is the only root of unit modulus.

A key ingredient of our analysis is the asymptotic expansion of the global error. This goes back to Gragg's thesis, see Stetter (1973). A proof due to Hairer and Lubich may be seen in Hairer *et al* (1993). Here we only write the expansion up to $O(h^{2r-1})$ terms because this is all we need (see the discussion in Section 8 of Cano & Sanz-Serna (1995)).

THEOREM 1 Assume that a strongly stable LMM of order $r \geqslant 1$, using a smooth starting procedure of order r is applied to solve (1)–(2). Then

$$y_n = y(t_n) + \sum_{j=r}^{2r-1} h^j e_j(t_n) + O(h^{2r}), \quad h \to 0, \tag{6}$$

with $t_n = t_0 + nh$, $n > 0$, where y_n is the numerical solution given by the method and $\{e_j\}_{j=r}^{2r-1}$ are smooth functions that obey the variational equations

$$\dot{e}_j(t) = f'(y(t))e_j(t) - c_j y^{(j+1)}(t), \tag{7}$$

where the c_j are the constants in (4).

The constant implied in the $O(h^{2r})$ remainder in (6) can be chosen to be independent of t_n for t_n in each compact interval $[\delta, t_{\max}]$ with $t_0 < \delta < t_{\max}$.

In the variational equation (7) the terms in the expansion of the truncation error (4) act as forcing terms; this is similar to the situation for one-step methods. However there are some differences between the expansion (6) and the expansion corresponding to one-step methods. First, the initial condition $e_j(t_0)$ for (7) is in general $\neq 0$; its value is determined in a complicated way matching the expansion of the global error and the expansion of the starting procedure (5). It is possible, but not practical, to ensure $e_j(t_0) = 0$ by carefully choosing the starting procedure. A second difference to the one-step case is that here the expansion (6) is not valid up to t_0.

2.2 *Error growth in periodic solutions*

We now assume that the solution of (1)–(2) is T-periodic and investigate the growth with t of the functions $e_j(t)$ in (6). Our main tool is the *transition matrix* $M(t, s)$ associated with the homogeneous variational equation

$$\dot{\delta}(t) = f'(y(t))\delta(t) \tag{8}$$

of (1)–(2). By definition, for each vector δ_0, $M(t, s)\delta_0$ is the solution of the initial value problem given by (8) and the initial condition $\delta(t = s) = \delta_0$. Thus, for ϵ small, $M(t, s)\epsilon\delta_0$ is approximately the effect that a perturbation of size $\epsilon\delta_0$ at time s has at time t on the solution of (1)–(2). Of particular significance is the matrix $M_{t_0} = M(t_0+T, t_0)$ that governs the amplification of errors after one period; this is called the *monodromy matrix* of the periodic solution and its eigenvalues are the corresponding *Floquet multipliers*. The magnitude of the Floquet multipliers thus governs the growth of perturbations of the periodic orbit.

By decomposing (7) according to the effects of the source term and the initial condition, we may write

$$e_j(t) = e_j^I(t) + e_j^{II}(t), \quad j = r, \ldots, 2r-1,$$

with

$$e_j^I(t) = -c_j \int_{t_0}^{t} M(t, s) y^{(j+1)}(s)\, \mathrm{d}s, \quad e_j^{II}(t) = M(t, t_0) e_j^{II}(t_0). \tag{9}$$

Next, we introduce the notation

$$\begin{aligned} e_j[N] &= e_j(t_0 + NT), \\ e_j^I[N] &= e_j^I(t_0 + NT), \\ e_j^{II}[N] &= e_j^{II}(t_0 + NT), \end{aligned}$$

for the values of e_j, e_j^I, e_j^{II} after a whole number $N \geqslant 0$ periods. A key observation is that the growth of $e_j(t)$ as a function of t is essentially determined by the growth of $e_j[N]$ as a function of N. In fact, if $t \in [t_0 + (N-1)T, t_0 + NT]$, then

$$e_j^{II}(t) = M(t - (N-1)T, t_0) e_j^{II}(t_0 + (N-1)T), \tag{10}$$

so that $e_j^{II}(t)$ grows like $e_j^{II}(t_0 + (N-1)T)$ because $M(t - (N-1)T, t_0)$ is uniformly bounded in view of the bound $|t - (N-1)T - t_0| \leqslant T$. For e_j^I, the following lemma shows similarly that $e_j^I(t)$ grows like $e_j^I(t_0 + (N-1)T)$.

LEMMA 1 If $t \in [t_0 + (N-1)T, t_0 + NT]$, then, for $r \leqslant j \leqslant 2r-1$,

$$\begin{aligned} e_j^I(t) = {} & M(t - (N-1)T, t_0) e_j^I(t_0 + (N-1)T) \\ & - c_j \int_{t_0}^{t-(N-1)T} M(t - (N-1)T, s) y^{(j+1)}(s)\, \mathrm{d}s. \end{aligned}$$

Proof. From (9), we have

$$\begin{aligned} e_j^I(t) &= -c_j \int_{t_0}^{t} M(t,s) y^{(j+1)}(s)\,\mathrm{d}s \\ &= -c_j \int_{t_0}^{t_0+(N-1)T} M(t, t_0 + (N-1)T) M(t_0 + (N-1)T, s) y^{(j+1)}(s)\,\mathrm{d}s \\ &\quad -c_j \int_{t_0+(N-1)T}^{t} M(t,s) y^{(j+1)}(s)\,\mathrm{d}s. \end{aligned}$$

The proof follows from the periodicity of $y^{(j+1)}$. □

In what follows we therefore restrict our attention to the values $e_j[N]$ rather than considering the functions $e_j(t)$ for real t. The next result expresses $e_j[N]$ in terms of $e_j^I[1]$, $e_j[0]$ and the monodromy matrix M_{t_0}.

THEOREM 2 With the preceding notation, for $N = 2, 3, \ldots$

$$e_j^I[N] = M_{t_0} e_j^I[N-1] + e_j^I[1],$$
$$e_j^{II}[N] = M_{t_0} e_j^{II}[N-1],$$

and therefore

$$e_j^I[N] = \left(\sum_{i=0}^{N-1} M_{t_0}^i \right) e_j^I[1], \tag{11}$$

$$e_j^{II}[N] = M_{t_0}^{N-1} e_j^{II}[1] = M_{t_0}^N e_j[0]. \tag{12}$$

Proof. The first formula is obtained by setting $t = t_0 + NT$ in Lemma 1. The second formula is similarly derived from (10). Then (11) and (12) follow easily. □

The growth of the matrices in (11) and (12) is governed by the growth of the corresponding Jordan blocks. In this connection we have the following lemma, whose proof is a simple exercise in linear algebra.

LEMMA 2 Assume that M is a $\mu \times \mu$ Jordan block with eigenvalue λ. Then, as $N \uparrow \infty$:

(i) If $|\lambda| \geqslant 1$, $\lambda \neq 1$, then

$$\left\| \sum_{i=0}^{N-1} M^i \right\| = O(N^{\mu-1}|\lambda|^N), \qquad \|M^N\| = O(N^{\mu-1}|\lambda|^N).$$

(ii) If $|\lambda| < 1$, then

$$\left\| \sum_{i=0}^{N-1} M^i \right\| = O(1), \qquad \|M^N\| = o(1).$$

(iii) If $\lambda = 1$, $\mu > 1$ then

$$\left\| \sum_{i=0}^{N-1} M^i \right\| = O(N^{\mu}), \qquad \|M^N\| = O(N^{\mu-1}).$$

(iv) If $\lambda = 1$, $\mu = 1$, then

$$\sum_{i=0}^{N-1} M^i = N, \qquad M^N = 1.$$

From the preceding results we conclude:

THEOREM 3 With the hypotheses of Theorem 1, assume that the solution of (1)–(2) is T-periodic. Then the following mutually exclusive possibilities arise:

(G1) The solution $y(\cdot)$ has a Floquet multiplier of modulus > 1, or in other words the monodromy matrix M_{t_0} has spectral radius $R > 1$. Then, for $j = r, \dots, 2r-1$, $N \to \infty$, $e_j[N] = O(N^{\mu-1}R^N)$, where μ is the size of the largest Jordan block of M_{t_0} corresponding to the eigenvalues of modulus R.

(G2) All Floquet multipliers have modulus $\leqslant 1$. Denote by μ the size of the largest Jordan block of M_{t_0} corresponding to eigenvalues $\neq 1$ of modulus 1 and denote by μ_1 the size of the largest Jordan block of M_{t_0} with eigenvalue 1 ($\mu_1 \geqslant 1$). Then, for $j = r, \dots, 2r-1$,

$$\|e_j^I[N]\| = O(N^\nu), \quad \nu = \max(\mu - 1, \mu_1),$$

while

$$\|e_j^{II}[N]\| = O(N^{\nu'}), \quad \nu' = \max(\mu - 1, \mu_1 - 1).$$

Therefore, the error growth is polynomial.

In the cases (G1) or (G2) with $\mu - 1 \geqslant \mu_1$, the growth of the bound for $e_j^{II}[N]$ is not faster than that of the bound for $e_j^I[N]$. In the case (G2) with $\mu - 1 < \mu_1$, the growth of the bound of $e_j^{II}[N]$ is actually slower than that of the bound for $e_j^I[N]$. For this reason, there is no interest in trying to find special starting procedures to ensure $e_j(t_0) = 0$ and therefore $e_j^{II} \equiv 0$.

The following particular case of (G2) deserves special attention.

(G2′) The periodic solution is hyperbolic and attracting, i.e. 1 is a simple Floquet multiplier and the remaining $D - 1$ multipliers have modulus < 1. This corresponds to case (G2) above with $\mu = 0$, $\mu_1 = 1$. Therefore, $\|e_j^I[N]\| = O(N)$ and $\|e_j^{II}[N]\| = O(1)$. If we decompose $e_j^I[N]$ according to eigenvectors and generalized eigenvectors of M_{t_0}, then the components of $e_j^I[N]$ corresponding to multipliers $\neq 1$ remain bounded by (ii) in Lemma 2. Therefore, the only component which grows linearly is the one associated to the eigenvalue 1, that is to say, to the eigenvector $f(y_0)$. This means that the error committed is basically a phase error.

The situation (G2′) is *generic:* if a differential system has a periodic orbit in (G2′) then all neighbouring differential systems have a periodic orbit in (G2′).

REMARK 1 In each of the previous cases, when the starting procedure is of order $r + 1$, the initial condition for e_r can be shown to be zero. It follows that the only component in the principal term $e_r(t)$ is $e_r^I(t)$.

2.3 *Reversible systems*

We now consider the case where the system (1) being integrated is reversible (Arnold & Sevryuk (1986), Sevryuk (1986)). Let Λ be a linear involution in R^D, i.e. a linear mapping in R^D with $\Lambda^2 = I$. To avoid trivial cases we assume that $\Lambda \neq \pm I$. Then R^D is decomposed as a direct sum $R^D = X_+ \oplus X_-$, where $\Lambda v = \pm v$ if $v \in X_\pm$ and the subspaces X_+ and X_- have dimension $\geqslant 1$. The system (1) is said to be Λ-reversible if

$$f(\Lambda x) \equiv -\Lambda f(x). \tag{13}$$

Reversible systems often arise in many applications including mechanics, see Cano & Sanz-Serna (1995), Sanz-Serna (1997).

A nontrivial periodic solution $y(\cdot)$ of a Λ-reversible system (13) is called *symmetric* if the corresponding trajectory in phase space R^D intersects the invariant subspace X_+ of Λ. The monodromy matrix of a symmetric orbit has special properties (Cano & Sanz-Serna (1995)) that, as we will show next, have an impact on the error growth of numerical integrators. The following result is analogous to Lemma 5.7 of Cano & Sanz-Serna (1995). The situation here is more favourable than for one-step methods because the method is not supposed to be time-reversible.

LEMMA 3 When a strongly stable LMM is employed to integrate a reversible initial value problem (1)–(2), (13) where $a \in X_+$, and the solution is a symmetric periodic orbit, the coefficients e_j^I with even j $(j = r, \ldots, 2r-1)$ of the asymptotic expansion of the error satisfy

$$M_{t_0} \Lambda e_j^I[N] = -e_j^I[N]. \tag{14}$$

Proof. From the reversibility

$$\Lambda M(t_0 + t, t_0 + s) = M(t_0 - t, t_0 - s)\Lambda,$$

so that from (9), we may write

$$\begin{aligned} M_{t_0} \Lambda e_j^I[N] &= -c_j \int_{t_0}^{t_0+T} M(t_0+T, t_0)\Lambda M(t_0+T, s) y^{(j+1)}(s)\, \mathrm{d}s \\ &= -c_j \int_{t_0}^{t_0+T} M(t_0+T, t_0) M(t_0 - T, 2t_0 - s)\Lambda y^{(j+1)}(s)\, \mathrm{d}s. \end{aligned}$$

Making the change of variables $u = 2t_0 + T - s$, we have

$$M_{t_0} \Lambda e_j^I[N] = -c_j \int_{t_0}^{t_0+T} M(t_0+T, t_0) M(t_0, u)\Lambda y^{(j+1)}(2t_0 + T - u)\, \mathrm{d}u.$$

Now the periodicity and symmetry of $y(\cdot)$ lead to the result. □

THEOREM 4 Assume that the solution of the reversible initial value problem (1)–(2), (13) is a symmetric periodic orbit and that $a \in X_+$. When integrating a strongly stable LMM as in Theorem 1, the following possibilities arise:

(R1) There is a Floquet multiplier of modulus $\neq 1$. Then, $e_j[N]$ ($j = r, \ldots, 2r-1$) grows exponentially with N.

(R2) Every Floquet multiplier has modulus 1. Then, $e_j[N]$ ($j = r, \ldots, 2r-1$) grows polynomially with N.

Let us consider the following particular cases of (R2):

(R2′) Every Floquet multiplier $\neq 1$ has Jordan blocks of size $\leqslant 2$ and the multiplier 1 only possesses trivial Jordan blocks (of size 1). Then, $e_j[N]$ grows linearly with N.

(R2″) Every Floquet multiplier has Jordan blocks of size $\leqslant 2$, and for the multiplier 1 there are no generalized eigenvectors in X_-. Then,

- $e_j[N]$ grows linearly if j is even and quadratically if j is odd.
- In particular, if the order r of the method is even, the leading $O(h^r)$ error term in (6) grows linearly and the $O(h^{r+1})$ error term grows quadratically.

Proof. The case (R1) is a consequence of the behaviour of (G1) in Theorem 3, because for a symmetric orbit the Floquet multipliers appear in pairs λ, $1/\lambda$. The cases (R2) and (R2′) are straightforward applications of (G2) in Theorem 3.

For the case (R2″) we begin by noticing that it is easy to prove that if a vector $\tilde{e}$ belongs to the invariant subspace of M_{t_0} associated with a Floquet multiplier λ, then $M_{t_0}\Lambda\tilde{e}$ belongs to the invariant subspace of M_{t_0} associated with the multiplier $1/\lambda$. By setting in particular $\lambda = 1$, we conclude from (14) that, for even j,

$$M_{t_0}\Lambda\tilde{e}_j = -\tilde{e}_j,$$

where $\tilde{e}_j$ denotes the component of $e_j^I[1]$ in the invariant subspace of M_{t_0} associated with the multiplier 1. After this the proof is concluded by using the argument in Theorem 5.1 of Cano & Sanz-Serna (1995). □

Some remarks are in order.

The hypothesis $a \in X_+$ is not necessary. This can be shown by an argument similar to that in the remark that follows Theorem 5.1 of Cano & Sanz-Serna (1995).

The case (R2″) includes many examples found in applications, including the periodic solutions of Kepler's problem. A discussion may be seen in Section 5.4 of Cano & Sanz-Serna (1995).

In the case (R2″) it is possible to determine those directions in which the error growth takes place, see Cano (1996).

3. Weakly stable methods

3.1 *Preliminaries*

We now consider a weakly stable LMM and denote by x_i, $i = 1, \ldots, m$, $2 \leqslant m \leqslant k$, the (simple) roots of unit modulus of the polynomial ρ, with $x_1 = 1$; the roots of ρ different from the x_i have modulus < 1. Associated with each x_i there is a *growth parameter* λ_i

$$\lambda_i = \frac{\sigma(x_i)}{x_i\rho'(x_i)}, \quad i = 1, \ldots, m. \tag{15}$$

Note that $\lambda_1 = 1$ by consistency.

In lieu of Theorem 1 we now have the following result, where the main feature is the appearance of terms $x_i^n e_{ji}(t_n)$, $j = r, \ldots, 2r-1$, $i = 2, \ldots, m$ that do not vary smoothly with t_n.

THEOREM 5 Using the above notation, assume that a weakly stable LMM of order $r \geqslant 1$, using a smooth starting procedure of order r, is applied to solve (1)–(2). Then

$$y_n = y(t_n) + \sum_{j=r}^{2r-1} h^j \left[\sum_{i=1}^{m} x_i^n e_{ji}(t_n) \right] + O(h^{2r}), \quad h \to 0, \tag{16}$$

where e_{ji}, $j = r, \ldots, 2r-1$, $i = 1, \ldots, m$ are smooth functions that satisfy the variational equations

$$\dot{e}_{ji}(t) = \lambda_i f'(y(t)) e_{ji}(t) + b_{ji}(t), \tag{17}$$

with

$$b_{j1}(t) = -c_j y^{(j+1)}(t), \quad j = r, \ldots, 2r-1,$$

and, for $2 \leqslant i \leqslant m$,

$$b_{ri}(t) = 0,$$

$$b_{ji}(t) = -\sum_{l=1}^{j-r} c_l^{(i)} e_{j-l,i}^{(l+1)}(t), \quad j = r+1, \ldots, 2r-1.$$

Here the c_j are the constants in (4) and $c_l^{(i)}$ are constants depending on the polynomials ρ, σ.

The constant implied in the $O(h^{2r})$ remainder in (16) can be chosen to be independent of t_n for t_n in each compact interval $[\delta, t_{\max}]$ with $t_0 < \delta < t_{\max}$.

Again the initial values for the variational equations are $\neq 0$ and may be found by matching the starting procedure.

3.2 *Symmetric methods*

The most important example of weakly stable methods is given by symmetric methods, i.e. methods that satisfy

$$\rho(x) = -x^k \rho\left(\frac{1}{x}\right), \quad \sigma(x) = x^k \sigma\left(\frac{1}{x}\right), \tag{18}$$

or

$$\alpha_j = -\alpha_{k-j}, \quad \beta_j = \beta_{k-j}, \quad j = 0, \ldots, k.$$

It is clear that for a symmetric method the roots of ρ other than ± 1 appear in pairs x, $1/x$. Therefore a symmetric method cannot be strongly stable; it is either unstable or weakly stable.

Assume that a symmetric k-step method is applied to the solution of a Λ-reversible system (13). If $y_n, y_{n+1}, \ldots, y_{n+k}$ are $k+1$ consecutive values of a numerical trajectory, then $\Lambda y_{n+k}, \Lambda y_{n+k-1}, \ldots, \Lambda y_n$ are also consecutive values of a numerical trajectory (Stoffer (1988)). This is the discrete analogue of the fact that if $y(t)$ is a solution of a reversible system then $\Lambda y(-t)$ is also a solution. Therefore symmetric methods are of potential interest in the integration of reversible problems. It has also been suggested that they may be of interest in the solution of Hamiltonian problems (Eirola & Sanz-Serna (1991)).

The following lemma summarizes some well-known properties of symmetric methods (Stetter (1973)).

LEMMA 4 Every symmetric LMM satisfies:

(i) The growing parameters λ_i ($i = 2, \ldots, m$) defined in (15) are real.
(ii) The coefficients $\{c_j\}$ which define the truncation error (4) vanish for odd j.
(iii) For $i = 2, \ldots, m$, the constants $c_l^{(i)}$ which appear in the definition of the coefficients e_{ji} in (16) are imaginary for odd l, and real for even j.
(iv) If $x_2 = -1$, $c_l^{(2)} = 0$ for odd l.

3.3 *Error growth in periodic solutions*

When $i = 1$ (i.e. for the principal root $x_1 = 1$ of ρ), $\lambda_1 = 1$ and the variational equation (17) reduces to the variational equation (7). Therefore all the results for the coefficients $e_j(t)$, $j = r, \ldots, 2r-1$, obtained in Sections 2.2 and 2.3 can readily be translated into results for the coefficients $e_{j1}(t)$, $j = r, \ldots, 2r-1$ in the expansion (16) of the error in a weakly stable LMM. Let us study in particular the case of a symmetric orbit of type (R2″) integrated by a weakly stable symmetric LMM. For the $e_{j1}(t)$, $j = r, \ldots, 2r-1$, with even j the growth is linear as in Theorem 3. For j odd we have, with a notation similar to that in Section 2.2, $e_{j1}^{I}(t) \equiv 0$ because $c_j = 0$ (see Lemma 4). Since $e_{j1}^{II}(t)$ grows linearly (all Jordan blocks have size $\leqslant 2$) then $e_{j1}(t)$ grows linearly for $j = r, \ldots, 2r-1$. This is analogous to the situation for a (R2″) symmetric orbit integrated with a symmetric one-step method (Cano & Sanz-Serna (1995)).

However, we still have to study the growth of the $e_{ji}(t)$, $j = r, \ldots, 2r-1$, $i = 2, \ldots, m$, associated with the roots $x_i \neq 1$. Proceeding as in Section 2.2,

$$e_{ji}(t) = e_{ji}^{I}(t) + e_{ji}^{II}(t),$$

with

$$e_{ji}^{I}(t) = \int_{t_0}^{t} M^{(i)}(t,s) b_{ji}(s)\, \mathrm{d}s, \quad e_{ji}^{II}(t) = M^{(i)}(t, t_0) e_{ji}(t_0),$$

where $M^{(i)}(t,s)$ is the transition matrix of the linear system

$$\dot{\delta}(t) = \lambda_i f'(y(t))\delta(t), \tag{19}$$

($y(t)$ is the solution of (1)–(2)). We therefore have to investigate the growth of the powers $[M_{t_0}^{(i)}]^N$ with $M_{t_0}^{(i)} = M^{(i)}(t_0 + T, t_0)$. Unfortunately the systems (19) have no relation whatsoever with the variational equation (8) of the orbit being integrated. As a consequence, the powers $[M_{t_0}^{(i)}]^N$ typically grow *exponentially* even in cases where the powers

$M_{t_0}^N$ only grow polynomially, i.e. where perturbations of the initial value problem (1)–(2) only grow as a polynomial in t. We present two examples.

EXAMPLE 1 Let us consider Newton's second law for the motion of a particle of unit mass with a potential $V(q) = 2q\,\mathrm{sign}(q)$, where q is the (scalar) coordinate. The equations of motion are

$$\dot{p} = -V'(q),$$
$$\dot{q} = p.$$

This system is reversible with respect to $\Lambda(p, q) = (-p, q)$ and Hamiltonian. If $q(t_0) = 1$, $p(t_0) = 0$, the particle undergoes a periodic motion of period $T = 4$. The monodromy matrix is found to be

$$\begin{pmatrix} 1 & 4 \\ 0 & 1 \end{pmatrix},$$

with 1 as a double eigenvalue: an initial perturbation grows linearly with time. On the other hand a simple computation reveals that

$$M_{t_0}^{(i)} = \begin{pmatrix} 1 - 8\lambda_i^2 + 8\lambda_i^4 & -4\lambda_i + 8\lambda_i^3 \\ \lambda_i(4 - 12\lambda_i^2 + 8\lambda_i^4) & 1 - 8\lambda_i^2 + 8\lambda_i^4 \end{pmatrix}.$$

Since

$$\det M_{t_0}^{(i)} \equiv 1,$$
$$\mathrm{trace}(M_{t_0}^{(i)}) = 2 + 16\lambda_i^2(\lambda_i^2 - 1),$$

for real λ_i with $|\lambda_i| > 1$, $M_{t_0}^{(i)}$ has real eigenvalues and one of them is of modulus > 1, leading to exponential growth of the powers $[M_{t_0}^{(i)}]^N$. In this example the potential is not smooth; it is possible to regularize the potential by changing its values in a small neighbourhood of the origin. By continuity, the regularized problem would still lead to matrices with eigenvalues of modulus > 1.

EXAMPLE 2 For the reversible, Hamiltonian Kepler problem in Sanz-Serna & Calvo (1994, Example 1.1), we have computed numerically (Cano (1996)) that $M_{t_0}^{(i)}$ has spectral radius > 1 as soon as $\lambda_i \neq \pm 1$.

In view of this exponential growth, *weakly stable LMM, symmetric or otherwise, cannot be recommended for the integration of reversible or Hamiltonian problems.* Let us present some numerical illustrations. We have integrated the symmetric orbit arising in the Kepler problem in Sanz-Serna & Calvo (1994, Example 1.1) (eccentricity $e = 0{\cdot}5$) by means of the symmetric LMM specified by $\rho(x) = (1/3)(y^3 - 1)$, $\sigma(x) = (1/2)(y^2 + y)$. In a first experiment, the missing starting values are found by Euler's rule, $y_0 = y(0)$, $y_1 = y_0 + hf(y_0)$, $y_2 = y_1 + hf(y_1)$. The norm of the error as a function of t is given in Fig. 1 (here norm means the maximum norm in the four-dimensional space of the (p, q) variables). The exponential error growth is apparent and at $t \approx 50$ the errors are large in spite of the tiny stepsizes used, $h = 2\pi \times 10^{-4}/J$, $J = 36, 72, 144, 288, 576$. Fig. 2 corresponds to a second case where y_0, y_1, y_2 are taken from the 'exact' solution and $h =$

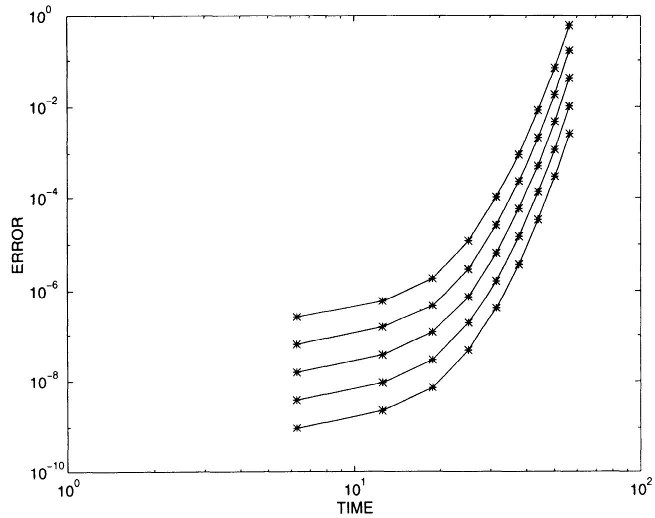

FIG. 1. Exponential error growth in the numerical integration of the Kepler problem with a symmetric linear multistep method for first-order systems. The starting values are found by Euler's rule.

$2\pi \times 10^{-4}/J$, $J = 9, 18, 36, 72$. A careful analysis (see Cano (1996)) shows that the leading $O(h^2)$ error term grows linearly due to the more accurate choice of starting values. Nevertheless the next $O(h^3)$ term grows exponentially. In the figure the growth appears to be linear in the initial time interval where the $O(h^3)$ term is negligible; after nine periods the $O(h^3)$ term dominates and the exponential growth manifests itself.

Before closing this section we should point out that the weakly stable explicit midpoint rule, used in extrapolation codes, is exceptional: the error grows as in a one-step method. This can be shown by rewriting the method as a one-step method as in Stetter (1970). A detailed discussion can be seen in Cano (1996).

4. Second-order systems

4.1 *Preliminaries*

Finally, we study the solution of the initial value problems

$$\ddot{Y}(t) = F(Y(t)), \tag{20}$$

$$Y(t_0) = A, \quad \dot{Y}(t_0) = B, \tag{21}$$

(F is smooth in R^d) by an LMM2

$$\sum_{l=0}^{k} A_l Y_{n+l} = h^2 \sum_{l=0}^{k} B_l F(Y_{n+l}). \tag{22}$$

Now the characteristic polynomials are

$$R(x) = A_k x^k + A_{k-1} x^{k-1} + \cdots + A_0,$$
$$S(x) = B_k x^k + B_{k-1} x^{k-1} + \cdots + B_0.$$

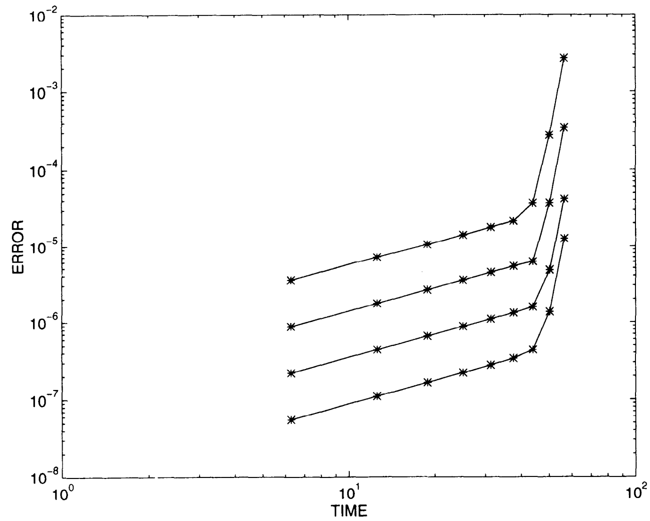

FIG. 2. Error growth in the numerical integration of the Kepler problem with a symmetric linear multistep method for first-order systems. The starting values are exact. An exponential error growth manifests itself after nine periods.

We assume throughout that $A_k \neq 0$ and that the method is irreducible (i.e. R and S have no common factors) and consistent (i.e. $R(1) = R'(1) = 0$, $R''(1) = 2S(1)$). Furthermore we normalize the method coefficients so that $S(1) = 1$.

It is well known that if (20) is rewritten as a first-order system in $\mathcal{R}^D$, $D = 2d$,

$$\dot{V} = F(Y), \quad \dot{Y} = V, \tag{23}$$

then the applications to (23) of the LMM specified by the polynomials ρ, σ is equivalent, after eliminating the velocities V_n, to the application to (20) of the LMM2 specified by $R = \rho^2$, $S = \sigma^2$.

For a method of order r there is an expansion

$$\tilde{L}(Z, t, h) = S(E)\left(\sum_{l=r}^{J-1} c_l h^{l+2} Z^{(l+2)}(t)\right) + O(h^{J+2}), \tag{24}$$

of the truncation error

$$\tilde{L}(Z, t, h) = R(E)Z(t) - h^2 S(E)\ddot{Z}(t).$$

The constants c_l in (24) only depend on R and S.

We say that the formula (22) is started with a procedure of order s if

$$Y_\nu - Y(t_\nu) = O(h^s), \quad \nu = 0, 1, \ldots, m-1,$$

as $h \to 0$, where $Y(t)$ is the solution of (20)–(21). Starting procedures are assumed to be smooth as in (5).

For LMMs, we studied separately the strongly and weakly stable cases; we treat all

LMM2s at once. We denote by x_i, $i = 1, \ldots, m$, the double roots of unit modulus of R, with $x_1 = 1$. Furthermore, let x_i, $i = m+1, \ldots, m+l$, be the simple roots of R with unit modulus. The roots of R different from x_i, $i = 1, \ldots, m+l$, are supposed to have modulus < 1, so as to have stability. Each x_i, $i = 2, \ldots, m$, leads to a growth parameter

$$\mu_i = \frac{2\sigma(x_i)}{x_i^2 \rho''(x_i)}. \tag{25}$$

The asymptotic expansion of the global error is presented in the following theorem, where we will need the polynomial

$$R_2(x) = \frac{R(x)}{\prod_{i=1}^m (x - x_i)}.$$

THEOREM 6 Assume that a stable LMM2 of order $r \geqslant 1$, using a smooth starting procedure of order r, with

$$R_2(E)[Y_l - Y(t_l)] = O(h^{r+1}), \quad l = 0, 1, \ldots, m-1,$$

is applied to solve (20)–(21). Then,

$$Y_n = Y(t_n) + \sum_{j=r}^{2r-1} h^j \left(\sum_{i=1}^{m+l} x_i^n \mathcal{E}_{ji}(t_n) \right) + O(h^{2r}), \quad h \to 0, \tag{26}$$

where the $\mathcal{E}_{ji}$, $j = r, \ldots, 2r-1$, $i = 1, \ldots, m+l$, are smooth functions that we describe next.

(i) For $i = 1$, $\mathcal{E}_{j1}$ solves the equation

$$\ddot{\mathcal{E}}_{j1}(t) = F'(Y(t))\mathcal{E}_{j1}(t) - c_j Y^{(j+2)}(t), \tag{27}$$

where c_j are the constants in (24).

(ii) For $i = 2, \ldots, m$, the $\mathcal{E}_{ji}$ satisfy

$$\ddot{\mathcal{E}}_{ji}(t) = \mu_i F'(Y(t))\mathcal{E}_{ji}(t) + b_{ji}(t),$$

with

$$\begin{aligned} b_{ri}(t) &= 0 \\ b_{ji}(t) &= -\sum_{l=1}^{j-r} \tilde{c}_l^{(i)} \mathcal{E}_{j-l,i}^{(l+2)}(t), \quad j = r+1, \ldots, 2r-1. \end{aligned}$$

Here μ_i are the growth parameters in (25) and $\tilde{c}_l^{(i)}$ are constants that only depend on the characteristic polynomials R and S.

(iii) For $i = m+1, \ldots, m+l$, the $\mathcal{E}_{ji}$ satisfy

$$\begin{aligned} \dot{\mathcal{E}}_{ji}(t) = \frac{1}{\alpha_{i,1}} \Bigg[&- \sum_{l=2}^{j-r+1} \alpha_{i,l} \mathcal{E}_{j-l+1,i}^{(l)}(t) \\ &+ \sum_{l=0}^{j-r-1} \beta_{i,l} \frac{\mathrm{d}^l}{\mathrm{d}t^l} [f'(y(t))\mathcal{E}_{j-l-1,i}(t)] \Bigg], \end{aligned} \tag{28}$$

where α_{il}, β_{il} are method-dependent constants.

The constant implied in the $O(h^{2r})$ remainder in (26) can be chosen independent of t_n for $t_n \in [\delta, t_{\max}]$, where $0 < \delta < t_{\max}$.

An idea of a proof is given in Hairer *et al* (1993). Full details of an alternative proof may be seen in Cano (1996).

4.2 *Error growth for periodic orbits*

Our task is now to study the behaviour of the functions $\mathcal{E}_{ji}(t)$ in (26) where the solution of (20)–(21) is a T-periodic function.

Let us begin with the $\mathcal{E}_{j1}(t)$ associated with the root $x_1 = 1$. We rewrite the variational equation (27) in first-order form as

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix} v(t) \\ \mathcal{E}(t) \end{pmatrix} = \begin{pmatrix} 0 & F'(y(t)) \\ I & 0 \end{pmatrix}\begin{pmatrix} v(t) \\ \mathcal{E}(t) \end{pmatrix} - c_j \begin{pmatrix} y^{(j+2)}(t) \\ 0 \end{pmatrix},$$

and consider the transition and monodromy matrices of this first-order system with the corresponding Floquet multipliers. Then, it is a simple matter to derive formulae for $\mathcal{E}_{j1}(t_0 + NT)$ similar to those we obtained for $e_j[N]$ in Section 2.2. From there, we can ascertain the behaviour of the $\mathcal{E}_{j1}(t_0 + NT)$ in terms of the Floquet multipliers as in Theorem 3.

For the $\mathcal{E}_{ji}(t)$ with $i = 2, \ldots, m$, we have to deal with variational equations that in first-order form are

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix} \frac{1}{\sqrt{\mu}}v(t) \\ \mathcal{E}(t) \end{pmatrix} = \sqrt{\mu}\begin{pmatrix} 0 & F'(y(t)) \\ I & 0 \end{pmatrix}\begin{pmatrix} \frac{1}{\sqrt{\mu}}v(t) \\ \mathcal{E}(t) \end{pmatrix} + \begin{pmatrix} b(t) \\ 0 \end{pmatrix}. \qquad (29)$$

As Examples 1 and 2 in Section 3.3 show, the transition matrices for (29) have properties that do not relate to the Floquet multipliers of the periodic solution being studied. Thus in general the $\mathcal{E}_{ji}(t)$, $i = 2, \ldots, m$, grow exponentially and *methods with double roots x_i of unit modulus, $x_i \neq 1$, cannot be recommended.* In this connection note that a weakly stable LMM applied to (23) induces a LMM2 with parasitic double roots of unit modulus because $R(x) = \rho^2(x)$.

Finally let us study the behaviour of the function $\mathcal{E}_{ji}$, $i = m + 1, \ldots, m + l$, associated with simple roots of unit modulus.

THEOREM 7 Given the situation of Theorem 6 and assuming that the solution of (20)–(21) is T-periodic, the functions $\mathcal{E}_{ji}(t)$, $j = r, \ldots, 2r - 1$, $i = m + 1, \ldots, m + l$, grow like $O(t^{j-r})$.

If, in addition, the starting procedure is of order $r + 1$, then, for $i = m + 1, \ldots, m + l$, $\mathcal{E}_{ri}(t) \equiv 0$ and $\mathcal{E}_{ji}$ grows like $O(t^{j-r-1})$, $j = r, \ldots, 2r - 1$.

If, furthermore, the starting procedure is of order $r + 2$, then, for $i = m + 1, \ldots, m + l$, $\mathcal{E}_{ri}(t) \equiv \mathcal{E}_{r+1,i}(t) \equiv 0$ and $\mathcal{E}_{ji}$ grows like $O(t^{j-r-2})$, $j = r, \ldots, 2r - 1$.

Proof. The first part is settled by inductively showing in (28) that $\mathcal{E}^{(l)}_{j,i}$ is $O(t^{j-r-l})$ if $j - r - l \geqslant 0$ and $O(1)$ if $j - r - l < 0$.

The second part is proved by showing that, when deriving the initial values $\mathcal{E}_{ri}(t_0)$ by matching the starting procedure, one obtains $\mathcal{E}_{ri}(t_0) = 0$ and hence $\mathcal{E}_{ri}(t) \equiv 0$. From there the proof proceeds by induction.

The proof of the third part is analogous. More details can be found in Cano (1996). □

REMARK 2 The use of starting procedures of order $r+3, r+4, \dots$ does not bring any further reduction in the growth of the $\mathcal{E}_{ji}(t)$, $i = m+1, \dots, m+l$, see Cano (1996).

4.3 *Reversible systems*

For second-order equations (20) each linear involutive map Ξ in R^d with

$$\Xi \circ F \circ \Xi = F, \tag{30}$$

induces an involution Λ

$$\Lambda \begin{pmatrix} V \\ Y \end{pmatrix} = \begin{pmatrix} -\Xi V \\ \Xi Y \end{pmatrix}, \tag{31}$$

for the associated first-order system (23). The choice $\Xi = I$ gives an important particular example. Note that for this choice, the subspaces X_+ and X_- associated with Λ consist of vectors of the form $(0, Y)$ and $(V, 0)$ respectively.

The proof of the following result is similar to that of Lemma 3. The notation is as in Section 2.

LEMMA 5 Assume that an LMM2 is used to integrate an initial value problem (20)–(21) that is reversible with respect to Λ in (31). If $(A, B) \in X_+(\Lambda)$ and the solution is T-periodic, then the functions $\mathcal{E}^I_{j1}$ with even j, $r \leqslant j \leqslant 2r-1$, satisfy

$$M_{t_0} \Lambda \begin{pmatrix} \dot{\mathcal{E}}^I_{j1}[N] \\ \mathcal{E}^I_{j1}[N] \end{pmatrix} = - \begin{pmatrix} \dot{\mathcal{E}}^I_{j1}[N] \\ \mathcal{E}^I_{j1}[N] \end{pmatrix}. \tag{32}$$

From this lemma we can obtain the following result for the growth of the functions $\mathcal{E}_{j1}$ associated with the principal root $x_1 = 1$ of R.

THEOREM 8 Assume that the initial value problem (20)–(21) is reversible with respect to Λ in (31) and has a symmetric, T-periodic solution.

Assume that all the Floquet multipliers have unit modulus (case (R2) in Theorem 4). Then in the asymptotic expansion (26) the functions $\mathcal{E}_{j1}$, $j = r, \dots, 2r-1$, grow polynomially with t.

The following cases are important.

(R2′) All Floquet multipliers $\neq 1$ have Jordan blocks of size $\leqslant 2$ and the multiplier 1 only possesses trivial Jordan blocks (of size 1). Then $\mathcal{E}_{j1}(t)$, $j = r, \dots, 2r-1$, grow linearly with t.

(R2″) Every Floquet multiplier has Jordan blocks of size $\leqslant 2$, and for the multiplier 1 there are no generalized eigenvectors in the space of fixed points of $-\Lambda$. Then,

- $\mathcal{E}_{j1}[N]$ grows linearly if j is even and quadratically if j is odd.
- In particular, if the order r of the method is even, the coefficient $\mathcal{E}_{r1}(t)$ in the leading term in (26) grows linearly and the coefficient $\mathcal{E}_{r+1,1}(t)$ grows quadratically.

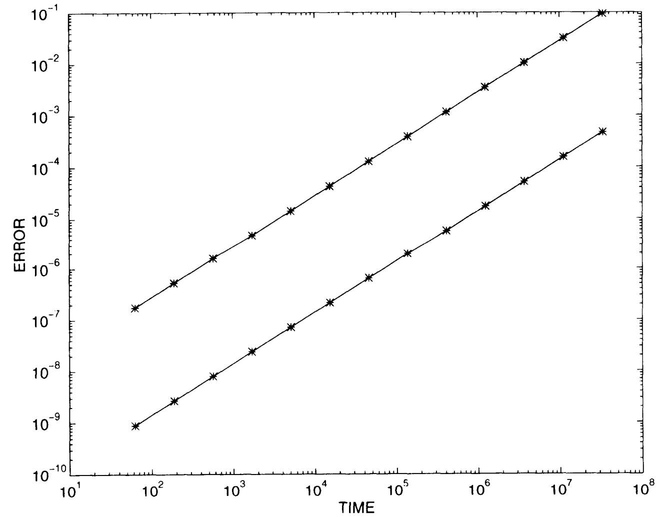

FIG. 3. Linear error growth in the numerical solution of the Kepler problem with a symmetric linear multistep method for second-order systems.

This result explains why, in the integration of Kepler's problem with Störmer methods ($m = 1, l = 0$) of even order (Quinlan & Tremaine (1990)), the error grows first linearly with t (when t is small and the leading $O(h^r)$ term of the expansion dominates) and later quadratically with t.

4.4 *Symmetric methods*

We finally study the situation when the method in (22) is symmetric, i.e.

$$R(x) = x^k R\left(\frac{1}{x}\right), \qquad S(x) = x^k S\left(\frac{1}{x}\right)$$

or

$$A_k = A_{k-j}, \quad B_k = B_{k-j}, \quad j = 0, \ldots, k.$$

For a symmetric method the truncation error constants c_l in (24) vanish for odd l; the order r is then even.

For a stable symmetric method all roots of R have unit modulus. If one of these roots, different from $x_1 = 1$, is double, then, for the reasons discussed in Section 4.2, the use of the method cannot be recommended. Hence we restrict our attention to symmetric methods for which $x_1 = 1$ is the only double root of R and all other roots are simple (with unit modulus), i.e. $m = 1, l = k - 2$.

Just as for LMMs, symmetric LMM2s inherit a reversibility property from the system being integrated, this makes them appealing for reversible systems. In fact, for a symmetric method some of the conclusions of Theorem 8 may be strengthened. In the case (R2$''$), the functions $\mathcal{E}_{j1}$ with odd j, $j = r, \ldots, 2r - 1$, that, in principle, may grow quadratically, only grow linearly because the coeffecient c_l in the source term in (27) vanishes. Then $\mathcal{E}_{j1}$ grows linearly for $j = r, \ldots, 2r-1$. Furthermore, according to Theorem 7, the remaining $\mathcal{E}_{ji}$, $i \neq 1$, grow at most linearly for $r \leqslant j \leqslant \min(r+3, 2r-1)$, if the starting procedure is sufficiently accurate. As a result, when h is small enough for the asymptotic expansion to capture the behaviour of the global error, the global error will show a linear behaviour as a function of t. This was experimentally found in Quinlan & Tremaine (1990). A numerical illustration follows. We have integrated the Kepler problem of Sanz-Serna & Calvo (1994), this time with the order 8, explicit, symmetric LMM2

$$\begin{aligned}
R(x) &= x^8 - 2x^7 + 2x^6 - x^5 - x^3 + 2x^2 - 2x + 1, \\
S(x) &= \frac{1}{12096}[17671x^7 - 23622x^6 + 61449x^5 - 50516x^4 \\
&\quad + 61449x^3 - 23622x^2 + 17671x],
\end{aligned}$$

derived in Quinlan & Tremaine (1990). The roots of R are $(1 \pm \sqrt{3}i)/2$ and the fifth roots of 1, with 1 a double root. To decrease the effects of round-off, we have used compensated summation and rewritten the method in first-order form (see Hairer *et al* (1993)). The starting values are computed 'exactly' by means of a Runge–Kutta package. The results, for eccentricity $e = 0{\cdot}2$, are given in Fig. 3, for $h = 2\pi/150, 2\pi/300$. The linear growth makes it possible to integrate accurately as far as $t \approx 5 \times 10^7$.

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