STABILITY AND RESONANCES OF MULTISTEP COSINE METHODS*

B. Cano

Departamento de Matemática Aplicada, IMUVA. Facultad de Ciencias. Paseo Belén 7, CP 47011 Valladolid, Spain

 $Email:\ bego@mac.uva.es$

M.J. Moreta

Departamento de Fundamentos del Análisis Económico I. Universidad Complutense de Madrid. Campus de Somosaguas, Pozuelo de Alarcón, 28223 Madrid, Spain

Email: mjesusmoreta@ccee.ucm.es

Abstract

In a previous paper, some particular multistep cosine methods were constructed which proved to be very efficient because of being able to integrate in a stable and explicit way linearly stiff problems of second-order in time. In the present paper, the conditions which guarantee stability for general methods of this type are given, as well as a thorough study of resonances and filtering for symmetric ones (which, in another paper, have been proved to behave very advantageously with respect to conservation of invariants in Hamiltonian wave equations). What is given here is a systematic way to analyse and treat any of the methods of this type in the mentioned aspects.

Mathematics subject classification: 35L70, 65M12, 65M99.

Key words: Exponential integrators, Multistep cosine methods, Second-order partial differential equations, Stability, Resonances.

1. Introduction

In this paper we deal with the stability and phenomenon of resonances of multistep cosine methods. These methods are designed to integrate systems of the form

$$\ddot{y}(t) = -\Omega^2 y(t) + g(t, y(t)),$$
(1.1)

with g a smooth function and Ω some matrix which we assume to be diagonal with real eigenvalues, in such a way that the linear part is integrated exactly. These methods have been proved to turn up very efficient when integrating the system which arises after the space discretization of a partial differential equation of second-order in time when the 'stiff' part is linear [2,3,5,6,9,10,13] and $High\ order\ symmetric\ multistep\ cosine\ methods$, by B. Cano and M. J. Moreta (unpublished). In such a way, explicit and stable methods can be obtained. We remark that the methods suggested in [5,6,9,10,13] lead to at most second-order in time under a finite-energy and non-resonance condition, but without assuming any regularity of the solution of the continuous problem. On the contrary, the methods suggested and analysed in [2,3] and $High\ order\ symmetric\ multistep\ cosine\ methods\ (unpublished)\ can lead to higher order in time without assuming any finite-energy condition but taking as a strong hypothesis enough$

^{*} Received August 12, 2010 / Revised version received January 11, 2012 / Accepted March 28, 2012 / Published online September 24, 2012 /

regularity of the solution of the continuous problem. The study of stability (independent of the degree of stiffness of the problem) has been done for particular cases as Gautschi, MC3 and SMC4 methods in [3] but a general study is lacking in the literature yet which can be applied to methods of higher order for regular solutions, as those suggested in *High order symmetric multistep cosine methods* (unpublished). That is the first aim of the present paper.

For the sake of simplicity, we will consider explicit methods with an even number of steps, which are the ones recommended in the literature [3] and *High order symmetric multistep cosine methods* (unpublished). These methods are determined by a difference equation like

$$\rho_{h\Omega}(E)y_n = h^2 \sigma_{h\Omega}(E)g(t_n, y_n), \tag{1.2}$$

where y_n approximates the exact solution $y(t_n)$, with $t_n = t_0 + nh$ (natural n), E is the operator which advances a stepsize from n to n + 1 and

$$\rho_{\epsilon}(z) = z^{2k} + \alpha_{2k-1}(\epsilon)z^{2k-1} + \dots + \alpha_0(\epsilon), \quad \sigma_{\epsilon}(z) = \gamma_{2k-1}(\epsilon)z^{2k-1} + \dots + \gamma_0(\epsilon),$$

with $\{\alpha_j\}_{j=0}^{2k-1}, \{\gamma_j\}_{j=0}^{2k-1}$ certain real functions.

When the methods of this type are consistent and stable convergence follows, which implies that, for a fixed value of time, when the timestepsize diminishes, the error goes to zero (see [3] and High order symmetric multistep cosine methods (unpublished)). However, the values of the timestepsizes h for which clean numerical convergence of the corresponding order is observed vary a lot depending on the possible diagonal elements λ of Ω . That may lead to 'not so good' numerical results. The phenomenon which we try to avoid is called 'resonance', since it is caused by the fact that $h\lambda$ is at or near certain real distinguished values. This phenomenon has been well studied in [3] for the symmetric Gautschi and SMC4 methods for the scalar equation

$$\ddot{y}(t) = -\lambda^2 y(t) - y(t),\tag{1.3}$$

and our second aim here is to give a more general study in order to understand it, only for this equation, but for every symmetric multistep cosine method. This will allow to construct filters which avoid those resonances. We remark that the filters suggested here may not lead to uniform second-order convergence for problem (1.3), as distinct from some of the filters well discussed in [10]. However, these filters make the methods conserve its order of consistency (as high as we want) when integrating regular solutions of Hamiltonian wave or beam equations, as it is well justified in *High order symmetric multistep cosine methods* (unpublished). Remark 4.1 means to be clarifying in that sense. Besides, for space discretizations of this type of equations (much more complicated than (1.3)), we have numerically observed that resonances are also avoided in *High order symmetric multistep cosine methods* (unpublished). We also remark that symmetry of these methods is a key condition to guarantee a good behaviour with respect to conservation of invariants with time when integrating space discretizations of Hamiltonian wave equations (see [2]).

The paper is structured as follows. Section 2 deals with conditions under which stability can be assured. Section 3 gives a detailed study of resonances. Section 4 analyses how filtering must be done in order to avoid them. Finally, in Section 5 some numerical experiments are shown which corroborate previous results. For the sake of readability, the more technical proofs of the provided theorems have been written in an appendix.

2. Stability

It is well known that (1.2) can be written as a one-step method by introducing the vector $Y_n = [y_{n+2k-1}, \dots, y_n]^T$, since

$$Y_{n+1} = R(h\Omega)Y_n + h^2B(h\Omega)G(t_n, Y_n),$$

with $G(t_n, Y_n) = [g(t_{n+2k-1}, y_{n+2k-1}), \dots, g(t_n, y_n)]^T$,

$$R(h\Omega) = \begin{pmatrix} -\alpha_{2k-1}(h\Omega) & -\alpha_{2k-2}(h\Omega) & -\alpha_{0}(h\Omega) \\ I & 0 & \cdots & 0 \\ 0 & I & \cdots & 0 \\ \vdots & & \ddots & \vdots \\ 0 & 0 & \cdots & I & 0 \end{pmatrix},$$

$$B(h\Omega) = \begin{pmatrix} \gamma_{2k-1}(h\Omega) & \gamma_{2k-2}(h\Omega) & \cdots & \gamma_{0}(h\Omega) \\ 0 & \cdots & \cdots & 0 \\ \vdots & & & \vdots \\ 0 & \cdots & \cdots & 0 \end{pmatrix}.$$

Then, the stability consists of obtaining the following bound

$$||R^n(h\Omega)|| < Cn$$
,

for every natural value n and some constant C which does not depend on Ω , h and n, and where $\|\cdot\|$ denotes the Euclidean matrix norm. Notice that in case g=0 (and therefore G=0),

$$Y_n = R(h\Omega)^n Y_0. (2.1)$$

Besides, in such a case, the exact solution of (1.1) would grow at most linearly. However, the fact that these methods integrate the linear part exactly does not directly imply that the methods are stable in the indicated sense. Notice that this would be true if Y_0 in (2.1) always corresponded to an exact starting procedure. However, in order to have convergence, $||R(h\Omega)^n\delta||$ must be controlled for any possible perturbation δ . In fact, a multistep cosine method which is not stable in the sense mentioned above is given in [3]. We would also like to remark that Kreiss matrix theorems [1] cannot be applied for our stability bound since the Schur decomposition of $R(h\Omega)$ is not diagonal, as it was studied in [3] for Gautschi and SMC4 methods.

Due to a well-known spectral result, as $h\Omega$ is a normal matrix,

$$||R(h\Omega)^n|| \le \sup_{\lambda \in \sigma(\Omega)} ||R(h\lambda)^n||.$$

Therefore, we are interested in bounding $||R^n(\epsilon)||/n$ uniformly on real ϵ . In fact, we obtain a finer result since, for many values of ϵ , $||R^n(\epsilon)||$ does not grow with n. Here is the precise result, which proof is given in the appendix because of its technicality.

Theorem 2.1. Let us assume that

- (i) $\rho_{\epsilon}(z)$ has coefficients which are continuous and periodic on ϵ .
- (ii) For every value of ϵ , all the roots of $\rho_{\epsilon}(z)$ have modulus less than or equal to one and those of modulus one are at most double.

(iii) There exist just a finite number of values of ϵ_l in each period for which double roots are met.

Then, the stability matrix associated to this polynomial $R(\epsilon)$ satisfies

$$||R^n(\epsilon)|| \le Cn, \quad \epsilon \in \mathbb{R}, n \in \mathbb{N},$$
 (2.2)

for some constant C which does not depend on n either on ϵ .

Besides, there exists $\eta > 0$ such that if $|\epsilon - \epsilon_l| > \eta$ for every ϵ_l which leads to double roots,

$$||R^n(\epsilon)|| \le K, \quad n \in \mathbb{N},$$

for some constant K which does not depend on n either on ϵ .

3. Resonances

As it was explained in the introduction, in spite of having convergence when integrating space discretizations of regular solutions of continuous problems, some times the size of the errors is very big for moderately small values of the timestepsize. In order to understand this, we will consider the integration of the simplified problem (1.3) as in the previous paper [3]. As distinct from there, instead of studying just Gautschi and SMC4 method, we will consider here any stable symmetric multistep cosine method for which the coefficients of the second characteristic polynomial are bounded for real ϵ . Although the last hypothesis is weaker than that assumed in [3], Lemmas 6.1 and 6.2 there are still valid with the same proof. We state them here again for clarity.

It is well known that the numerical solution of (1.3) consists of a linear combination of powers of the roots $z_j(\epsilon, h)_{j=1}^{2k}$ of the polynomial

$$\rho_{\epsilon}(z) + h^2 \sigma_{\epsilon}(z), \tag{3.1}$$

where $\epsilon = \lambda h$. Then, the following lemmas hold.

Lemma 3.1. Let us assume hypotheses of Theorem 2.1 for $\rho_{\epsilon}(z)$ and that the coefficients of $\sigma_{\epsilon}(z)$ are bounded for real ϵ . Then, for small enough $\delta > 0$, it happens that for every $\epsilon \in \mathbb{R} \setminus \bigcup_{l=0}^{\infty} (\epsilon_{l} - \delta, \epsilon_{l} + \delta)$, there exist positive values $h_{0}, r_{1}, \ldots, r_{2k}$ (depending on δ but not on ϵ) satisfying that, for every positive h such that $h \leq h_{0}(\delta)$, each of the roots $\{z_{j}(\epsilon, h)\}_{j=1}^{2k}$ remains in one of the balls $\{B(z_{j}(\epsilon, 0), r_{j})\}_{j=1}^{2k}$, where these balls are disjoint to each other. On the other hand, if for some natural l, $\epsilon \in (\epsilon_{l} - \delta, \epsilon_{l} + \delta)$, the same result is true with the exception that $d(\epsilon_{l})$ pairs of the balls may not be disjoint to each other in each pair but are disjoint to all the other ones. (Here $d(\epsilon_{l})$ denotes the number of double roots of $\rho_{\epsilon_{l}}(z)$.)

Lemma 3.2. Under the same hypotheses of Lemma 3.1, if the method is also symmetric (i.e. $\alpha_j(\epsilon) = \alpha_{2k-j}(\epsilon), j = 0, \ldots, k, \gamma_j(\epsilon) = \gamma_{2k-j}(\epsilon), j = 1, \ldots, k-1$), the following statements hold.

- (a) $|z_j(\epsilon,0)| = 1$, for every $j = 1, \ldots, 2k$.
- (b) For small enough δ , if $\epsilon \in \mathbb{R} \setminus \bigcup_{l=0}^{\infty} (\epsilon_l \delta, \epsilon_l + \delta)$, there exists $h_1(\delta)$ such that, for $h \leq h_1(\delta)$, $|z_j(\epsilon,h)| = 1$ for every $j = 1, \ldots, 2k$.
- (c) If for some natural l, $\epsilon \in (\epsilon_l \delta, \epsilon_l + \delta)$, either it happens the situation before either $|z_j(\epsilon, h)| = 1$ for at least $2k 2d(\epsilon_l)$ roots and the other roots have not modulus one but, by pairs, they are one the conjugate inverse of the other.

(d) If, in situation (c), l is such that $\rho_{\epsilon_l}(z)$ has a real double root $z_j(\epsilon_l, 0) = z_r(\epsilon_l, 0) \in \mathbb{R}$, the pair of roots $z_j(\epsilon, h)$ and $z_r(\epsilon, h)$ satisfy that either both have modulus one and conjugate to each other or both are real and inverse to each other.

These lemmas are crucial to study resonances. Notice that, for small h, $z_j(\epsilon,h)$ will be a perturbation of $z_j(\epsilon,0)$, which is a root of the first characteristic polynomial $\rho_{\epsilon}(z)$. Notice also that all the solutions of (1.3) are bounded with time while in case $|z_j(\epsilon,h)| > 1$ for some j, the numerical solution can grow exponentially with n. This is the fact which leads to resonance. Therefore, we are interested in cases (c) and (d) in Lemma 6.2, which are the ones which produce resonance.

In order to understand which double roots produce resonances, the following Taylor series expansion of (3.1) is used,

$$\eta \frac{d\rho_{\epsilon}}{d\epsilon}(z_{l})|_{\epsilon_{l}} + \frac{\eta^{2}}{2} \frac{d^{2}\rho_{\epsilon}}{d\epsilon^{2}}|(z_{l})_{\epsilon_{l}} + \eta r \frac{d}{d\epsilon}\rho_{\epsilon}'(z_{l})|_{\epsilon_{l}} + \frac{r^{2}}{2}\rho_{\epsilon_{l}}''(z_{l}) \\
+ \dots + h^{2} \left[\sigma_{\epsilon_{l}}(z_{l}) + \eta \frac{d\sigma_{\epsilon}}{d\epsilon}(z_{l})|_{\epsilon_{l}} + r\sigma_{\epsilon_{l}}'(z_{l}) + \frac{\eta^{2}}{2} \frac{d^{2}\sigma_{\epsilon}}{d\epsilon^{2}}(z_{l})|_{\epsilon_{l}} \right] \\
+ \eta r \frac{d}{d\epsilon}\sigma_{\epsilon}'(z_{l})|_{\epsilon_{l}} + \frac{r^{2}}{2}\sigma_{\epsilon_{l}}''(z_{l}) + \dots = 0,$$
(3.2)

where $\epsilon = \epsilon_l + \eta$, $z = z_l + r$, with z_l a double root of $\rho_{\epsilon_l}(z)$.

In the following, we will say that no resonance occurs at ϵ_l if, for small enough h and ϵ near enough ϵ_l the roots $z_j(\epsilon,h)$ of (3.1) have modulus one. On the contrary, we will say that resonance occurs if that situation does not happen.

Also in the following we will consider the following hypotheses:

- (a) the coefficients of $\rho_{\epsilon}(z)$ are twice continuously differentiable at all the values ϵ_l which lead to double roots of $\rho_{\epsilon_l}(z)$.
- (b) the coefficients of $\sigma_{\epsilon}(z)$ are continuous at the same values of ϵ_l mentioned in (a) and once differentiable at the same values of ϵ_l when σ_{ϵ_l} vanishes at some of its double roots.

For the values of ϵ_l which lead to the double root 1 or -1, the sign of $\sigma_{\epsilon_l}(\pm 1)$ is very important in order to know whether that ϵ_l will produce resonance. The precise result is the following theorem which proof is again in the appendix.

Theorem 3.1. Let us assume hypotheses of Lemma 3.2, (a), (b) and that 1 or -1 is a double root of $\rho_{\epsilon_l}(z)$. Then,

- (i) If $\sigma_{\epsilon_l}(\pm 1) > 0$ or $\sigma_{\epsilon_l}(\pm 1) = \sigma'_{\epsilon_l}(\pm 1) = \frac{d\sigma_{\epsilon_l}}{d\epsilon}(\pm 1)|_{\epsilon = \epsilon_l} = 0$, no resonance occurs at ϵ_l .
- (ii) If $\sigma_{\epsilon_l}(\pm 1) < 0$, resonance occurs at ϵ_l .

Remark 3.1. Notice that for every consistent method $\rho_0(z)$ has the double root 1. Besides, $\sigma_0(1) = \rho_0''(1)/2$ and therefore, by looking at the proof of the previous theorem, $\sigma_0(1)$ is always positive. Besides, when the underlying multistep method is s-stable [4,12], 1 is the only double root of $\rho_0(z)$. As a consequence, in that case, resonance never occurs by applying (i) in Theorem 3.1.

Finally, for the values of ϵ_l which lead to non-real double roots of $\rho_{\epsilon_l}(z)$, both phenomena of resonance and non-resonance can be observed. The key point to obtain one or other behaviour is given by the following theorem, which proof is again in the appendix.

Theorem 3.2. Let us assume hypotheses of Lemma 3.2, (a), (b) and that \tilde{z} is a complex double root of $\rho_{\epsilon_l}(z)$. Then,

- (i) $\rho_{\epsilon_l}''(\tilde{z})/\tilde{z}^{k-2}$ and $\sigma_{\epsilon_l}(\tilde{z})/\tilde{z}^k$ take real values.
- (ii) If the previous values take the same sign or $\sigma_{\epsilon_l}(\tilde{z}) = \frac{d}{d\epsilon}\sigma_{\epsilon}(\tilde{z})|_{\epsilon=\epsilon_l} = \sigma'_{\epsilon_l}(\tilde{z})| = 0$, no resonance turns up at ϵ_l .
- (iii) If the values in (i) take different signs, resonance turns up at ϵ_l .

4. Filters to Avoid Resonance

In this section we consider the technique of filter functions to avoid resonances. In such a way, the new method would read

$$\rho_{h\Omega}(E)y_n = h^2 \sigma_{h\Omega}(E)g(t_n, \phi(y_n)), \tag{4.1}$$

for some filter function ϕ . Therefore, when integrating (1.3), the numerical solution would be linear combinations of powers of the roots of the following polynomial (with $\epsilon = h\lambda$)

$$\rho_{\epsilon}(z) + h^2 \tilde{\sigma}_{\epsilon}(z), \tag{4.2}$$

where $\tilde{\sigma}_{\epsilon}(z) = \phi(\epsilon)\sigma_{\epsilon}(z)$. Notice that this polynomial is again symmetric. The following theorem states under which conditions on the filter function ϕ , all the roots of this polynomial have modulus one and therefore no resonance turns up. We omit the proof since that follows from Lemmas 6.1 and 6.2 in [3] and Theorems 3.1, 3.2 in this paper just by considering also that

$$\frac{d\tilde{\sigma}_{\epsilon}}{d\epsilon}(z) = \phi'(\epsilon)\sigma_{\epsilon}(z) + \phi(\epsilon)\frac{d\sigma_{\epsilon}}{d\epsilon}(z), \quad \tilde{\sigma}'_{\epsilon}(z) = \phi(\epsilon)\sigma'_{\epsilon}(z).$$

Theorem 4.1. Under the same hypotheses of Theorems 3.1 and 3.2, the roots of (4.2) have modulus one and therefore no resonance turns up if the filter function ϕ satisfies the following conditions:

- (i) $\phi: \mathbb{R} \to \mathbb{R}$ is a bounded function on the real axis.
- (ii) $\phi(\epsilon)$ is continuous at the values ϵ_l which lead to double roots of $\rho_{\epsilon}(z)$ and continuously differentiable at the values ϵ_l such that, for the corresponding double roots \tilde{z} , $\sigma_{\epsilon_l}(\tilde{z}) = 0$.
- (iii) $\phi(\epsilon_l) < 0$ or $\phi(\epsilon_l) = \phi'(\epsilon_l) = 0$ for every real value ϵ_l which leads to the double root ± 1 of $\rho_{\epsilon}(z)$ and for which $\sigma_{\epsilon_l}(\pm 1) < 0$.
- (iv) $\phi(\epsilon_l) > 0$ or $\phi(\epsilon_l) = \phi'(\epsilon_l) = 0$ for every real value ϵ_l which leads to the double root ± 1 of $\rho_{\epsilon}(z)$ and for which $\sigma_{\epsilon_l}(\pm 1) > 0$.
- (v) $\phi(\epsilon_l) = 0$ for every real value ϵ_l which leads to the double root ± 1 of $\rho_{\epsilon}(z)$ and for which $\sigma_{\epsilon_l}(\pm 1) = 0$.

- (vi) $\phi(\epsilon_l) > 0$ or $\phi(\epsilon_l) = \phi'(\epsilon_l) = 0$ for every real value ϵ_l which leads to a non-real double root \tilde{z} of $\rho_{\epsilon}(z)$ and for which $\rho''_{\epsilon_l}(\tilde{z})/\tilde{z}^{k-2}$ and $\sigma_{\epsilon_l}(\tilde{z})/\tilde{z}^k$ take the same sign.
- (vii) $\phi(\epsilon_l) < 0$ or $\phi(\epsilon_l) = \phi'(\epsilon_l) = 0$ for every real value ϵ_l which leads to a non-real double root \tilde{z} of $\rho_{\epsilon}(z)$ and for which $\rho''_{\epsilon_l}(\tilde{z})/\tilde{z}^{k-2}$ and $\sigma_{\epsilon_l}(\tilde{z})/\tilde{z}^k$ take different signs.
- (viii) $\phi(\epsilon_l) = 0$ for every real value ϵ_l which leads to a non-real double root \tilde{z} of $\rho_{\epsilon}(z)$ and for which $\sigma_{\epsilon_l}(\tilde{z}) = 0$.

On the other hand, it is also necessary to ask for some requirements to the filter function ϕ so that the filtered multistep cosine method conserves the order of consistency. Let us denote by d_n to the local truncation error when applied to (1.1), which is defined as

$$d_n = \rho_{h\Omega}(E)y(t_n) - h^2\sigma_{h\Omega}(E)g(t_n, y(t_n)).$$

Then the following theorem follows.

Theorem 4.2. Whenever g is Lipschitz on its second variable with Lipschitz constant L and the coefficients of $\sigma_{\epsilon}(z)$ are bounded by a certain constant Γ , the local truncation error corresponding to the filtered method (4.1) d_n^* satisfies for every vector norm $\|\cdot\|$,

$$||d_n^*|| \le ||d_n|| + 2kh^2\Gamma L \max_{l \in \{0,\dots,2k-1\}} ||[I - \phi(h\Omega)]y(t_{n+l})||.$$
(4.3)

Proof. The proof is straightforward by taking into account that

$$d_n^* = \rho_{h\Omega}(E)y(t_n) - h^2\sigma_{h\Omega}(E)g(t_n, \phi(h\Omega)y(t_n))$$

= $d_n + h^2\sigma_{h\Omega}(E)[g(t_n, y(t_n)) - g(t_n, \phi(h\Omega)y(t_n))].$

This completes the proof of the theorem.

Remark 4.1. As it was justified in [3] and B. Cano and M. J. Moreta, High order symmetric multistep cosine methods, unpublished, for all the methods recommended there, when integrating regular solutions of PDEs, after a pseudospectral discretization Ω is a diagonal matrix and $||d_n||$ behaves as $O(h^{2k+2})$. On the other hand, y(t) in such a case contains the approximation to the Fourier coefficients of the solution. Therefore, for regular solutions, the components corresponding to the higher frequencies are very small, even negligible. Because of this, we suggest considering a filter function for which $\phi(\epsilon)$ is at least bounded and not very big when ϵ grows and such that $(\phi(\epsilon) - 1)/\epsilon^{2k}$ is bounded (and as small as possible) for small ϵ so that the second term in (4.3) at least behaves also as $O(h^{2k+2})$. In any case, a detailed proof of the conservation of the order of consistency in that case is given in the same references.

Remark 4.2. For the choice of that function we must also take into account that $\phi''(\epsilon_l)$ must not be too big for the values of ϵ_l for which we are imposing that $\phi(\epsilon_l) = \phi'(\epsilon_l) = 0$ since, in that case, the higher order terms in (3.2) may be too large and h should be very small so as not to observe resonance.

Remark 4.3. The filter functions suggested in [3] for Gautschi and SMC4 methods satisfied all the conditions stated in Theorem 4.1 and Remarks 4.1, 4.2.

5. Numerical Experiments

In this section, our aim is to numerically corroborate the results of Sections 3 and 4. We numerically integrate problem (1.3) with initial conditions such that the exact solution of the problem is $y(t) = \cos(\sqrt{1+\lambda^2}t)/\sqrt{1+\lambda^2}$. We have considered the cosine 8-step method SMC8 described in High order symmetric multistep cosine methods (unpublished). For that method, double roots of the first characteristic polynomial were met for $\epsilon = 2m\pi$, $\pi/3 + 2m\pi$, $2\pi/5 + 2m\pi$, $4\pi/5 + 2m\pi$, $\pi + 2m\pi$, $6\pi/5 + 2m\pi$, $8\pi/5 + 2m\pi$, $5\pi/3 + 2m\pi$, integer m. An obvious function ϕ which satisfies all the conditions stated in Theorems 4.1 and Remarks 4.1, 4.2 is

$$\phi(\epsilon) = \begin{cases} 1 \text{ if } \epsilon \in [-1.2, 1.2] \\ 0 \text{ if } \epsilon \notin [-1.2, 1.2]. \end{cases}$$

$$(5.1)$$

In the left plot of Fig. 5.1 we show the local error committed just after advancing one stepsize with the values h=0.1,0.05,0.025. We have considered the values $\lambda=1,2,\ldots,1000$. Then, in the right plot of Fig. 5.1 we show the same local error when using filter (5.1). We notice that the errors are the same for values of λ such that $h\lambda < 1.2$. Then, there is a range of values for which the errors are noticeably different. That is because the second term in (4.3) becomes important then. However, for bigger values of λ , as it was well justified in [3] for this problem, the second term becomes less important and the size of the errors of both figures are very similar.

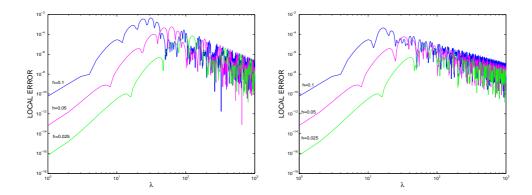


Fig. 5.1. Growth of local error with λ for problem (1.3) and SMC8 method without filtering (left) and filtering (right)

In any case, the advantages of filtering are not seen in the local error but in the global error. In Fig. 5.2, we show the global error committed after time T=40 for the same values of h and λ . In the left plot, no filter function was used and therefore the error is enormously big, mainly when $h\lambda$ is near the values of ϵ_l which lead to resonances: $2\pi/5 + 2m\pi$, $\pi + 2m\pi$, $8\pi/5 + 2m\pi$, integer m, according to Theorems 3.1, 3.2 and the calculations made in *High order symmetric multistep cosine methods* (unpublished).

However, in the right plot of Fig. 5.2, after applying the filter function (5.1), those resonances disappear. Notice also that, as it is justified in the above reference, the first characteristic polynomial associated to this method satisfies hypotheses of Theorem 2.1. Therefore, following the same argument as that in Subsection 5.2 of [3], this justifies that the method converges

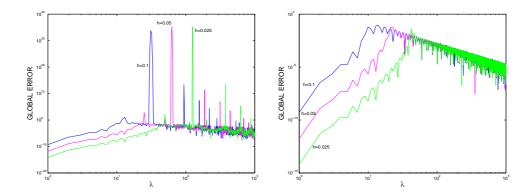


Fig. 5.2. Growth of global error with λ for problem (1.3) and SMC8 method without filtering (left) and filtering (right)

for the smallest values of λ as $O(h^8)$ but the error does not decrease when h diminishes but is controlled for the biggest values of λ .

Appendix

A. Proof of Theorem 2.1

Before proving the main theorem of stability, we consider the following lemma.

Lemma A.1. Let $r \geq 1$ be an integer and $z_0, \ldots, z_{r-1}, t_0, \ldots, t_r$ some complex values of unit modulus such that z_0, \ldots, z_{r-1} are well apart from each other and from the value 1 and t_0, \ldots, t_r are near enough the value 1. More precisely, there exists $\delta > 0$ such that $|arg(z_j)| \geq 2\delta$ $(j = 0, \ldots, r-1), |arg(z_j/z_l)| \geq 2\delta$ $(j, l = 0, \ldots, r-1, j \neq l)$ and $|arg(t_j)| \leq \delta$ $(j = 0, \ldots, r)$. Then,

$$\sum_{e_0, \dots, e_{r-1} = 0}^{n} z_0^{e_0} \dots z_{r-1}^{e_{r-1}} \left(\sum_{s=0}^{e_0-1} t_0^s \right) \left(\sum_{s_1=0}^{e_1-1} t_1^{s_1} \right) \dots \left(\sum_{s_r=0}^{n-e_0-\dots-e_{r-1}-1} t_r^{s_r} \right)$$

$$= z_0^n C_{0,r}(z_0, \dots, z_{r-1}, t_0, \dots, t_r) \left(\sum_{s=0}^{n} t_0^s \right) + \dots$$

$$+ z_{r-1}^n C_{r-1,r}(z_0, \dots, z_{r-1}, t_0, \dots, t_r) \left(\sum_{s_r=0}^{n} t_r^{s_{r-1}} \right)$$

$$+ C_{r,r}(z_0, \dots, z_{r-1}, t_0, \dots, t_r) \left(\sum_{s_r=0}^{n} t_r^{s_r} \right) + z_0^n C_{0,r}'(z_0, \dots, z_{r-1}, t_0, \dots, t_r)$$

$$+ \dots + z_{r-1}^n C_{r-1,r}'(z_0, \dots, z_{r-1}, t_0, \dots, t_r) + C_{r,r}'(z_0, \dots, z_{r-1}, t_0, \dots, t_r)$$

$$+ (z_0 t_0)^n C_{0,r}''(z_0, \dots, z_{r-1}, t_0, \dots, t_r) + \dots + (z_{r-2} t_{r-2})^n C_{r-2,r}''(z_0, \dots, z_{r-1}, t_0, \dots, t_r),$$

where the functions $C_{j,r}(z_0,\ldots,z_{r-1},t_0,\ldots,t_r)$, $C'_{j,r}(z_0,\ldots,z_{r-1},t_0,\ldots,t_r)$ and $C''_{j,r}(z_0,\ldots,z_{r-1},t_0,\ldots,t_r)$ do not depend on n and are bounded independently of the considered values $z_0,\ldots,z_{r-1},t_0,\ldots,t_r$.

Proof. The result follows by induction on r. For r = 1, let us first assume that $t_0 \neq 1$ and $t_1 \neq 1$. Then,

$$\sum_{e_{0}=0}^{n} z_{0}^{e_{0}} \left(\sum_{s=0}^{e_{0}-1} t_{0}^{s} \right) \left(\sum_{s_{1}=0}^{n-e_{0}-1} t_{1}^{s_{1}} \right) \\
= \sum_{e_{0}=0}^{n} z_{0}^{e_{0}} \frac{1-t_{0}^{e_{0}}}{1-t_{0}} \frac{1-t_{1}^{n-e_{0}}}{1-t_{1}} \\
= \frac{1}{1-t_{0}} \frac{1}{1-t_{1}} \left[\sum_{e_{0}=0}^{n} z_{0}^{e_{0}} - \sum_{e_{0}=0}^{n} (z_{0}t_{0})^{e_{0}} - t_{1}^{n} \sum_{e_{0}=0}^{n} \left(\frac{z_{0}}{t_{1}} \right)^{e_{0}} + t_{1}^{n} \sum_{e_{0}=0}^{n} \left(\frac{z_{0}t_{0}}{t_{1}} \right)^{e_{0}} \right] \\
= \frac{1}{1-t_{0}} \frac{1}{1-t_{1}} \left[\frac{1-z_{0}^{n+1}}{1-z_{0}} - \frac{1-z_{0}^{n+1}t_{0}^{n+1}}{1-z_{0}t_{0}} - t_{1}^{n+1} \frac{1-\left(\frac{z_{0}}{t_{1}}\right)^{n+1}}{t_{1}-z_{0}} + t_{1}^{n+1} \frac{1-\left(\frac{z_{0}t_{0}}{t_{1}}\right)^{n+1}}{t_{1}-z_{0}t_{0}} \right]. \quad (A.1)$$

After making the corresponding calculations to sum the four rational expressions in the bracket, (A.1) becomes

$$\frac{1}{1-t_0} \frac{1}{1-t_1} \frac{Dt_0^{n+1} + Et_0^2 + Ft_0 + G}{(1-z_0)(1-z_0t_0)(t_1-z_0)(t_1-z_0t_0)},$$

with

$$\begin{split} D &= z_0^{n+2} - z_0^{n+3} - t_1 z_0^{n+1} + t_1^2 z_0^{n+1} - t_1^2 z_0^{n+2} + t_1 z_0^{n+3}, \\ E &= t_1 z_0^2 - z_0^3 - t_1 z_0^{n+3} + z_0^3 t_1^{n+1} + z_0^{n+3} - z_0^2 t_1^{n+1}, \\ F &= -z_0 t_1^2 + z_0^3 + t_1^2 z_0^{n+2} + z_0 t_1^{n+1} - z_0^{n+2} - z_0^3 t_1^{n+1}, \\ G &= -t_1^2 z_0^{n+1} + z_0 t_1^2 - z_0^2 t_1 - z_0 t_1^{n+1} + z_0^2 t_1^{n+1}. \end{split}$$

Notice that D + E + F + G = 0 since it is clear that the term in brackets in (A.1) vanishes when $t_0 = 1$. This implies that (A.1) can also be written as

$$\frac{1}{t_1-1}\frac{Dt_0^n+\cdots+Dt_0^2+(D+E)t_0+(D+E+F)}{(1-z_0)(1-z_0t_0)(t_1-z_0)(t_1-z_0t_0)},$$

or equivalently, in terms of t_1 .

$$\frac{1}{t_1 - 1} \frac{Ht_1^{n+1} + It_1^2 + Jt_1 + K}{(1 - z_0)(1 - z_0t_0)(t_1 - z_0)(t_1 - z_0t_0)},$$

with

$$\begin{split} H &= z_0^3 t_0 - z_0^2 t_0 + z_0 - z_0^2, \\ I &= (z_0^{n+1} - z_0^{n+2}) \bigg(\sum_{l=1}^n t_0^l \bigg) + z_0^{n+1} - z_0, \\ J &= (z_0^{n+3} - z_0^{n+1}) \bigg(\sum_{l=2}^n t_0^l \bigg) + (z_0^2 - z_0^{n+1}) (t_0 + 1), \\ K &= (z_0^{n+2} - z_0^{n+3}) \bigg(\sum_{l=2}^n t_0^l \bigg) + (z_0^{n+2} - z_0^3) t_0. \end{split}$$

Notice that now H + I + J + K = 0 since it is again clear that the term in brackets in (A.1) vanishes when $t_1 = 1$. This implies that (A.1) can also be written as

$$\frac{H(\sum_{l=0}^{n} t_1^l) + I(t_1+1) + J}{(1-z_0)(1-z_0t_0)(t_1-z_0)(t_1-z_0t_0)}.$$
(A.2)

From here, as the denominator is far from zero for the considered values of z_0, t_0, t_1 , and taking into account the expressions for H, I, J, the result follows for r = 1 and $t_0, t_1 \neq 1$. On the other hand, for $t_0 = 1$ and $t_1 = 1$ the result comes from applying Gosper's algorithm [8, 15] to find closed forms for hypergeometric identities, and can be seen to be the same as (A.2) substituting t_0 and t_1 by 1.

It is quite straightforward except for extremely tedious expressions that the result can be proved for general r once it is assumed for r-1 and r=1.

From this lemma and for simplicity, we will show here the proof for the most unfavourable case in which all the roots of $\rho_{\epsilon}(z)$ have unit modulus. Notice that, by a Schur decomposition [9], the matrix $R(\epsilon)$ is unitary equivalent to

$$T(\epsilon) = \begin{pmatrix} T_{11}(\epsilon) & T_{12}(\epsilon) & \dots & T_{1k}(\epsilon) \\ 0 & T_{22}(\epsilon) & \dots & T_{2k}(\epsilon) \\ \vdots & & \ddots & \\ 0 & 0 & \dots & T_{kk}(\epsilon) \end{pmatrix},$$

where each $T_{jl}(\epsilon)$ is a 2 × 2-matrix and

$$T_{jj}(\epsilon) = \begin{pmatrix} e^{i\theta_{j,1}(\epsilon)} & a_j(\epsilon) \\ 0 & e^{i\theta_{j,2}(\epsilon)} \end{pmatrix},$$

with $e^{i\theta_{j,1}(\epsilon)}$ and $e^{i\theta_{j,2}(\epsilon)}$ $(j=1,\ldots,k)$ the eigenvalues of $R(\epsilon)$, for which we can assume that $e^{i\theta_{j,1}(\epsilon)}$ and $e^{i\theta_{j,2}(\epsilon)}$ may be close to each other but $e^{i\theta_{j,m}(\epsilon)}$ (m=1,2) are always well apart from $e^{i\theta_{k,r}(\epsilon)}$ (r=1,2) whenever $j \neq k$. Notice that

$$||R(\epsilon)|| \le \sqrt{||R(\epsilon)||_1 \cdot ||R(\epsilon)||_{\infty}},\tag{A.3}$$

and therefore, using hypothesis (i), $||R(\epsilon)||$ is uniformly bounded on ϵ . On the other hand, it always happens that

$$||R^n(\epsilon)|| = ||T^n(\epsilon)||, \tag{A.4}$$

and, by using the notation,

$$T^{n}(\epsilon) = \begin{pmatrix} T_{11,n}(\epsilon) & T_{12,n}(\epsilon) & \dots & T_{1k,n}(\epsilon) \\ 0 & T_{22,n}(\epsilon) & \dots & T_{2k,n}(\epsilon) \\ \vdots & & \ddots & \\ 0 & 0 & \dots & T_{kk,n}(\epsilon) \end{pmatrix},$$

it can be inductively proved that

$$T_{jl,n} = \sum_{r=1}^{l-j} \sum_{j < j_1 < \dots < j_r = l} \sum_{\substack{e_0, \dots, e_r = 0 \\ e_0 + \dots + e_r = n - r}}^{n-r} T_{jj}^{e_0} T_{jj_1} T_{j_1j_1}^{e_1} T_{j_1j_2} T_{j_2j_2}^{e_2} \dots T_{j_rj_r}^{e_r}.$$
(A.5)

Our aim now is to bound the coefficients of these 2×2 -matrices and by using (A.3) applied to T^n and (A.4), we will get bound (2.2).

Notice that

$$T_{jj}^n(\epsilon) = \begin{pmatrix} e^{in\theta_{j,1}(\epsilon)} & a_j(\epsilon) \sum_{s=0}^{n-1} e^{i[s\theta_{j,1}(\epsilon) + (n-s)\theta_{j,2}(\epsilon)]} \\ 0 & e^{in\theta_{j,2}(\epsilon)} \end{pmatrix},$$

and then, using (A.5), we need to bound appropriately the most unfavourable terms, which are of the form

$$\sum_{\substack{e_0, \dots, e_r = 0 \\ e_0 + \dots + e_r = n - r}}^{n - r} e^{ie_0 \theta_{j,2}(\epsilon)} \left(\sum_{s=0}^{e_0 - 1} e^{is(\theta_{j,1}(\epsilon) - \theta_{j,2}(\epsilon))} \right) \dots e^{ie_r \theta_{j_r,2}(\epsilon)} \left(\sum_{s_r = 0}^{e_r - 1} e^{is_r(\theta_{j_r,1}(\epsilon) - \theta_{j_r,2}(\epsilon))} \right).$$
(A.6)

This can also be written as

$$\begin{split} \sum_{\substack{e_0, \dots, e_{r-1} = 0 \\ e_0 + \dots + e_{r-1} \le n - r}}^{n - r} e^{ie_0\theta_{j,2}(\epsilon)} \bigg(\sum_{s = 0}^{e_0 - 1} e^{is(\theta_{j,1}(\epsilon) - \theta_{j,2}(\epsilon))} \bigg) \dots \\ e^{ie_{r-1}\theta_{j_{r-1},2}(\epsilon)} \bigg(\sum_{s_{r-1} = 0}^{e_{r-1} - 1} e^{is_{r-1}(\theta_{j_{r-1},1}(\epsilon) - \theta_{j_{r-1},2}(\epsilon))} \bigg) \\ e^{i(n - r - e_0 - \dots - e_{r-1})\theta_{j_r,2}(\epsilon)} \bigg(\sum_{s_r = 0}^{n - r - e_0 - \dots - e_{r-1} - 1} e^{is_r(\theta_{j_r,1}(\epsilon) - \theta_{j_r,2}(\epsilon))} \bigg), \end{split}$$

which, except for the factor $e^{i(n-r)\theta_{j_r,2}(\epsilon)}$ (which is obviously bounded by 1), is equal to

$$\sum_{\substack{e_0, \dots, e_{r-1} = 0 \\ e_0 + \dots + e_{r-1} \leq n - r}}^{n-r} e^{ie_0(\theta_{j,2}(\epsilon) - \theta_{j_r,2}(\epsilon))} \dots e^{ie_{r-1}(\theta_{j_{r-1},2}(\epsilon) - \theta_{j_r,2}(\epsilon))} \left(\sum_{s=0}^{e_0 - 1} e^{is(\theta_{j,1}(\epsilon) - \theta_{j,2}(\epsilon))}\right) \\ \dots \left(\sum_{s_{r-1} = 0}^{e_{r-1} - 1} e^{is_{r-1}(\theta_{j_{r-1},1}(\epsilon) - \theta_{j_{r-1},2}(\epsilon))}\right) \left(\sum_{s_r = 0}^{n-r-e_0 - \dots - e_{r-1} - 1} e^{is_r(\theta_{j_r,1}(\epsilon) - \theta_{j_r,2}(\epsilon))}\right).$$

This summation corresponds to the result in Lemma A.1 for

$$z_{0} = e^{i(\theta_{j,2}(\epsilon) - \theta_{j_{r},2}(\epsilon))}, \quad z_{1} = e^{i(\theta_{j_{1},2}(\epsilon) - \theta_{j_{r},2}(\epsilon))}, \quad \cdots, \quad z_{r-1} = e^{i(\theta_{j_{r-1},2}(\epsilon) - \theta_{j_{r},2}(\epsilon))},$$

$$t_{0} = e^{i(\theta_{j,1}(\epsilon) - \theta_{j,2}(\epsilon))}, \quad t_{1} = e^{i(\theta_{j_{1},1}(\epsilon) - \theta_{j_{1},2}(\epsilon))}, \quad \cdots, \quad t_{r} = e^{i(\theta_{j_{r},1}(\epsilon) - \theta_{j_{r},2}(\epsilon))},$$

where z_0, \ldots, z_{r-1} are clearly far from 1 but t_0, \ldots, t_r can be as closer as we want to 1. Notice also that $z_0, \ldots, z_{r-1}, t_0, \ldots, t_r$ are continuous and periodic functions on ϵ and therefore, taking also (iii) into account, when applying the result on Lemma A.1, the constant which appears in Landau notation there can be bounded independently of ϵ .

Let us assume now that ϵ is far enough from the values of ϵ_l which lead to double roots of $\rho_{\epsilon}(z)$ so that $|1 - e^{i(\theta_{j,1}(\epsilon) - \theta_{j,2}(\epsilon))}|$ and $|1 - e^{i(\theta_{j_m,1}(\epsilon) - \theta_{j_m,2}(\epsilon))}|$ (m = 1, ..., r) are always bigger than a certain quantity δ . (Because of hypotheses (i) and (iii) this will happen whenever $|\epsilon - \epsilon_l| > \eta$ for some positive value η .) Then, the previous sum can be written as

$$\sum_{\substack{e_0, \dots, e_{r-1} = 0 \\ e_0 + \dots + e_{r-1} \le n - r}} e^{ie_0(\theta_{j,2}(\epsilon) - \theta_{j_r,2}(\epsilon))} \dots e^{ie_{r-1}(\theta_{j_{r-1},2}(\epsilon) - \theta_{j_r,2}(\epsilon))} \\ \frac{1 - e^{ie_0(\theta_{j,1}(\epsilon) - \theta_{j,2}(\epsilon))}}{1 - e^{i(\theta_{j,1}(\epsilon) - \theta_{j,2}(\epsilon))}} \dots \frac{1 - e^{ie_{r-1}(\theta_{j_{r-1},1}(\epsilon) - \theta_{j_{r-1},2}(\epsilon))}}{1 - e^{i(\theta_{j_{r-1},1}(\epsilon) - \theta_{j_{r-1},2}(\epsilon))}} \frac{1 - e^{i(n-r-e_0 - \dots - e_{r-1})(\theta_{j_r,1}(\epsilon) - \theta_{j_r,2}(\epsilon))}}{1 - e^{i(\theta_{j_r,1}(\epsilon) - \theta_{j_r,2}(\epsilon))}},$$

which, except for a factor which can be bounded independently of ϵ and n, is a sum of 2^{r+1} terms of the following form

$$\sum_{\substack{e_0, \dots, e_{r-1} = 0 \\ e_0 + \dots + e_{r-1} \le n - r}}^{n-r} e^{ie_0(\theta_{j,m}(\epsilon) - \theta_{j_r,m_r}(\epsilon))} \dots e^{ie_{r-1}(\theta_{j_{r-1},m_{r-1}}(\epsilon) - \theta_{j_r,m_r}(\epsilon))}, \tag{A.7}$$

where $m, m_1, \ldots, m_{r-1}, m_r$ will take the values 1 or 2. Then, this term can also be written like

$$\sum_{\substack{e_0, \dots, e_{r-2} = 0 \\ e_0 + \dots + e_{r-2} \le n - r}}^{n-r} e^{ie_0(\theta_{j,m}(\epsilon) - \theta_{j_r,m_r}(\epsilon))} \dots e^{ie_{r-2}(\theta_{j_{r-2},m_{r-2}}(\epsilon) - \theta_{j_r,m_r}(\epsilon))}$$

$$\sum_{\substack{e_{r-1} = 0}}^{n-r} e^{ie_{r-1}(\theta_{j_{r-1},m_{r-1}}(\epsilon) - \theta_{j_r,m_r}(\epsilon))}$$

$$= \sum_{\substack{e_0, \dots, e_{r-2} = 0 \\ e_0 + \dots + e_{r-2} \le n - r}}^{n-r} e^{ie_0(\theta_{j,m}(\epsilon) - \theta_{j_r,m_r}(\epsilon))} \dots e^{ie_{r-2}(\theta_{j_{r-2},m_{r-2}}(\epsilon) - \theta_{j_r,m_r}(\epsilon))}$$

$$\frac{1 - e^{i(n-r-e_0 - \dots - e_{r-2} + 1)(\theta_{j_{r-1},m_{r-1}}(\epsilon) - \theta_{j_r,m_r}(\epsilon))}}{1 - e^{i(\theta_{j_{r-1},m_{r-1}}(\epsilon) - \theta_{j_r,m_r}(\epsilon))}},$$

which can be expressed (except for a factor which is bounded independently of ϵ and n) as a sum of two terms of the following form

of two terms of the following form
$$\sum_{\substack{e_0,\ldots,e_{r-2}=0\\e_0+\cdots+e_{r-2}< n-r}}^{n-r} e^{ie_0(\theta_{j,m}(\epsilon)-\theta_{j_s,m_s}(\epsilon))} \ldots e^{ie_{r-2}(\theta_{j_{r-2},m_{r-2}}(\epsilon)-\theta_{j_s,m_s}(\epsilon))}, \quad s=r,r-1.$$

By proceeding inductively, (A.7) and therefore (A.6) can be finally written like a number (dependent of r) of terms of the following form (except for a factor which does not depend on n either on ϵ):

$$\sum_{e_0=0}^{n-r} e^{ie_0(\theta_{j,m}(\epsilon)-\theta_{j_s,m_s}(\epsilon))} = \frac{1-e^{i(n-r+1)(\theta_{j,m}(\epsilon)-\theta_{j_s,m_s}(\epsilon))}}{1-e^{i(\theta_{j,m}(\epsilon)-\theta_{j_s,m_s}(\epsilon))}}, \quad s=1,\ldots,r,$$

and each of these terms is obviously bounded.

B. Proof of Theorem 3.1

In such a case, situation (d) of Lemma 6.2 in [3] applies. Therefore, the perturbed roots satisfy that either both have modulus one and are conjugate to each other or both are real and inverse to each other. To deduce which case applies, we will consider Taylor series expansion (3.2).

Notice that the assumptions on $\rho_{\epsilon}(z)$ imply that

$$\rho_{\epsilon}(z) = \prod_{l=1}^{k} (z - e^{i\theta_{l}(\epsilon)})(z - e^{-i\theta_{l}(\epsilon)})$$

$$= \prod_{l=1}^{k} (z^{2} - 2\cos(\theta_{l}(\epsilon))z + 1), \tag{B.1}$$

for some real functions $\theta_l(\epsilon)$ (l = 1, ..., k) which are twice differentiable on ϵ at $\epsilon = \epsilon_l$. First notice that, according to (B.1),

$$\frac{d}{d\epsilon}\rho_{\epsilon}(z) = \sum_{r=1}^{k} 2\sin(\theta_{r}(\epsilon))\theta'_{r}(\epsilon)z\Pi^{k}_{\substack{j=1\\j\neq r}} (z^{2} - 2\cos(\theta_{j}(\epsilon))z + 1). \tag{B.2}$$

Now, as $\rho_{\epsilon_l}(\pm 1) = 0$, for some $\tilde{r} \in \{1, \dots, k\}$ it happens that $\cos(\theta_{\tilde{r}}(\epsilon_l)) = \pm 1$. Then, it is easy to deduce from (B.2) that

$$\frac{d}{d\epsilon}\rho_{\epsilon}(\pm 1)|_{\epsilon=\epsilon_l}=0.$$

Now, differentiating (B.2) again with respect to ϵ and with respect to z and evaluating at $\epsilon = \epsilon_l$, $z = \pm 1$, leads to

$$\frac{d^2}{d\epsilon^2} \rho_{\epsilon}(\pm 1)|_{\epsilon=\epsilon_l} = 2^k (\theta'_{\tilde{r}}(\epsilon_l))^2 \prod_{\substack{j=1\\j\neq \tilde{r}}}^k \left(1 \mp \cos(\theta_j(\epsilon_l))\right) > 0, \qquad \frac{d}{d\epsilon} \rho'_{\epsilon}(\pm 1)|_{\epsilon=\epsilon_l} = 0.$$

On the other hand, differentiating now (B.1) just with respect to z,

$$\rho'_{\epsilon}(z) = \sum_{r=1}^{k} (2z - 2\cos(\theta_r(\epsilon))) \prod_{\substack{j=1 \ j \neq r}}^{k} \left(z^2 - 2\cos(\theta_j(\epsilon))z + 1\right),$$

which evaluated at $z=\pm 1, \epsilon=\epsilon_l$ vanishes by similar arguments. Differentiating again, it can be deduced that

$$\rho_{\epsilon_l}''(\pm 1) = 2^k \prod_{\substack{j=1\\j \neq \bar{r}}}^k \left(1 \mp \cos(\theta_j(\epsilon_l)) \right) > 0.$$

From here, in case (i), and by considering (3.2), in first approximation $r^2 < 0$, so r is purely imaginary, from what the perturbed corresponding roots lie on the unit circle.

In case (ii), if $\sigma_{\epsilon_l}(\pm 1) < 0$ notice that in first approximation

$$r^2 = -\frac{2}{\rho_{\epsilon_l}''(\pm 1)} \left(h^2 \sigma_{\epsilon_l}(\pm 1) + \frac{\eta^2}{2} \frac{d^2}{d\epsilon^2} \rho_{\epsilon}(\pm 1)|_{\epsilon = \epsilon_l} \right),$$

and therefore for $|\eta|^2 < 2h^2\sigma_{\epsilon_l}(\pm 1)/\frac{d^2}{d\epsilon^2}\rho_{\epsilon}(\pm 1)|_{\epsilon=\epsilon_l}$, $r^2 > 0$ and therefore the two perturbed roots are real and one of them of modulus greater than 1.

C. Proof of Theorem 3.2

To prove (i), notice that

$$\sigma_{\epsilon}(z) = \gamma_1(\epsilon)z^{2k-1} + \dots + \gamma_{k-1}(\epsilon)z^{k+1} + \gamma_k(\epsilon)z^k + \gamma_{k-1}(\epsilon)z^{k-1} + \dots + \gamma_1(\epsilon)z^{k-1}$$

can also be written as

$$\sigma_{\epsilon}(z) = z^{k} \left(\gamma_{1}(\epsilon)(z^{k-1} + z^{1-k}) + \dots + \gamma_{k-1}(\epsilon)(z + z^{-1}) + \gamma_{k}(\epsilon) \right), \tag{C.1}$$

for which the bracket when evaluated at \tilde{z} is real because $\tilde{z} = \tilde{z}^{-1}$. On the other hand, by proceeding in a similar manner, just taking into account that $\rho_{\epsilon}(z)$ is also symmetric, it can be proved that

$$\frac{z\frac{d}{dz}(z\rho'_{\epsilon}(z))}{z^k}|_{z=\tilde{z}}$$

is real.

Now, taking into account that \tilde{z} is a double root of $\rho_{\epsilon_l}(z)$,

$$z\frac{d}{dz}(z\rho_{\epsilon}'(z))\bigg|_{\substack{z=\tilde{z}\\\epsilon=\epsilon_{l}}}=z\left[\rho_{\epsilon}'(z)+z\rho_{\epsilon}''(z)\right]_{\substack{z=\tilde{z}\\\epsilon=\epsilon_{l}}}=\tilde{z}^{2}\rho_{\epsilon_{l}}''(\tilde{z}),$$

from what (i) follows. Now, in order to prove (ii-iii), let us consider the notation $\tilde{z} = e^{i\theta_{\tilde{r}}(\epsilon_l)}$. Then, as

$$\begin{split} \rho_{\epsilon}(z) &= (z - e^{i\theta_{\bar{r}}(\epsilon)})^2 (z - e^{-i\theta_{\bar{r}}(\epsilon)})^2 \prod_{\substack{l=1\\l\neq\bar{r}}}^k (z - e^{i\theta_l(\epsilon)}) (z - e^{-i\theta_l(\epsilon)}), \\ \frac{d}{d\epsilon} \rho_{\epsilon}(z) &= -2i\theta'_{\bar{r}}(\epsilon) e^{i\theta_{\bar{r}}(\epsilon)} (z - e^{i\theta_{\bar{r}}(\epsilon)}) (z - e^{-i\theta_{\bar{r}}(\epsilon)})^2 \prod_{\substack{l=1\\l\neq\bar{r}}}^k (z - e^{i\theta_l(\epsilon)}) (z - e^{-i\theta_l(\epsilon)}) \\ &+ 2i\theta'_{\bar{r}}(\epsilon) e^{-i\theta_{\bar{r}}(\epsilon)} (z - e^{i\theta_{\bar{r}}(\epsilon)})^2 (z - e^{-i\theta_{\bar{r}}(\epsilon)}) \prod_{\substack{l=1\\l\neq\bar{r}}}^k (z - e^{i\theta_l(\epsilon)}) (z - e^{-i\theta_l(\epsilon)}) \\ &+ (z - e^{i\theta_{\bar{r}}(\epsilon)})^2 (z - e^{-i\theta_{\bar{r}}(\epsilon)})^2 \sum_{\substack{l=1\\l\neq\bar{r}}}^k \left(-i\theta'_l(\epsilon) e^{i\theta_l(\epsilon)} (z - e^{-i\theta_l(\epsilon)}) \right) \\ &+ i\theta'_l(\epsilon) e^{-i\theta_l(\epsilon)} (z - e^{i\theta_l(\epsilon)}) \right) \cdot \prod_{\substack{r=1\\r\neq\bar{r}\\r\neq\bar{r}\\r\neq l}}^k (z - e^{i\theta_l(\epsilon)}) (z - e^{-i\theta_l(\epsilon)}), \end{split}$$

from what clearly $\frac{d}{d\epsilon}\rho_{\epsilon}(\tilde{z})|_{\epsilon=\epsilon_l}=0$. Then,

$$\frac{d^{2}}{d\epsilon^{2}}\rho_{\epsilon}(\tilde{z})\Big|_{\epsilon=\epsilon_{l}} = -8e^{2i\theta_{\tilde{r}}(\epsilon_{l})}(\theta'_{\tilde{r}}(\epsilon))^{2}\cos^{2}(\theta_{\tilde{r}}(\epsilon_{l})) \prod_{\substack{l=1\\l\neq\tilde{r}}}^{k} (e^{i\theta_{\tilde{r}}(\epsilon_{l})} - e^{i\theta_{l}(\epsilon_{l})})(e^{i\theta_{\tilde{r}}(\epsilon_{l})} - e^{-i\theta_{l}(\epsilon_{l})}),$$

$$\frac{d^{2}}{d\epsilon dz}\rho_{\epsilon}(z)\Big|_{\substack{\epsilon=\epsilon_{l}\\z=\tilde{z}}} = -8ie^{i\theta_{\tilde{r}}(\epsilon_{l})}\theta'_{\tilde{r}}(\epsilon_{l})\cos^{2}(\theta_{\tilde{r}}(\epsilon_{l})) \prod_{\substack{l=1\\l\neq\tilde{r}}}^{k} (e^{i\theta_{\tilde{r}}(\epsilon_{l})} - e^{i\theta_{l}(\epsilon_{l})})(e^{i\theta_{\tilde{r}}(\epsilon_{l})} - e^{-i\theta_{l}(\epsilon_{l})}),$$

$$\frac{d^{2}}{dz^{2}}\rho_{\epsilon}(z)\Big|_{\substack{\epsilon=\epsilon_{l}\\z=\tilde{z}}} = 8\cos^{2}(\theta_{\tilde{r}}(\epsilon_{l})) \prod_{\substack{l=1\\l\neq\tilde{r}}}^{k} (e^{i\theta_{\tilde{r}}(\epsilon_{l})} - e^{i\theta_{l}(\epsilon_{l})})(e^{i\theta_{\tilde{r}}(\epsilon_{l})} - e^{-i\theta_{l}(\epsilon_{l})}).$$

Inserting all this in (3.2) it follows that in first approximation

$$[-\tilde{z}^2(\theta_{\tilde{x}}'(\epsilon_l))^2\eta^2 - 2i\tilde{z}\theta_{\tilde{x}}'(\epsilon_l)\eta r + r^2]\rho_{\epsilon_l}''(\tilde{z}) + 2h^2\sigma_{\epsilon_l}(\tilde{z}) = 0.$$

Then, let us denote by C to $\sigma_{\epsilon_l}(\tilde{z})/\tilde{z}^2\rho_{\epsilon_l}''(\tilde{z})$, which is real because of (i). If C>0,

$$r = \frac{1}{2} \left(2i\tilde{z}\theta_{\tilde{r}}'(\epsilon_l)\eta \pm \sqrt{-4\tilde{z}^2(\theta_{\tilde{r}}'(\epsilon_l))^2\eta^2 - 4\tilde{z}^2(-(\theta_{\tilde{r}}'(\epsilon_l))^2\eta^2 + 2Ch^2)} \right)$$
$$= i\tilde{z}(\eta\theta_{\tilde{r}}'(\epsilon_l) \pm h\sqrt{2C}),$$

so the perturbations of the double root are orthogonal to the root \tilde{z} in first approximation. This means that both perturbations lie on the unit circle because if that did not happen, according to part (c) of Lemma 6.2 of [3] or Lemma 3.2 here, one of the roots should be the inverse conjugate of the other and therefore if one had modulus greater than 1, the other should have modulus less than 1, which is in contradiction with the fact that the perturbation is tangent to the circumference in the point where \tilde{z} lies.

In case

$$\sigma_{\epsilon_l}(\tilde{z}) = \frac{d}{d\epsilon} \sigma_{\epsilon}(\tilde{z})|_{\epsilon = \epsilon_l} = \sigma'_{\epsilon_l}(\tilde{z}) = 0,$$

in first approximation $r = i\tilde{z}\theta_{\tilde{r}}'(\epsilon_l)\eta$ and the conclusions would be the same.

In case C < 0, $r = \tilde{z}(i\theta'_{\tilde{r}}(\epsilon_l)\eta \mp h\sqrt{-2C})$ and therefore when h does not vanish, one of the perturbations will lie outside the unit circle.

Acknowledgements. This research was supported by MTM 2011-23417.

References

- [1] M.L. Buchanon, A necessary and sufficient condition for stability of difference shemes for initial value problems, SIAM J. Appl. Math., 11 (1963), 919-935.
- [2] B. Cano, Conservation of invariants by symmetric multistep cosine methods, in press in *BIT Numer. Math.*.
- [3] B. Cano and M.J. Moreta, Multistep cosine methods for second-order partial differential equations, *IMA J. Numer. Anal.*, **30** (2010), 431-461.
- [4] B. Cano and J.M. Sanz-Serna, Error growth in the numerical integration of periodic orbits by multistep methods, with application to reversible systems, IMA J. Numer. Anal., 18 (1998), 57-75.
- [5] D. Cohen, E. Hairer and C. Lubich, Numerical energy conservation for multi-frequency oscillatory differential equations, *BIT Numer. Math.*, **45** (2005), 287-305.
- [6] D. Cohen, E. Hairer and C. Lubich, Conservation of energy, momentum and actions in numerical discretizations of non-linear wave equations, *Numer. Math.*, 110 (2008), 113-143.
- [7] G.H. Golub and C.F. Van Loan, Matrix Computations (Second Edition), The Johns Hopkins University Press, Baltimore and London, 1990.
- [8] R.W. Gosper, Decision procedure for indefinite hypergeometric summation, *Proc. Nat. Acad. Sci. USA*, **75** (1978), 40-42.
- [9] V. Grimm, A note on the Gautschi-type method for oscillatory differential equations, *Numer. Math.*, **102** (2005), 61-66.
- [10] V. Grimm and M. Hochbruck, Error analysis of exponential integrators for oscillatory second-order differential equations, *J. Phys. A: Math. Gen.*, **39** (2006), 5495-5507.
- [11] E. Hairer, S. Norsett and G. Wanner, Solving Ordinary Differential Equations I, Second Revised Edition, Springer-Verlag, 2000.
- [12] E. Hairer, S. Norsett and G. Wanner, Geometric Numerical Integration, Second Edition, Springer-Verlag, 2006.
- [13] M. Hochbruch and C. Lubich, A Gautschi-type method for oscillatory second-order differential equations, *Numer. Math.*, **83** (1999), 403-426.
- [14] P. Lancaster and M. Tismenetsky, The Theory of Matrices, Second Edition with Applications, Academic Press, London, 1985.
- [15] E.W. Weisstein, Gosper's algorithm, from MathWorld-A Wolfram Web Resource, http://mathworld.wolfram.com/GospersAlgorithm.html.