BACKWARD DIFFERENCE FORMULAE: NEW MULTIPLIERS AND STABILITY PROPERTIES FOR PARABOLIC EQUATIONS

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Abstract. We determine new, more favourable, and in a sense optimal, multipliers for the three- and five-step backward difference formula (BDF) methods. We apply the new multipliers to establish stability of these methods as well as of their implicit–explicit counterparts for parabolic equations by energy techniques, under milder conditions than the ones recently imposed in [4, 1].

1. Introduction

The aims of this paper are twofold: the determination of multipliers for the three- and five-step BDF methods that are more favourable than the Nevanlinna–Odeh multipliers, and their use in the derivation of stability estimates for parabolic equations under relaxed stability conditions.

We first recall the multiplier concept of Nevanlinna and Odeh as well as their multipliers for BDF methods of order up to five. We determine new, more favourable, and in a sense optimal, multipliers for the three- and five-step BDF methods, and show that the Nevanlinna–Odeh multiplier for the four-step BDF method is optimal.

Then, we consider initial value problems for two abstract parabolic equations, one linear and one possibly nonlinear, and discuss their discretization in time by BDF methods and by implicit–explicit BDF methods, respectively. We give necessary conditions for the stability of these methods as well as known and new sufficient stability conditions; stability is established by the energy technique, and the advantage of the new multipliers is that they lead to relaxed sufficient stability conditions.

1.1. **Multipliers for BDF methods.** We consider the $q-$step BDF method (α, β), described by the polynomials α and β,

$$\alpha(\zeta) = \sum_{j=1}^{q} \frac{1}{j}\zeta^{q-j}(\zeta-1)^j = \sum_{j=0}^{q} \alpha_j \zeta^j, \quad \beta(\zeta) = \zeta^q. \tag{1.1}$$

The BDF methods are $A-$stable for $q = 1$ and $q = 2$, i.e., $A(\vartheta_q)-$stable with $\vartheta_1 = \vartheta_2 = 90°$, and $A(\vartheta_q)-$stable for $q = 3, \dots, 6$ with $\vartheta_3 = 86.03°$, $\vartheta_4 = 73.35°$, $\vartheta_5 = 51.84°$ and $\vartheta_6 = 17.84°$; see [10, Section V.2]. Their order is q.

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A set of real numbers $(\mu_1,\dots,\mu_q)$ is called *multiplier* for the $q-$step BDF method, if, with $\tilde\mu(\zeta):=1-\mu_1\zeta^{-1}-\dots-\mu_q\zeta^{-q}$, there holds

$$\operatorname{Re}\frac{\alpha(\zeta)}{\tilde\mu(\zeta)\beta(\zeta)}>0\quad\forall\zeta\in\mathbb{C},|\zeta|>1,$$

i.e., if

$$\operatorname{Re}\frac{\alpha(\zeta)}{\mu(\zeta)}>0\quad\forall\zeta\in\mathbb{C},|\zeta|>1, \tag{1.2}$$

with $\mu(\zeta):=\tilde\mu(\zeta)\beta(\zeta)=\zeta^q-\mu_1\zeta^{q-1}-\dots-\mu_q$, and, in addition, the polynomials α and μ have no common divisor; consequently, the $q-$step scheme described by the parameters $\alpha_q,\dots,\alpha_0,1,-\mu_1,\dots,-\mu_q$ is $A-$stable. The motivation for this definition is the equivalence between the $A-$stability of this scheme and the $G-$stability of the corresponding one-leg method.

The concept of multipliers for multistep methods was introduced by Nevanlinna and Odeh; see [12]. In [12] the multipliers $(\eta_q,0,\dots,0)$ for the $q-$step BDF methods, with

$$\eta_1=\eta_2=0,\quad \eta_3=0.0836,\quad \eta_4=0.2878,\quad \eta_5=0.8160, \tag{1.3}$$

were also determined; these multipliers are optimal among the multipliers with vanishing $\mu_2,\dots,\mu_q$, in the sense that η_q cannot be replaced by a smaller number.

In this paper, we show that

$$\mu_1=\frac{2}{169},\quad \mu_2=\frac{11}{169},\quad \mu_3=0, \tag{1.4}$$

$$\mu_1=\eta_4,\quad \mu_2=\mu_3=\mu_4=0, \tag{1.5}$$

and

$$\mu_1=0.7321818449,\quad \mu_4=0.07755190105,\quad \mu_2=\mu_3=\mu_5=0, \tag{1.6}$$

are also multipliers for the three-, four- and five-step BDF methods, respectively, which are optimal among the multipliers $(\mu_1,\dots,\mu_q)$, in the sense that they are the only multipliers for which the sum $\hat\eta_q:=|\mu_1|+\dots+|\mu_q|$ of the absolute values of $\mu_1,\dots,\mu_q$ attains its minimal value. While $\hat\eta_4=\eta_4$, the new multipliers for the three- and five-step BDF methods are more favourable than the corresponding Nevanlinna–Odeh multipliers, since

$$\hat\eta_3=\frac{1}{13}=0.076923076<\eta_3=0.0836\quad\text{and}\quad \hat\eta_5=0.8097337459<\eta_5=0.8160.$$

The improvement for the five-step BDF method is only minor, while for the three-step BDF method it is rather considerable.

A straightforward application of Dahlquist's G-stability theory ensures then existence of a positive definite symmetric matrix $G=(g_{ij})_{i,j=1,\dots,q}$ and reals $\delta_0,\dots,\delta_q$ such that for $v^0,\dots,v^q$ in an inner product space, with inner product $(\cdot,\cdot)$ and corresponding norm $|\cdot|$, there holds

$$\operatorname{Re}\Big(\sum_{i=0}^q\alpha_iv^i,v^q-\sum_{j=1}^q\mu_jv^{q-j}\Big)=\sum_{i,j=1}^q g_{ij}(v^i,v^j)-\sum_{i,j=1}^q g_{ij}(v^{i-1},v^{j-1})+\Big|\sum_{i=0}^q\delta_iv^i\Big|^2. \tag{1.7}$$

Indeed, following the Baiocchi–Crouzeix approach [7], see also [10, Section V.6], we explicitly determine the matrix G and the constants $\delta_0, \dots, \delta_3$ for the three-step BDF method; see Lemma 2.3.

Identity (1.7) plays a key role in our stability analysis of the $q-$step BDF and the implicit–explicit $q-$step BDF methods, $q = 3, 5$, for parabolic equations; it leads to slightly relaxed stability conditions compared to the ones recently imposed in [4, 1].

The Nevanlinna–Odeh multipliers were for the first time used in the analysis of BDF methods for parabolic equations in [11].

1.2. **Abstract parabolic equations and time-stepping methods.** Let $T > 0, u^0 \in H$, and consider two abstract initial value problems, one for a linear parabolic equation,

$$\begin{cases} u'(t) + A(t)u(t) = 0, \quad 0 < t < T, \\ u(0) = u^0, \end{cases} \tag{1.8}$$

and one for a possibly nonlinear parabolic equation,

$$\begin{cases} u'(t) + A(t)u(t) = B(t, u(t)), \quad 0 < t < T, \\ u(0) = u^0, \end{cases} \tag{1.9}$$

in a usual triplet of separable complex Hilbert spaces $V \subset H = H' \subset V'$, with V densely and continuously embedded in H. Here $A(t) : V \to V'$ are linear operators, while the operators $B(t, \cdot) : V \to V'$ may be nonlinear. We denote by $(\cdot, \cdot)$ both the inner product in H and the antiduality pairing between V' and V, and by $|\cdot|$ and $\|\cdot\|$ the norms in H and V, respectively. The space V' may be considered the completion of H with respect to the dual norm $\|\cdot\|_\star$,

$$\forall v \in V' \quad \|v\|_\star := \sup_{w \in V \setminus \{0\}} \frac{|(v, w)|}{\|w\|} = \sup_{\substack{w \in V \\ \|w\|=1}} |(v, w)|.$$

Besides the $q-$step BDF method (α, β) we consider also the explicit $q-$step method (α, γ) described by the polynomials α and γ with

$$\gamma(\zeta) = \zeta^q - (\zeta - 1)^q = \sum_{i=0}^{q-1} \gamma_i \zeta^i. \tag{1.10}$$

The scheme (α, γ) is the unique explicit $q-$step method of order q; the order of all other explicit $q-$step schemes $(\alpha, \tilde{\gamma})$ is at most $q - 1$.

Let $N \in \mathbb{N}, N \geq q$, and consider a uniform partition $t^n := nk, n = 0, \dots, N$, of the interval $[0, T]$, with time step $k := T/N$. Assuming we are given starting approximations $U^0, \dots, U^{q-1} \in V$, we discretize (1.8) in time by the $q-$step BDF method, i.e., we define approximations $U^m \in V$ to the nodal values $u^m := u(t^m)$ of the exact solution as follows:

$$\sum_{i=0}^{q} \alpha_i U^{n+i} + kA(t^{n+q})U^{n+q} = 0, \tag{1.11}$$

$n = 0, \dots, N-q$. With the same notation, we discretize (1.9) in time by the implicit–explicit $q-$step BDF method,

$$\sum_{i=0}^{q} \alpha_i U^{n+i} + kA(t^{n+q})U^{n+q} = k \sum_{i=0}^{q-1} \gamma_i B(t^{n+i}, U^{n+i}), \tag{1.12}$$

$n = 0, \dots, N-q$. The unknown U^{n+q} appears only on the left-hand side of (1.12); therefore, to advance in time, we only need to solve one linear equation, which reduces to a linear system if we discretize also in space, at each time level.

Implicit–explicit multistep methods, for linear parabolic equations, were introduced and analyzed in [8]; such methods for nonlinear parabolic equations are studied, e.g., in [2] and [1].

Natural conditions for the parabolicity of the abstract equation in (1.8) are *coercivity* and *boundedness* of the operators $A(t) : V \to V'$, i.e.,

$$\text{Re}(A(t)v, v) \ge \kappa(t)\|v\|^2 \quad \forall v \in V \tag{1.13}$$

and

$$\|A(t)v\|_\star \le \nu(t)\|v\| \quad \forall v \in V, \tag{1.14}$$

respectively, with two smooth positive functions $\kappa, \nu : [0, T] \to \mathbb{R}$.

In the stability analysis of the implicit–explicit scheme (1.12) we assume, in addition, that $B(t, \cdot)$ satisfies the following local Lipschitz condition in a ball $\mathscr{B}_{u(t)} := \{v \in V : \|v - u(t)\| \le 1\}$, centered at the value $u(t)$ of the solution u at time t, and, for simplicity, defined here in terms of the norm of V,

$$\|B(t, v) - B(t, \tilde{v})\|_\star \le \tilde{\lambda}(t)\|v - \tilde{v}\| + \tilde{\mu}|v - \tilde{v}| \quad \forall v, \tilde{v} \in \mathscr{B}_{u(t)}, \tag{1.15}$$

for all $t \in [0, T]$, with a smooth nonnegative function $\tilde{\lambda} : [0, T] \to \mathbb{R}$ and an arbitrary constant $\tilde{\mu}$.

Using (1.13) and (1.14), existence and uniqueness of the approximations $U^q, \dots, U^N$ can be easily established by the Lax–Milgram lemma.

1.3. **Stability conditions.**

1.3.1. *Necessary stability conditions.* Using the von Neumann stability criterion, it is easily seen that a necessary condition for the stability of the $q-$step BDF scheme (1.11), $q = 3, 5$, is

$$\frac{\nu(t)}{\kappa(t)} \le \frac{1}{\tilde{\eta}_3} = 14.45087 \quad \text{and} \quad \frac{\nu(t)}{\kappa(t)} \le \frac{1}{\tilde{\eta}_5} = 1.62892979, \tag{1.16}$$

for all $t \in [0, T]$, respectively, with $\tilde{\eta}_3 = \cos 86.03^\circ = 0.0692, \tilde{\eta}_5 = \cos 51.84^\circ = 0.6139$; see [1]. This result in combination with the stability result from [2] for the implicit-explicit $q-$step BDF scheme (1.12), $q = 3, 5$, in the case of a time-independent, positive definite self-adjoint operator A, shows that a necessary *linear* condition for the local stability of the implicit–explicit $q-$step BDF scheme (1.12), $q = 3, 5$, is

$$\tilde{\eta}_q \nu(t) + (2^q - 1)\tilde{\lambda}(t) < \kappa(t) \tag{1.17}$$

for all $t \in [0, T]$, in the sense that none of the coefficients $\tilde{\eta}_q$ and $2^q - 1$ can be replaced by a smaller one; see [1].

1.3.2. *Known sufficient stability conditions.* Stability of the $q-$step BDF scheme (1.11) as well as local stability of the implicit–explicit $q-$step BDF scheme (1.12), $q = 3, 5$, were recently established by energy techniques in [4, 1], based on the Nevanlinna–Odeh multipliers, under the sufficient stability conditions

$$\frac{\nu(t)}{\kappa(t)} < \frac{1}{\eta_3} = 11.9617 \quad \text{and} \quad \frac{\nu(t)}{\kappa(t)} < \frac{1}{\eta_5} = 1.2254902, \tag{1.18}$$

for all $t \in [0, T]$, for $q = 3$ and $q = 5$, respectively, and

$$\eta_q \nu(t) + (2^q - 1)(1 + \eta_q)\tilde{\lambda}(t) < \kappa(t), \tag{1.19}$$

for all $t \in [0, T]$, respectively, with $\eta_3 = 0.0836, \eta_5 = 0.8160$.

1.3.3. *New sufficient stability conditions.* Using the new multipliers (1.4) and (1.6) for the three- and five-step BDF methods, respectively, we relax here the sufficient stability conditions (1.18) and (1.19) to

$$\frac{\nu(t)}{\kappa(t)} < \frac{1}{\hat{\eta}_3} = 13 \quad \text{and} \quad \frac{\nu(t)}{\kappa(t)} < \frac{1}{\hat{\eta}_5} = 1.23497392, \tag{1.20}$$

for all $t \in [0, T]$, for $q = 3$ and $q = 5$, respectively, and

$$\hat{\eta}_q \nu(t) + (2^q - 1)(1 + \hat{\eta}_q)\tilde{\lambda}(t) < \kappa(t), \tag{1.21}$$

for all $t \in [0, T]$, respectively, with $\hat{\eta}_3 = 1/13 = 0.076923076, \hat{\eta}_5 = 0.8097337459$.

1.3.4. *An example.* Let $\varphi : [0, T] \to (-\frac{\pi}{2}, \frac{\pi}{2})$ be a smooth function and consider the initial value problem for the parabolic equation

$$u_t = -A(t)u = -\mathrm{e}^{\mathrm{i}\varphi(t)}\tilde{A}u = -\cos\varphi(t)\tilde{A}u - \mathrm{i}\sin\varphi(t)\tilde{A}u, \quad t \in (0, T], \tag{1.22}$$

with $\tilde{A} : V \to V'$ a positive definite self-adjoint bounded operator.

The most suitable norm in V is $\|v\| := |\tilde{A}^{1/2}v| = (\tilde{A}v, v)^{1/2}$ in this case. Then, the dual norm $\|\cdot\|_\star$ in V' is $\|v\|_\star = |\tilde{A}^{-1/2}v| = (v, \tilde{A}^{-1}v)^{1/2}$. Now, for $v \in V$, we have

$$(\mathrm{e}^{\mathrm{i}\varphi(t)}\tilde{A}v, v) = \cos\varphi(t)(\tilde{A}v, v) + \mathrm{i}\sin\varphi(t)(\tilde{A}v, v),$$

whence $\operatorname{Re}(\mathrm{e}^{\mathrm{i}\varphi(t)}\tilde{A}v, v) = (\cos\varphi(t))\|v\|^2$; we infer that $\kappa(t) = \cos\varphi(t)$. Furthermore, obviously,

$$\|\mathrm{e}^{\mathrm{i}\varphi(t)}\tilde{A}\|_{L(V,V')} = |\mathrm{e}^{\mathrm{i}\varphi(t)}|\,\|\tilde{A}\|_{L(V,V')} = \|\tilde{A}\|_{L(V,V')} = 1,$$

whence $\nu(t) = 1$. Therefore, $\lambda(t) = 1/\cos\varphi(t)$.

The eigenvalues of $\mathrm{e}^{\mathrm{i}\varphi(t)}\tilde{A}$ are of the form $r\mathrm{e}^{\mathrm{i}\varphi(t)}$, with a positive number r, i.e., they lie on the half-line in the complex plane starting at the origin and forming angle $\varphi(t)$ with the positive real half-axis. For $|\varphi(t)| > \vartheta_q$, for some $t \in [0, T]$, this half-line is not contained in the stability sector $S_{\vartheta_q} := \{z \in \mathbb{C} : z = r\mathrm{e}^{\mathrm{i}\varphi}, r \geq 0, |\varphi| \leq \vartheta_q\}$ of the $q-$step BDF method; thus, according to the von Neumann criterion, the $q-$step BDF method (1.11) is unstable for this equation; see the necessary stability condition (1.16).

As far as the sufficient stability conditions in the case of equation (1.22) are concerned, the new multipliers ensure stability of the three- and five-step BDF scheme (1.11), respectively, provided $\varphi(t)$ is such that $\cos\varphi(t) > \hat{\eta}_q$, for all $t \in [0, T]$, for $q = 3, 5$, respectively; see the new sufficient stability condition (1.20). On the other hand, the Nevanlinna–Odeh multipliers ensure stability of these methods under the more stringent condition $\cos\varphi(t) > \eta_q$, for all $t \in [0,T]$, for $q = 3,5$, respectively; see the known sufficient stability condition (1.18). In other words, in case $\cos\varphi(t) > \hat\eta_q$, for all $t \in [0,T]$, but $\cos\varphi(t) \le \eta_q$, for some $t \in [0,T]$, the new sufficient stability condition (1.20) does ensure stability of the $q-$step BDF method (1.11), $q = 3,5$, while the known sufficient stability condition (1.18) fails to do so.

The new and known sufficient conditions (1.21) and (1.19) for the local stability of the implicit–explicit $q-$step BDF scheme (1.12), $q = 3,5$, can be compared analogously.

1.3.5. *Sufficient stability conditions in terms of time-dependent norms.* Proceeding as in [1] for the case of the stability conditions (1.18) and (1.19), we can relax the sufficient stability conditions (1.20) and (1.21) using time-dependent norms. Motivated by the approach in [11] and [4], where time-dependent norms were used in the case of self-adjoint operators, the operators $A(t)$ were decomposed in [1] in their self-adjoint and anti-self-adjoint parts $A_s(t)$ and $A_a(t)$, respectively,

$$A_s(t) := \frac{1}{2}\big[A(t) + A(t)^\star\big], \quad A_a(t) := \frac{1}{2}\big[A(t) - A(t)^\star\big],$$

and the time-dependent norm $\|\cdot\|_t$,

$$\|v\|_t := (A_s(t)v, v)^{1/2} \quad \forall v \in V,$$

was introduced in V. The corresponding dual norm on V' was denoted by $\|\cdot\|_{\star,t}$,

$$\forall v \in V' \quad \|v\|_{\star,t} := \sup_{w\in V\setminus\{0\}} \frac{|(v,w)|}{\|w\|_t} = \sup_{\substack{w\in V\\ \|w\|_t=1}} |(v,w)|.$$

An easy consequence of (1.13) and (1.14) is that the norms $\|\cdot\|_t$ and $\|\cdot\|$ are equivalent,

$$\sqrt{\kappa(t)}\,\|v\| \le \|v\|_t \le \sqrt{\nu(t)}\,\|v\| \quad \forall v \in V. \tag{1.23}$$

Let $\lambda_a(t) : [0,T] \to [1,\infty)$ be a smooth function such that

$$\|A(t)v\|_{\star,t} \le \lambda_a(t)\|v\|_t \quad \forall v \in V. \tag{1.24}$$

It easily follows from (1.13) and (1.14) that (1.24) is valid with $\lambda_a(t) = \lambda(t) = \nu(t)/\kappa(t)$. In general, however, (1.24) may be satisfied with $\lambda_a(t)$ much smaller than $\lambda(t)$; see [1]. In the case of positive definite self-adjoint operators $A(t)$, the estimate (1.24) holds as an equality with $\lambda_a(t) = 1$. The difference $\lambda_a(t) - 1$ may be viewed as a measure of the deviation of $A(t)$ from a positive definite self-adjoint operator.

Assume also that $A_s(t)$ satisfies a mild Lipschitz condition with respect to t, namely

$$\|\big(A_s(t) - A_s(\tilde t)\big)v\|_\star \le L|t - \tilde t|\,\|v\| \quad \forall t, \tilde t \in [0,T] \;\; \forall v \in V, \tag{1.25}$$

with a Lipschitz constant L.

In analogy to (1.15), assume that the operators B satisfy the local Lipschitz condition

$$\|B(t,v) - B(t,\tilde v)\|_{\star,t} \le \tilde\lambda_b(t)\|v - \tilde v\|_t + \tilde\mu_b|v - \tilde v| \quad \forall v, \tilde v \in \mathscr{B}_{u(t)}, \tag{1.26}$$

for all $t \in [0,T]$, with a smooth nonnegative function $\tilde\lambda_b : [0,T] \to \mathbb{R}$ and an arbitrary constant $\tilde\mu_b$. It follows easily from (1.15) and (1.13) that (1.26) is valid with $\tilde\lambda_b(t) = \tilde\lambda(t)/\kappa(t)$ and $\tilde\mu_b = \tilde\mu/\min_{0\le t\le T}\sqrt{\kappa(t)}$. In general, however, (1.26) may be satisfied with $\tilde\lambda_b(t)$ much smaller than $\tilde\lambda(t)/\kappa(t)$; see [1].

Combining the use of the time-dependent norms mentioned above with the new multipliers (1.4) and (1.6) along the lines of [1], one can show that the three- and five-step BDF methods (1.11) are stable, provided

$$\lambda_a(t) < \frac{1}{\hat{\eta}_q}, \quad q = 3, 5, \tag{1.27}$$

respectively, for all $t \in [0, T]$. Analogously, the implicit–explicit $q-$step BDF methods (1.12) are locally stable, provided

$$\hat{\eta}_q \lambda_a(t) + (2^q - 1)(1 + \hat{\eta}_q)\tilde{\lambda}_b(t) < 1, \quad q = 3, 5, \tag{1.28}$$

respectively, for all $t \in [0, T]$. These new sufficient stability conditions are relaxed versions of the corresponding conditions (2.29) and (3.30) in [1], respectively, in which η_q enters insted of $\hat{\eta}_q$.

Let us also note that all stability results for the schemes (1.11) and (1.12), respectively, mentioned here, combined with the easily established consistency of the methods for the underlying equations, lead to optimal order a priori error estimates for the initial value problems (1.8) for the (inhomogeneous) linear equation and for (1.9), respectively.

Extensive numerical experiments to investigate the accuracy and efficiency of the implicit–explicit BDF methods (1.12) were carried out in [5, 6, 3] with very satisfactory results. More precisely, these methods were used for the discretization in time of a nonlinear parabolic system arising in two-phase flows in [5], of a general class of dispersively modified Kuramoto–Sivashinsky equations arising in multiphase hydrodynamics in [6], and of two-dimensional active partial differential equations such as the Topper–Kawahara equation, which is a two-dimensional extension of the dispersively modified Kuramoto–Sivashinsky equation, found in falling film hydrodynamics in [3].

An outline of the paper is as follows: In Sections 2, 3 and 4 we show that (1.4), (1.5) and (1.6) are the unique optimal multipliers for the three-, four-, and five-step BDF methods, respectively. In Section 5 we establish stability of the three-step BDF scheme (1.11) for the linear parabolic equation (1.8) and local stability of the implicit–explicit three-step BDF scheme (1.12) for the nonlinear parabolic equation (1.9) under the stability conditions (1.20) and (1.21), respectively. These stability results can be easily extended to the case of the five-step methods and to the case of quasi-linear parabolic equations (see [4]); the case of time-dependent norms can also be easily handled (see [4, 1]).

2. A new multiplier for the three-step BDF method

In this section we show that the multiplier (1.4) is the unique optimal multiplier for the three-step BDF method.

2.1. Background and known multipliers.

First, we recall a result from Dahlquist's G-stability theory.

Lemma 2.1 ([9]; see also [7] and [10, Section V.6]). *Let $\alpha(\zeta) = \alpha_q\zeta^q + \cdots + \alpha_0$ and $\mu(\zeta) = \mu_q\zeta^q + \cdots + \mu_0$ be polynomials, with real coefficients, of degree at most q (and at least one of them of degree q) that have no common divisor. Let $(\cdot, \cdot)$ be an inner* *product with associated norm* $|\cdot|$. *If*

$$\operatorname{Re}\frac{\alpha(\zeta)}{\mu(\zeta)} > 0 \quad \text{for } |\zeta| > 1, \tag{2.1}$$

then there exists a positive definite symmetric matrix $G = (g_{ij}) \in \mathbb{R}^{q,q}$ *and real* $\delta_0, \dots, \delta_q$ *such that for* $v^0, \dots, v^q$ *in the inner product space,*

$$\operatorname{Re}\Big(\sum_{i=0}^{q} \alpha_i v^i, \sum_{j=0}^{q} \mu_j v^j\Big) = \sum_{i,j=1}^{q} g_{ij}(v^i, v^j) - \sum_{i,j=1}^{q} g_{ij}(v^{i-1}, v^{j-1}) + \Big|\sum_{i=0}^{q} \delta_i v^i\Big|^2. \qquad \square$$

In combination with the preceding result for $\mu(\zeta) = \zeta^q - \eta_q \zeta^{q-1}$, the following property of BDF methods up to order 5 was established in [12].

Lemma 2.2 ([12]; see also [10, Section V.8])**.** *For* $q \le 5$, *there exists* $0 \le \eta_q < 1$ *such that the generating polynomial* $\alpha(\zeta)$ *of the* $q-$*step BDF method, see* (1.1), *satisfies*

$$\operatorname{Re}\frac{\alpha(\zeta)}{\zeta^q - \eta_q \zeta^{q-1}} > 0 \quad \text{for } |\zeta| > 1.$$

The smallest possible values of η_q *are*

$$\eta_1 = \eta_2 = 0,\ \eta_3 = 0.0836,\ \eta_4 = 0.2878,\ \eta_5 = 0.8160. \qquad \square$$

Let now $\alpha \in \mathbb{P}_q$ be the generating polynomial of the $q-$step BDF method and $\mu \in \mathbb{P}_q$ be a polynomial, $\mu(\zeta) = \zeta^q - \mu_1 \zeta^{q-1} - \cdots - \mu_q$, with real coefficients and roots inside the unit disc, and assume that α and μ have no common divisor. Then $\alpha(z)/\mu(z)$ is holomorphic outside the unit disc in the complex plane, and

$$\lim_{|z|\to\infty} \frac{\alpha(z)}{\mu(z)} = \alpha_q > 0.$$

Therefore, according to the maximum principle for harmonic functions, (2.1) is equivalent to

$$\operatorname{Re}\frac{\alpha(\zeta)}{\mu(\zeta)} \ge 0 \quad \forall \zeta \in \mathscr{K},$$

with $\mathscr{K}$ the unit circle in the complex plane, $\mathscr{K} := \{\zeta \in \mathbb{C} : |\zeta| = 1\}$, i.e., equivalent to

$$\operatorname{Re}[\alpha(\mathrm{e}^{\mathrm{i}\varphi})\mu(\mathrm{e}^{-\mathrm{i}\varphi})] \ge 0 \quad \forall \varphi \in \mathbb{R}. \tag{2.2}$$

2.2. **New multiplier.** In the case of the three-step BDF method and the parameters given in (1.4), it is easily seen that α and μ have no common divisor, cf. §2.3, and

$$\operatorname{Re}[\alpha(\mathrm{e}^{\mathrm{i}\varphi})\mu(\mathrm{e}^{-\mathrm{i}\varphi})] = \frac{4}{3}(1 - \cos\varphi)\Big(\cos\varphi - \frac{7}{13}\Big)^2. \tag{2.3}$$

In particular, (2.2) is satisfied, whence (μ_1, μ_2, μ_3) is indeed a multiplier for the three-step BDF method.

More precisely, we have the following result:

Lemma 2.3 (New multiplier). *Let* $\alpha(\zeta)=\alpha_3\zeta^3+\cdots+\alpha_0$ *be the generating polynomial of the three-step BDF method, and* $G=(g_{ij})_{i,j=1,2,3}$ *the positive definite symmetric matrix*

$$G:=\frac{1}{6\cdot 169}\begin{pmatrix}169 & -362 & 349\\ -362 & 997 & -1181\\ 349 & -1181 & 1690\end{pmatrix}.$$

Then, for $v^0,\dots,v^3$ *in an inner product space, with inner product* $(\cdot,\cdot)$ *and corresponding norm* $|\cdot|$, *we have the identity*

$$\operatorname{Re}\Big(\sum_{i=0}^{3}\alpha_i v^i, v^3-\frac{2}{169}v^2-\frac{11}{169}v^1\Big)=\sum_{i,j=1}^{3}g_{ij}(v^i,v^j)-\sum_{i,j=1}^{3}g_{ij}(v^{i-1},v^{j-1})$$
$$+\frac{1}{6\cdot 169}\big|13v^3-27v^2+27v^1-13v^0\big|^2.$$

In particular,

$$\operatorname{Re}\Big(\sum_{i=0}^{3}\alpha_i v^i, v^3-\frac{2}{169}v^2-\frac{11}{169}v^1\Big)\ge\sum_{i,j=1}^{3}g_{ij}(v^i,v^j)-\sum_{i,j=1}^{3}g_{ij}(v^{i-1},v^{j-1}).\qquad\square$$

Remark 2.1 (Positive definiteness of the matrix G). The positive definiteness of the matrix G is a consequence of (2.2); see [9, 7]. Here, we give more precise information about the eigenvalues of G.

The characteristic polynomial p of the symmetric matrix $6\cdot169G$ is

$$p(\lambda)=-\lambda^3+2856\lambda^2-491427\lambda+4548960.$$

Now, $p(0)$ is positive and p' is negative in $(-\infty,0]$; thus, the eigenvalues of G are positive, i.e., G is positive definite. More precisely, it is easily seen that the roots of p are in the intervals $(9,10),(173,174)$ and $(2672,2673)$. Therefore, the smallest eigenvalue $\lambda^\star_{\min}$ of G is bounded from below by $9/(6\cdot169)$,

$$\lambda^\star_{\min}>\frac{3}{338}.\qquad\square$$

Remark 2.2 (Derivation of the identity in Lemma 2.3). Our derivation of the identity in Lemma 2.3 is based on the approach of Baiocchi and Crouzeix [7]: With the notation of Lemma 2.3 and

$$\mu(\zeta):=\zeta^3-\frac{2}{169}\zeta^2-\frac{11}{169}\zeta,$$

it is easily seen that

$$E(\zeta):=\alpha(\zeta)\mu(\frac{1}{\zeta})+\alpha(\frac{1}{\zeta})\mu(\zeta)=-\frac{(\zeta-1)^2}{3\cdot169\zeta^3}(13\zeta^2-14\zeta+13)^2,$$

whence

$$\alpha(\zeta)\mu(\frac{1}{\zeta})+\alpha(\frac{1}{\zeta})\mu(\zeta)=p(\zeta)p(\frac{1}{\zeta})\tag{2.4}$$

with

$$p(\zeta):=\frac{1}{13\sqrt{3}}(\zeta-1)(13\zeta^2-14\zeta+13)=\frac{1}{13\sqrt{3}}(13\zeta^3-27\zeta^2+27\zeta-13).\tag{2.5}$$

Furthermore,

$$\alpha(\zeta)\mu(\omega)+\alpha(\omega)\mu(\zeta)-p(\zeta)p(\omega)=2(\zeta\omega-1)\sum_{i,j=1}^{3}g_{ij}\zeta^{i-1}\omega^{j-1}; \tag{2.6}$$

(2.6) and (2.5) immediately lead to the identity in Lemma 2.3.

Notice that p has one real root, namely $\zeta_1=1$, and two complex conjugate roots ζ_2 and ζ_3; since, obviously, $\zeta_2\zeta_3=1$, we infer that $|\zeta_2|=|\zeta_3|=1$. Therefore, $|p(\zeta)|$ is positive in the exterior of the unit disc in the complex plane, i.e., for $|\zeta|>1$. Thus, it immediately follows from (2.6) that the real part of $\alpha(\zeta)\mu(\bar\zeta)$ is positive in the exterior of the unit disc in the complex plane, whence (2.1) is satisfied. □

2.3. **Optimality of the new multiplier.** Without loss of generality, we consider multipliers with $|\mu_1|+|\mu_2|+|\mu_3|<1/11$, say, since a multiplier with $|\mu_1|+|\mu_2|+|\mu_3|=0.0836$ is already known; see [12]. In the sequel, we call such multipliers *admissible*. Let $\alpha\in\mathbb{P}_3$ be the generating polynomial of the three-step BDF method, and let (μ_1,μ_2,μ_3) be an admissible multiplier for the three-step BDF method, i.e., satisfying (1.2) with $\mu(\zeta)=\zeta^3-\mu_1\zeta^2-\mu_2\zeta-\mu_3$. It is easily seen that the roots of μ are in the interior of the unit disc, whence $\alpha(\zeta)/\mu(\zeta)$ is holomorphic outside the unit disc. Furthermore, the polynomials α and μ have no common divisor; indeed, since

$$\alpha(\zeta)=\frac{11}{6}(\zeta-1)\big(\zeta^2-\frac{7}{11}\zeta+\frac{2}{11}\big),$$

if α and μ had a common divisor, then μ would be of the form

$$\mu(\zeta)=(\zeta-c)\big(\zeta^2-\frac{7}{11}\zeta+\frac{2}{11}\big)=\zeta^3-\big(\frac{7}{11}+c\big)\zeta^2+\frac{7c+2}{11}\zeta-\frac{2}{11}c \tag{2.7}$$

with $c\in(-1,1)$. It is easily seen that the sum of the absolute values of the constant term and the coefficients of ζ and ζ^2 of the polynomial μ in (2.7) is larger than $1/11$, for all possible choices of $c\in(-1,1)$, a contradiction.

2.3.1. *First claim.* A triplet (μ_1,μ_2,μ_3) is an admissible multiplier for the three-step BDF method, if and only if

$$(2\mu_1-11\mu_2-4\mu_3+5)^2-8(11\mu_3+2)(8\mu_1+\mu_2-8\mu_3+1)\le 0. \tag{2.8}$$

First, a straightforward but lengthy calculation shows that, in the case of the three-step BDF method, relation (2.2) can be equivalently written in the form

$$\begin{aligned}&-4(11\mu_3+2)\cos(3\varphi)+(2\mu_1-11\mu_2+18\mu_3+9)\cos(2\varphi)\\&-(20\mu_1-20\mu_2+9\mu_3+18)\cos\varphi+18\mu_1-9\mu_2+2\mu_3+11\ge 0,\end{aligned} \tag{2.9}$$

for all $\varphi\in\mathbb{R}$. Next, we use the substitution $x:=\cos\varphi$ and write (2.9) as

$$\begin{aligned}&-4(11\mu_3+2)(4x^3-3x)+(2\mu_1-11\mu_2+18\mu_3+9)(2x^2-1)\\&-(20\mu_1-20\mu_2+9\mu_3+18)x+18\mu_1-9\mu_2+2\mu_3+11\ge 0,\end{aligned}$$

i.e.,

$$(1-x)\big[2(11\mu_3+2)x^2-(2\mu_1-11\mu_2-4\mu_3+5)x+(8\mu_1+\mu_2-8\mu_3+1)\big]\ge 0,$$

or equivalently, since $x\le 1$,

$$2(11\mu_3+2)x^2-(2\mu_1-11\mu_2-4\mu_3+5)x+(8\mu_1+\mu_2-8\mu_3+1)\ge 0, \tag{2.10}$$

for all $x \in [-1, 1]$.

Let us now first consider the case that the quadratic polynomial on the left-hand side of (2.10) has two distinct real roots x_1, x_2. Since

$$x_1 + x_2 = \frac{2\mu_1 - 11\mu_2 - 4\mu_3 + 5}{22\mu_3 + 4}, \quad x_1 x_2 = \frac{8\mu_1 + \mu_2 - 8\mu_3 + 1}{22\mu_3 + 4}$$

are both positive and $x_1 x_2 < 1$, for all admissible multipliers, we see that x_1 and x_2 are positive, and at least one of them is less than 1. Therefore, in this case, (2.10) can obviously not be satisfied for all $x \in [-1, 1]$.

Thus, since the coefficient of x^2 is positive, we infer that (2.10) is satisfied for all $x \in [-1, 1]$, if and only if the discriminant of the quadratic polynomial on its left-hand side is nonpositive, i.e., if (2.8) holds true.

Remark 2.3 (The case of two vanishing μ_i's)**.** Let us first consider the case $\mu_2 = \mu_3 = 0$. Then, (2.8) takes the form

$$4\mu_1^2 - 108\mu_1 + 9 \le 0. \tag{2.11}$$

Now, the smallest real number satisfying (2.11) is the smallest root η_3 of the quadratic polynomial on its left-hand side, i.e.,

$$\eta_3 = \frac{3}{2}\big(\sqrt{5} - 2\big)^2 = 0.083592135. \tag{2.12}$$

Thus, in this case, we recover the corresponding Nevanlinna–Odeh multiplier; see [12].

Next, we consider the case $\mu_1 = \mu_3 = 0$. Then, (2.8) takes the form

$$121\mu_2^2 - 126\mu_2 + 9 \le 0; \tag{2.13}$$

the smallest μ_2 for which this relation is satisfied is

$$\mu_2 = \frac{63 - 24\sqrt{5}}{121} = 0.077143541. \tag{2.14}$$

This is a more favourable multiplier than the Nevanlinna–Odeh multiplier, and, indeed, only slightly worse than the optimal multiplier (1.4).

Finally, in the case $\mu_1 = \mu_2 = 0$, the quadratic polynomial on the left-hand side of (2.10) has two real roots; consequently, as we saw, (2.10) is not satisfied. ☐

Remark 2.4 (The case of vanishing μ_2, μ_3; alternative proof)**.** We give here an alternative proof of the fact that $\sigma := |\mu_1| + |\mu_2| + |\mu_3| = \mu_1 \ge \eta_3$ in the case $\mu_2 = \mu_3 = 0$; the idea of this proof will be useful in the sequel. First, we rewrite (2.10) in the form

$$f_0(x) + f_1(x)\mu_1 + f_2(x)\mu_2 + f_3(x)\mu_3 \ge 0 \quad \forall x \in [-1, 1], \tag{2.15}$$

with

$$f_0(x) := 4x^2 - 5x + 1, \quad f_1(x) := 8 - 2x, \quad f_2(x) := 11x + 1, \quad f_3(x) := 22x^2 + 4x - 8.$$

Then, for $\mu_2 = \mu_3 = 0$, we have

$$\mu_1 \ge -\frac{f_0(x)}{f_1(x)},$$

since $f_1(x)$ is positive in $[-1,1]$. It is easily seen that the derivative of the function on the right-hand side vanishes if and only if $4x^2-32x+19=0$ and that $-f_0(x)/f_1(x)$ attains its maximum η_3 at

$$x^\star := 4-\frac{3}{2}\sqrt{5}. \tag{2.16}$$

thus, $\mu_1 \ge \eta_3$ and the desired result follows. □

2.3.2. *Second claim.* If $\mu_2 \le 0$, then $\sigma \ge \eta_3$.

Indeed, for $x=x^\star$, with $x^\star$ as in (2.16), relation (2.15) yields

$$\mu_1 \ge \eta_3 - \frac{f_2(x^\star)}{f_1(x^\star)}\mu_2 - \frac{f_3(x^\star)}{f_1(x^\star)}\mu_3 \ge \eta_3 - a\mu_3,$$

since $f_2(x^\star)$ is positive and μ_2 nonpositive, with $a := f_3(x^\star)/f_1(x^\star) \in (0,1)$. Therefore,

$$\sigma = |\mu_1|+|\mu_2|+|\mu_3| \ge \mu_1 + |\mu_3| \ge \eta_3 - a\mu_3 + |\mu_3| = \eta_3 + (1-a\operatorname{sgn}\mu_3)|\mu_3| \ge \eta_3,$$

since $a\in(0,1)$. Furthermore, obviously, $\sigma=\eta_3$, if and only if $\mu_2=\mu_3=0$ and $\mu_1=\eta_3$.

Thus, from now on we assume that μ_2 is positive.

2.3.3. *Third claim.* Assuming $\mu_3=0$, the sum $\sigma=|\mu_1|+|\mu_2|+|\mu_3|$ of multipliers (μ_1,μ_2,μ_3) for the three-step BDF method attains its minimal value $1/13$, if and only if $\mu_1=2/169$ and $\mu_2=11/169$.

Indeed, we have $\sigma=|\mu_1|+|\mu_2|=|\mu_1|+\mu_2$, whence $\mu_2=\sigma-|\mu_1|$. We now distinguish two subcases, μ_1 positive and μ_1 nonpositive.

If μ_1 is positive, replacing μ_2 by $\sigma-\mu_1$ in (2.8), we rewrite it in the form

$$169\mu_1^2 + 2(9-143\sigma)\mu_1 + 121\sigma^2 - 126\sigma + 9 \le 0. \tag{2.17}$$

Obviously, a necessary condition for (2.17) is that the quadratic polynomial in μ_1 on its left-hand side has real roots; it is easily seen that this is the case if and only if $18720\sigma - 1440 \ge 0$, i.e.,

$$\sigma \ge \frac{1}{13}. \tag{2.18}$$

Now, for $\sigma=1/13$, (2.17) is satisfied if and only if $\mu_1=2/169$; then, $\mu_2=\sigma-\mu_1=11/169$.

If μ_1 is nonpositive, replacing μ_2 by $\sigma+\mu_1$ in (2.8), we rewrite it in the form

$$81\mu_1^2 - 2(99\sigma+117)\mu_1 + 121\sigma^2 - 126\sigma + 9 \le 0. \tag{2.19}$$

Now, if $121\sigma^2-126\sigma+9\le 0$, then it is easily seen that

$$\sigma \ge \frac{63-24\sqrt{5}}{121} > \frac{1}{13}. \tag{2.20}$$

Furthermore, if $121\sigma^2-126\sigma+9>0$, a necessary condition for (2.19) is that the quadratic polynomial in μ_1 on its left-hand side has real roots x_1 and x_2; it is easily seen that in this case both the sum x_1+x_2 and the product x_1x_2 are positive. Thus, if $x_1\le x_2$, we have $x_1\le\mu_1\le x_2$, whence μ_1 is positive, a contradiction.

2.3.4. *Fourth claim.* If (μ_1, μ_2, μ_3) is a multiplier for the three-step BDF method with $\mu_1 \neq 2/169$ or $\mu_2 \neq 11/169$, then $\sigma = |\mu_1| + |\mu_2| + |\mu_3| > 1/13$.

In fact, for $x = 7/13$, relation (2.15) yields

$$-\frac{90}{169} + \frac{90}{13}\mu_1 + \frac{90}{13}\mu_2 + \frac{90}{169}\mu_3 \geq 0, \quad \text{i.e.,} \quad \mu_1 + \mu_2 \geq \frac{1}{13} - \frac{1}{13}\mu_3.$$

Then, since μ_2 is positive,

$$\sigma = |\mu_1| + \mu_2 + |\mu_3| \geq \mu_1 + \mu_2 + |\mu_3| \geq \frac{1}{13} + \big(1 - \frac{1}{13}\operatorname{sgn}\mu_3\big)|\mu_3|.$$

The last expression attains its minimal value 1/13, if and only if $\mu_3 = 0$. We considered the latter case in §2.3.3.

We infer that if (μ_1, μ_2, μ_3) is a multiplier for the three-step BDF method, then $\sigma = |\mu_1| + |\mu_2| + |\mu_3| \geq 1/13$, and σ attains the minimal value 1/13 only for the multiplier given in (1.4).

3. Optimality of the Nevanlinna–Odeh multiplier for the four-step BDF method

Our goal here is not to improve the Nevanlinna–Odeh multiplier for the four-step BDF method but rather to give a precise expression for η_4 and to show that this multiplier is indeed optimal among all multipliers $(\mu_1, \mu_2, \mu_3, \mu_4)$ for the four-step BDF method.

Let α be the generating polynomial of the four–step BDF method,

$$\alpha(\zeta) = \sum_{j=1}^{4} \frac{1}{j}\zeta^{4-j}(\zeta - 1)^j = \frac{1}{12}\big(25\zeta^4 - 48\zeta^3 + 36\zeta^2 - 16\zeta + 3\big).$$

A quadruplet of real numbers $(\mu_1, \mu_2, \mu_3, \mu_4)$ is a multiplier for the four-step BDF method, if

$$\operatorname{Re}[\alpha(\mathrm{e}^{\mathrm{i}\varphi})\mu(\mathrm{e}^{-\mathrm{i}\varphi})] \geq 0 \quad \forall \varphi \in \mathbb{R}, \tag{3.1}$$

with $\mu(\zeta) := \zeta^4 - \mu_1\zeta^3 - \mu_2\zeta^2 - \mu_3\zeta - \mu_4$, provided that the roots of μ are inside the unit disc and α and μ have no common divisor; see (2.2).

In analogy to (2.9), it is easily seen that, with $x = \cos\varphi$, (3.1) takes the form

$$(1 - x)\big[f_0(x) + f_1(x)\mu_1 + f_2(x)\mu_2 + f_3(x)\mu_3 + f_4(x)\mu_4\big] \geq 0 \quad \forall x \in [-1, 1],$$

i.e.,

$$f_0(x) + f_1(x)\mu_1 + f_2(x)\mu_2 + f_3(x)\mu_3 + f_4(x)\mu_4 \geq 0 \quad \forall x \in [-1, 1], \tag{3.2}$$

with

$$\begin{aligned} &f_0(x) := -2(x-1)^2(3x+1), \quad &&f_1(x) := 3x^2 - 5x + 8, \quad f_2(x) := 2(7x - 1),\\ &f_3(x) := 25x^2 + x - 8, &&f_4(x) := 50x^3 + 2x^2 - 30x + 2. \end{aligned}$$

Assume first that $\mu_2 = 0$ and $\mu_3, \mu_4 \geq 0$. Since $f_1(x)$ is positive, (3.2) takes the form

$$\mu_1 \geq -\frac{f_0(x)}{f_1(x)} - \frac{f_3(x)}{f_1(x)}\mu_3 - \frac{f_4(x)}{f_1(x)}\mu_4 \quad \forall x \in [-1, 1]. \tag{3.3}$$

The derivative of the function $f_0(x)/f_1(x)$ vanishes at $x = 1$ and at $x = x^\star$, with $x^\star$ the real root of $9x^3 - 21x^2 + 73x - 13$, given by Cardano's formula,

$$x^\star = \frac{1}{9}\Big(7 + \sqrt[3]{90\sqrt{859} - 1430} - \sqrt[3]{90\sqrt{859} + 1430}\Big) = 0.18737068. \tag{3.4}$$

It is easily seen that $-f_0(x)/f_1(x)$ attains its maximum in $[-1, 1]$ at $x^\star$; the maximal value is

$$-\frac{f_0(x^\star)}{f_1(x^\star)} = \frac{2(x^\star - 1)^2(3x^\star + 1)}{3(x^\star)^2 - 5x^\star + 8} = \eta_4 = 0.287806557.$$

Since $f_3(x^\star)$ and $f_4(x^\star)$ are negative, μ_1 can attain its minimal value $-f_0(x^\star)/f_1(x^\star)$ if and only if $\mu_3 = \mu_4 = 0$. Summarizing, in the case $\mu_2 = 0$ and $\mu_3, \mu_4 \geq 0$, the sum $|\mu_1| + \cdots + |\mu_4|$ attains its minimal value for

$$\mu_1 = \eta_4 = 0.287806557, \quad \mu_3 = \mu_4 = 0. \tag{3.5}$$

Thus, in this case, we recover the Nevanlinna–Odeh multiplier for the four-step BDF method; see [12].

We next consider the general case. With $x^\star$ as in (3.4), let now

$$a := \frac{f_2(x^\star)}{f_1(x^\star)}, \quad b := -\frac{f_3(x^\star)}{f_1(x^\star)}, \quad c := -\frac{f_4(x^\star)}{f_1(x^\star)}.$$

It is easily seen that $a, b, c \in (0, 1)$. Now, for $x = x^\star$, relation (3.2) yields

$$\mu_1 \geq \eta_4 - a\mu_2 + b\mu_3 + c\mu_4.$$

Consequently,

$$\begin{aligned}\sigma &:= |\mu_1| + |\mu_2| + |\mu_3| + |\mu_4| \geq \mu_1 + |\mu_2| + |\mu_3| + |\mu_4| \\ &\geq \eta_4 + (1 - a\operatorname{sgn}\mu_2)|\mu_2| + (1 + b\operatorname{sgn}\mu_3)|\mu_3| + (1 + c\operatorname{sgn}\mu_4)|\mu_4|.\end{aligned}$$

Since $a, b, c \in (0, 1)$, the last expression attains its minimal value η_4, if and only if $\mu_2 = \mu_3 = \mu_4 = 0$ and $\mu_1 = \eta_4$.

We infer that if $(\mu_1, \ldots, \mu_4)$ is a multiplier for the four-step BDF method, then $\sigma = |\mu_1| + \cdots + |\mu_4| \geq \eta_4$, and σ attains the minimal value η_4 only for the Nevanlinna–Odeh multiplier $(\eta_4, 0, 0, 0)$.

4. A new multiplier for the five-step BDF method

In this section we show that the multiplier (1.6) is the unique optimal multiplier for the five-step BDF method.

Let α be the generating polynomial of the five–step BDF method,

$$\alpha(\zeta) = \sum_{j=1}^{5} \frac{1}{j}\zeta^{5-j}(\zeta - 1)^j = \frac{1}{60}\big(137\zeta^5 - 300\zeta^4 + 300\zeta^3 - 200\zeta^2 + 75\zeta - 12\big).$$

A set of real numbers $(\mu_1, \mu_2, \mu_3, \mu_4, \mu_5)$ is a multiplier for the five-step BDF method, if

$$\operatorname{Re}[\alpha(e^{i\varphi})\mu(e^{-i\varphi})] \geq 0 \quad \forall \varphi \in \mathbb{R}, \tag{4.1}$$

with $\mu(\zeta) := \zeta^5 - \mu_1\zeta^4 - \mu_2\zeta^3 - \mu_3\zeta^2 - \mu_4\zeta - \mu_5$, provided that the roots of μ are inside the unit disc and α and μ have no common divisor; see (2.2).

First, as in the previous cases, with $x = \cos\varphi$, (4.1) takes the form $(1-x)f(x) \geq 0$, for $x \in [-1,1]$, with

$$\begin{aligned} f(x) := {} & 4(12+137\mu_5)x^4 - (102+24\mu_1 - 274\mu_4 + 52\mu_5)x^3 \\ & + (38+51\mu_1 - 12\mu_2 + 137\mu_3 - 26\mu_4 - 437\mu_5)x^2 \\ & + (38 - 25\mu_1 + 94\mu_2 - 19\mu_3 - 150\mu_4 + 63\mu_5)x \\ & - 22 + 28\mu_1 - 22\mu_2 - 28\mu_3 + 22\mu_4 + 28\mu_5; \end{aligned}$$

thus, (4.1) can be equivalently written as

$$f(x) \geq 0 \quad \forall x \in [-1,1]. \tag{4.2}$$

We let

$$\begin{aligned} & f_0(x) := (x-1)^2(48x^2 - 6x - 22), && f_1(x) := -24x^3 + 51x^2 - 25x + 28, \\ & f_2(x) := -12x^2 + 94x - 22, && f_3(x) := 137x^2 - 19x - 28, \\ & f_4(x) := 274x^3 - 26x^2 - 150x + 22, && f_5(x) := 548x^4 - 52x^3 - 437x^2 + 63x + 28, \end{aligned}$$

and write (4.2) in the form

$$f_0(x) + f_1(x)\mu_1 + f_2(x)\mu_2 + f_3(x)\mu_3 + f_4(x)\mu_4 + f_5(x)\mu_5 \geq 0 \quad \forall x \in [-1,1]. \tag{4.3}$$

We observe that f_1 takes on only positive values in the interval $[-1,1]$ while f_2, f_3, f_4 and f_5 take on both positive and negative values.

4.1. **The case $\mu_4 = \mu_5 = 0$ and $\mu_2, \mu_3 \geq 0$.** In this case, (4.3) takes the form

$$\mu_1 \geq -\frac{f_0(x)}{f_1(x)} - \frac{f_2(x)}{f_1(x)}\mu_2 - \frac{f_3(x)}{f_1(x)}\mu_3 \quad \forall x \in [-1,1]. \tag{4.4}$$

The function $-f_0(x)/f_1(x)$ attains its maximum in $[-1,1]$ at $x^\star = -0.0907628$; we have $-f_0(x^\star)/f_1(x^\star) = 0.815980225$. Now, since $f_2(x^\star)$ and $f_3(x^\star)$ are negative, μ_1 can attain its minimal value $-f_0(x^\star)/f_1(x^\star)$ if and only if $\mu_2 = \mu_3 = 0$. Summarizing, in the case $\mu_4 = \mu_5 = 0$ and $\mu_2, \mu_3 \geq 0$, the sum $|\mu_1| + \cdots + |\mu_5|$ attains its minimal value for

$$\mu_1 = 0.815980225, \quad \mu_2 = \mu_3 = 0. \tag{4.5}$$

Thus, in this case, we recover the Nevanlinna–Odeh multiplier for the five-step BDF method; see [12].

4.2. **If $\mu_4 \leq 0$, then $\sigma \geq \eta_5$.** Indeed, with $x^\star = -0.0907628$ as above, and

$$a := -\frac{f_2(x^\star)}{f_1(x^\star)}, \quad b := -\frac{f_3(x^\star)}{f_1(x^\star)}, \quad c := \frac{f_4(x^\star)}{f_1(x^\star)}, \quad d := \frac{f_5(x^\star)}{f_1(x^\star)},$$

it is easily seen that $a, b, d \in (0,1)$ while $c > 1$. Now, for $x = x^\star$, relation (4.3) yields

$$\mu_1 \geq \eta_5 + a\mu_2 + b\mu_3 - c\mu_4 - d\mu_5,$$

whence, since μ_4 is nonpositive,

$$\mu_1 \geq \eta_5 + a\mu_2 + b\mu_3 - d\mu_5,$$

Consequently,

$$\begin{aligned}\sigma &:= |\mu_1| + \dots + |\mu_5| \geq \mu_1 + |\mu_2| + |\mu_3| + |\mu_5|\\ &\geq \eta_5 + (1 + a \operatorname{sgn} \mu_2)|\mu_2| + (1 + b \operatorname{sgn} \mu_3)|\mu_3| + (1 - d \operatorname{sgn} \mu_5)|\mu_5|.\end{aligned}$$

Since $a, b, d \in (0, 1)$, the last expression is at least η_5. Furthermore, obviously, $\sigma = \eta_5$, if and only if $\mu_2 = \dots = \mu_5 = 0$ and $\mu_1 = \eta_5$.

Thus, it suffices to consider the case μ_4 positive.

4.3. **The case $\mu_5 = 0, \mu_1, \mu_2, \mu_3 \geq 0$ and $\mu_4 > 0$.** We let $\lambda := \mu_1/\mu_4 \geq 0$. First, we note that, for $x = 0$, (4.3) yields $\mu_4 \geq 11/(11 + 14\lambda)$, whence, for $\lambda < 4$,

$$\sigma = |\mu_1| + \dots + |\mu_5| \geq \mu_1 + \mu_4 = (\lambda + 1)\mu_4 \geq \frac{11(\lambda + 1)}{11 + 14\lambda} > 0.82 > \eta_5.$$

Therefore, it suffices to consider the case $\lambda \geq 4$. In this case, $f_4 + \lambda f_1$ takes on only positive values in the interval $[-1, 1]$, and (4.3) can be written as

$$\mu_4 \geq \varphi_\lambda(x) + \Phi_\lambda(x)\mu_2 + \Psi_\lambda(x)\mu_3 \quad \forall x \in [-1, 1] \tag{4.6}$$

with

$$\varphi_\lambda(x) := \frac{-f_0(x)}{f_4(x) + \lambda f_1(x)}, \quad \Phi_\lambda(x) := \frac{-f_2(x)}{f_4(x) + \lambda f_1(x)}, \quad \Psi_\lambda(x) = \frac{-f_3(x)}{f_4(x) + \lambda f_1(x)}.$$

Now

$$f_4(x) + \lambda f_1(x) = (\lambda + 1)f_1(x) \iff f_4(x) = f_1(x) \iff (2x + 1)(149x^2 - 113 - 6) = 0.$$

At the root x_0,

$$x_0 = \frac{113 - \sqrt{16345}}{298} = -0.049824045,$$

of this equation, we have

$$\forall \lambda > 0 \quad F_\lambda(x_0) = -\frac{f_0(x_0)}{f_1(x_0)} = 0.809733746, \quad \text{where} \quad F_\lambda(x) := (\lambda + 1)\varphi_\lambda(x).$$

Now, for $\mu_2 = \mu_3 = 0$ and for all $\lambda \geq 4$, from (4.6), we obtain

$$\min \sigma = \max_{-1 \leq x \leq 1} [(\lambda + 1)\varphi_\lambda(x)] = \max_{-1 \leq x \leq 1} F_\lambda(x) \geq F_\lambda(x_0) = 0.809733746. \tag{4.7}$$

On the other hand, we observe that, for $\lambda = 9.441185$, (4.6) yields

$$\min \mu_4 = \max_{-1 \leq x \leq 1} \varphi_\lambda(x) = \varphi_\lambda(\tilde{x}) = 0.07755190105, \quad \text{with} \quad \tilde{x} = -0.049824 \approx x_0,$$

if and only if $\mu_2 = \mu_3 = 0$, since both $f_2(\tilde{x})$ and $f_3(\tilde{x})$ are negative. Then, the minimum of σ is $(9.441185 + 1)0.07755190105 = 0.8097337459$, that is, for $\lambda = \lambda_0, \lambda_0 = 9.441185$, (4.7) holds essentially as an equality.

We infer that

$$\mu_1 = 9.441185\mu_4 = 0.7321818449, \quad \mu_4 = 0.07755190105, \quad \mu_2 = \mu_3 = \mu_5 = 0, \tag{4.8}$$

and

$$\sigma_0 := \mu_1 + \dots + \mu_5 = 0.8097337459, \tag{4.9}$$

provided there exist points $x^\star_\lambda$ such that $f_2(x^\star_\lambda)$ and $f_3(x^\star_\lambda)$ are negative, in which case $\mu_2 = \mu_3 = 0$, and $F_\lambda(x^\star_\lambda) > 0.809733746$. Taking, now, $x^\star_\lambda = -0.04982$ $x^\star_\lambda = -0.04985$, points at which both f_2 and f_3 are negative, we have

$$F_\lambda(-0.04982) = \frac{23.78593427(\lambda+1)}{29.37458573 + 29.37505137\lambda} > 0.809733746 \iff \lambda < \lambda_1$$

and

$$F_\lambda(-0.04985) = \frac{23.78693713(\lambda+1)}{29.37894674 + 29.37595923\lambda} > 0.809733746 \iff \lambda > \lambda_2$$

with $\lambda_1 := 9.440374924$ and $\lambda_2 := 9.444166548$.

We thus see that for $\lambda \notin [\lambda_1, \lambda_2]$, suitable $x^\star_\lambda$ do exist. Now, if we take an $x^\star_\lambda \in (\tilde{x}, -0.04982)$ and an $x^\star_\lambda \in (-0.04985, \tilde{x})$, and repeat the above calculations, we see that, for $\lambda \geq 4$, outside a new subinterval $[\lambda_3, \lambda_4]$ of $[\lambda_1, \lambda_2]$, suitable $x^\star_\lambda$ do exist. We note that both f_2 and f_3 are negative in the whole interval $[-0.04985, -0.04982]$. By the continuity of F_λ, we infer that, if $x^\star_\lambda$ tends to $\tilde{x}$, then λ tends to λ_0; thus, for all $\lambda \neq \lambda_0$, suitable $x^\star_\lambda$ do exist.

4.4. **Optimality of the multiplier** (4.8)**.** Let us first note that the parameters $\mu_1, \dots, \mu_5$ given in (4.8) constitute a multiplier for the five-step BDF method. Indeed, as we saw, (4.1) is satisfied for these values of the parameters. Furthermore, the roots of the polynomial $\mu, \mu(\zeta) = z^5 - \mu_1 z^4 - \mu_4 z$, are $0, -0.40819, 0.85589$, and $0.14224 \pm 0.44919\mathrm{i}$, while the roots of the generating polynomial $\alpha \in \mathbb{P}_5$ of the five-step BDF method are $1, 0.38485 \pm 0.16212\mathrm{i}$, and $0.21004 \pm 0.67687\mathrm{i}$; thus, the roots of μ are in the interior of the unit disc, and μ and α have no common divisor. Therefore, $(\mu_1, \dots, \mu_5)$ is a multiplier for the five-step BDF method.

Now, let $\mu_1, \dots, \mu_5$ be such that (4.3) is satisfied. Then, with $x_0 = -0.049824045$ as in §4.3, since $f_1(x_0) = f_4(x_0)$, for $x = x_0$ relation (4.3) yields

$$f_1(x_0)(\mu_1 + \mu_4) \geq -f_0(x_0) - f_2(x_0)\mu_2 - f_3(x_0)\mu_3 - f_5(x_0)\mu_5,$$

i.e.,

$$\mu_1 + \mu_4 \geq \sigma_0 + a\mu_2 + b\mu_3 - c\mu_5,$$

with

$$a := -\frac{f_2(x_0)}{f_1(x_0)}, \quad b := -\frac{f_3(x_0)}{f_1(x_0)}, \quad c := \frac{f_5(x_0)}{f_1(x_0)}.$$

It is easily seen that $a, b, c \in (0, 1)$. Consequently,

$$\begin{aligned}\sigma = |\mu_1| + \cdots + |\mu_5| &\geq \mu_1 + \mu_4 + |\mu_2| + |\mu_3| + |\mu_5| \\ &\geq \sigma_0 + (1 + a\operatorname{sgn}\mu_2)|\mu_2| + (1 + b\operatorname{sgn}\mu_3)|\mu_3| + (1 - c\operatorname{sgn}\mu_5)|\mu_5|.\end{aligned}$$

Since $a, b, c \in (0, 1)$, the last expression attains its minimal value σ_0, if and only if $\mu_1 \geq 0$ and $\mu_2 = \mu_3 = \mu_5 = 0$.

We considered the latter case in §4.3. We infer that if $(\mu_1, \dots, \mu_5)$ is a multiplier for the five-step BDF method, then $\sigma = |\mu_1| + \cdots + |\mu_5| \geq \sigma_0$, and σ attains the minimal value σ_0 only for the multiplier given in (4.8).

5. Stability of the three-step BDF method for parabolic equations

This section is devoted to the analysis of stability properties of the three-step BDF method (1.11) for the linear parabolic equation (1.8) as well as of the implicit–explicit three-step BDF method (1.12) for the nonlinear equation (1.9). The analysis can be easily extended to the five-step BDF method.

5.1. **The implicit method for the linear equation.** We shall derive a sufficient stability condition, expressed in terms of the ratio $\lambda(t) = \nu(t)/\kappa(t)$, for the scheme (1.11). The proof proceed along the lines of corresponding results in [4, 1]; we employ the energy technique and make use of Lemma 2.3, while Lemma 2.2 was used in [4, 1]. This allows us to slightly relax the stability conditions of [4, 1] for the three-step BDF method.

Proposition 5.1 (Stability of the three-step BDF scheme (1.11))**.** *Assume* (1.13) *and* (1.14)*. Then, under the stability condition*

$$\kappa(t) - \frac{1}{13}\nu(t) \geq \rho > 0, \tag{5.1}$$

the three-step BDF method (1.11) *is stable in the sense that, for k sufficiently small,*

$$\frac{3}{338}|U^n|^2 + \frac{1}{2}\rho k \sum_{\ell=3}^{n} \|U^\ell\|^2 \leq C_3 \sum_{j=0}^{2} |U^j|^2 + ck\big(\|U^1\|^2 + \|U^2\|^2\big), \tag{5.2}$$

for $n = 3, \dots, N$, with C_3 a positive constant, and c a constant depending only on the maximum of ν.

Proof. We let $q = 3$ in (1.11) and take the inner product with $U^{n+3} - \mu_1 U^{n+2} - \mu_2 U^{n+1}$, with μ_1 and μ_2 as in (1.4), and then real parts to obtain

$$\operatorname{Re}\Big(\sum_{i=0}^{3} \alpha_i U^{n+i}, U^{n+3} - \mu_1 U^{n+2} - \mu_2 U^{n+1}\Big) + kI_{n+3} = 0 \tag{5.3}$$

with

$$I_{n+3} := \operatorname{Re}\big(A(t^{n+3})U^{n+3}, U^{n+3} - \mu_1 U^{n+2} - \mu_2 U^{n+1}\big). \tag{5.4}$$

The first term on the left-hand side of (5.3) can be taken care of using Lemma 2.3: With the notation $\mathcal{U}^n := (U^{n-2}, U^{n-1}, U^n)^T$ and the norm $|\mathcal{U}^n|_G$ given by

$$|\mathcal{U}^n|_G^2 = \sum_{i,j=1}^{3} g_{ij}(U^{n-3+i}, U^{n-3+j}),$$

from Lemma 2.3 we have

$$\operatorname{Re}\Big(\sum_{i=0}^{3} \alpha_i U^{n+i}, U^{n+3} - \mu_1 U^{n+2} - \mu_2 U^{n+1}\Big) \geq |\mathcal{U}^{n+3}|_G^2 - |\mathcal{U}^{n+2}|_G^2.$$

Thus, (5.3) yields

$$|\mathcal{U}^{n+3}|_G^2 - |\mathcal{U}^{n+2}|_G^2 + kI_{n+3} \leq 0. \tag{5.5}$$

It now remains to estimate I_{n+3} from below in a suitable way. First, we have

$$I_{n+3} = \operatorname{Re}\big(A(t^{n+3})U^{n+3}, U^{n+3}\big) - \sum_{i=1}^{2} \mu_{3-i} \operatorname{Re}\big(A(t^{n+3})U^{n+3}, U^{n+i}\big),$$

whence, in view of the coercivity condition (1.13),

$$I_{n+3} \geq \kappa(t^{n+3})\|U^{n+3}\|^2 - \sum_{i=1}^{2} \mu_{3-i} \operatorname{Re}\big(A(t^{n+3})U^{n+3}, U^{n+i}\big). \tag{5.6}$$

To estimate the sum on the right-hand side of (5.6), we notice that, for $i = 1, 2$,

$$\operatorname{Re}\big(A(t^{n+3})U^{n+3}, U^{n+i}\big) \leq \|A(t^{n+3})U^{n+3}\|_\star \, \|U^{n+i}\|,$$

whence, in view of the boundedness condition (1.14),

$$\operatorname{Re}\big(A(t^{n+3})U^{n+3}, U^{n+i}\big) \leq \nu(t^{n+3})\|U^{n+3}\| \, \|U^{n+i}\|,$$

and hence

$$\operatorname{Re}\big(A(t^{n+3})U^{n+3}, U^{n+i}\big) \leq \frac{\nu(t^{n+3})}{2}\big[\|U^{n+3}\|^2 + \|U^{n+i}\|^2\big]. \tag{5.7}$$

In view of (5.7) and the fact that $\mu_1 + \mu_2 = 1/13$, estimate (5.6) leads to

$$I_{n+3} \geq \Big[\kappa(t^{n+3}) - \frac{1}{26}\nu(t^{n+3})\Big]\|U^{n+3}\|^2 - \frac{1}{2}\nu(t^{n+3}) \sum_{i=1}^{2} \mu_{3-i}\|U^{n+i}\|^2. \tag{5.8}$$

From (5.3) and (5.8), we obtain

$$\begin{aligned} &|\mathcal{U}^{n+3}|_G^2 - |\mathcal{U}^{n+2}|_G^2 \\ &+ k\Big[\kappa(t^{n+3}) - \frac{1}{26}\nu(t^{n+3})\Big]\|U^{n+3}\|^2 - k\frac{1}{2}\nu(t^{n+3}) \sum_{i=1}^{2} \mu_{3-i}\|U^{n+i}\|^2 \leq 0, \end{aligned}$$

whence, in view also of the stability condition (5.1),

$$\begin{aligned} &|\mathcal{U}^{n+3}|_G^2 - |\mathcal{U}^{n+2}|_G^2 + \rho k\|U^{n+3}\|^2 \\ &+ \frac{1}{2}k\nu(t^{n+3}) \sum_{i=1}^{2} \mu_{3-i}\big[\|U^{n+3}\|^2 - \|U^{n+i}\|^2\big] \leq 0. \end{aligned} \tag{5.9}$$

Now, $|\nu(t^{m+i}) - \nu(t^m)| \leq \widetilde{L}k$, with $\widetilde{L}/2$ the Lipschitz constant of ν, whence

$$\nu(t^{n+3}) \leq \nu(t^{n+i}) + \widetilde{L}k, \quad i = 1, 2; \tag{5.10}$$

thus, estimate (5.9) yields

$$\begin{aligned} &|\mathcal{U}^{n+3}|_G^2 - |\mathcal{U}^{n+2}|_G^2 + \rho k\|U^{n+3}\|^2 \\ &+ \frac{1}{2}k \sum_{i=1}^{2} \mu_{3-i}\Big[\nu(t^{n+3})\|U^{n+3}\|^2 - \nu(t^{n+i})\|U^{n+i}\|^2\Big] \leq \frac{1}{2}\widetilde{L}k^2 \sum_{i=1}^{2} \mu_{3-i}\|U^{n+i}\|^2. \end{aligned} \tag{5.11}$$

Summing here from $n = 0$ to $n = m - 3$, we obtain

$$
\begin{aligned}
&|\mathcal{U}^m|_G^2 + \rho k \sum_{n=3}^{m} \|U^n\|^2 + \frac{1}{2} k \big[(\mu_1+\mu_2)\nu(t^m)\|U^m\|^2 + \mu_2 \nu(t^{m-1})\|U^{m-1}\|^2\big]\\
&\le |\mathcal{U}^2|_G^2 + \frac{1}{2} k(\mu_1+\mu_2)\big[\nu(t^2) + \widetilde{L}k\big]\|U^2\|^2 + \frac{1}{2} k\mu_2 \big[\nu(t^1)+\widetilde{L}k\big]\|U^1\|^2\\
&+ \ \frac{1}{2}(\mu_1+\mu_2)\widetilde{L}k^2 \sum_{n=3}^{m-1} \|U^n\|^2.
\end{aligned}
$$

For k sufficiently small such that $(\mu_1+\mu_2)\widetilde{L}k \le \rho$, the last term on the right-hand side can be absorbed into the second term on the left-hand side, and we get

$$
|\mathcal{U}^m|_G^2 + \frac{\rho}{2} k \sum_{n=3}^{m} \|U^n\|^2 \le |\mathcal{U}^2|_G^2 + c_1 k \big(\|U^1\|^2 + \|U^2\|^2\big).
$$

Using now the lower bound $|\mathcal{U}^m|_G^2 \ge \lambda^\star_{\min}|U^m|^2 \ge \frac{3}{338}|U^m|^2$, see Remark 2.1, as well as the obvious estimate $|\mathcal{U}^2|_G^2 \le \widehat{C}\big(|U^0|^2 + |U^1|^2 + |U^2|^2\big)$, we obtain the desired stability estimate (5.2). □

5.2. **The implicit–explicit method for the nonlinear equation.** In this section we prove local stability of the implicit–explicit three-step BDF method, (1.12) for $q = 3$, for the nonlinear parabolic equation (1.9).

Besides the approximations $U^n \in \mathscr{B}_{u(t^n)}$ satisfying (1.12), for $q = 3$, we consider implicit–explicit three-step BDF approximations $V^n \in \mathscr{B}_{u(t^n)}$ such that

$$
\sum_{i=0}^{3} \alpha_i V^{n+i} + kA(t^{n+3})V^{n+3} = k \sum_{i=0}^{2} \gamma_i B(t^{n+i}, V^{n+i}), \quad n = 0,\dots,N-3. \tag{5.12}
$$

Theorem 5.1 (Stability of the implicit–explicit three-step BDF scheme)**.** *Assume* (1.13)*,* (1.14) *and* (1.15)*. Then, under the stability condition*

$$
\forall t \in [0,T] \quad \kappa(t) - \frac{1}{13}\nu(t) - 7\cdot\frac{14}{13}\tilde{\lambda}(t) \ge \rho > 0, \tag{5.13}
$$

the implicit–explicit three-step BDF method, (1.12) *for* $q = 3$*, is locally stable in the sense that, with* $\vartheta^m := U^m - V^m$*, for* k *sufficiently small,*

$$
\frac{3}{338}|\vartheta^n|^2 + \frac{1}{2}\rho k \sum_{\ell=3}^{n} \|\vartheta^\ell\|^2 \le C \sum_{j=0}^{2} \big(|\vartheta^j|^2 + k\|\vartheta^j\|^2\big), \tag{5.14}
$$

for $n = 3,\dots,N$*, with* C *a constant independent of* ρ, k, n *and the approximations.*

Proof. Letting $b^m := B(t^m, U^m) - B(t^m, V^m)$ and subtracting (5.12) from (1.12), for $q = 3$, we obtain

$$
\sum_{i=0}^{3} \alpha_i \vartheta^{n+i} + kA(t^{n+3})\vartheta^{n+3} = k \sum_{i=0}^{2} \gamma_i b^{n+i}, \tag{5.15}
$$

$n = 0, \dots, N-3$. As in §5.1, we take in (5.15) the inner product with $\vartheta^{n+3} - \mu_1\vartheta^{n+2} - \mu_2\vartheta^{n+1}$, with μ_1 and μ_2 as in (1.4), and take real parts to obtain

$$\operatorname{Re}\Big(\sum_{i=0}^{3}\alpha_i\vartheta^{n+i}, \vartheta^{n+3} - \mu_1\vartheta^{n+2} - \mu_2\vartheta^{n+1}\Big) + kI_{n+3} = kJ_{n+3} \tag{5.16}$$

with

$$I_{n+3} := \operatorname{Re}\big(A(t^{n+3})\vartheta^{n+3}, \vartheta^{n+3} - \mu_1\vartheta^{n+2} - \mu_2\vartheta^{n+1}\big) \tag{5.17}$$

and

$$J_{n+3} := \operatorname{Re}\Big(\sum_{i=0}^{2}\gamma_i b^{n+i}, \vartheta^{n+3} - \mu_1\vartheta^{n+2} - \mu_2\vartheta^{n+1}\Big). \tag{5.18}$$

With the notation $\Theta^n := (\vartheta^{n-2}, \vartheta^{n-1}, \vartheta^n)^T$ and the norm $|\Theta^n|_G$ given by

$$|\Theta^n|_G^2 = \sum_{i,j=1}^{3} g_{ij}(\vartheta^{n-3+i}, \vartheta^{n-3+j}),$$

in view of (1.7), relation (5.16) yields the estimate

$$|\Theta^{n+3}|_G^2 - |\Theta^{n+2}|_G^2 + kI_{n+3} \le kJ_{n+3}. \tag{5.19}$$

Furthermore, I_{n+3} can be estimated from below exactly as in the case of the implicit three-step BDF scheme,

$$I_{n+3} \ge \Big[\kappa(t^{n+3}) - \frac{1}{26}\nu(t^{n+3})\Big]\|\vartheta^{n+3}\|^2 - \frac{1}{2}\nu(t^{n+3})\sum_{i=1}^{2}\mu_{3-i}\|\vartheta^{n+i}\|^2; \tag{5.20}$$

see (5.8). Therefore, all that remains to be done, is to estimate J_{n+3} from above in a suitable way. For simplicity of presentation, we assume in the following that $\tilde\mu = 0$ in (1.15); the general case can be treated similarly via a straightforward use of the discrete Gronwall inequality at the end of the proof. To simplify the notation, we set $\mu_0 := 1$. First, we have

$$J_{n+3} \le \sum_{i=0}^{2}|\gamma_i|\,\|b^{n+i}\|_\star \sum_{j=0}^{3}\mu_{3-j}\|\vartheta^{n+j}\|,$$

whence, in view of the local Lipschitz condition (1.15),

$$\begin{aligned}
J_{n+3} &\le \sum_{i=0}^{2}|\gamma_i|\tilde\lambda(t^{n+i})\|\vartheta^{n+i}\|\sum_{j=0}^{3}\mu_{3-j}\|\vartheta^{n+j}\| \\
&\le \frac{1}{2}\sum_{i=0}^{2}|\gamma_i|\tilde\lambda(t^{n+i})\sum_{j=0}^{3}\mu_{3-j}\big(\|\vartheta^{n+i}\|^2 + \|\vartheta^{n+j}\|^2\big) \\
&= \frac{1}{2}\cdot\frac{14}{13}\sum_{i=0}^{2}|\gamma_i|\tilde\lambda(t^{n+i})\|\vartheta^{n+i}\|^2 + \frac{1}{2}\Big(\sum_{i=0}^{2}|\gamma_i|\tilde\lambda(t^{n+i})\Big)\sum_{j=1}^{3}\mu_{3-j}\|\vartheta^{n+j}\|^2.
\end{aligned}$$

Now, since $\tilde\lambda(t^{n+i}) \le \tilde\lambda(t^{n+j}) + \widehat{L}k, i = 0,1,2, j = 1,2,3,$ and $|\gamma_0| + |\gamma_1| + |\gamma_2| = 7$, we easily see that

$$\sum_{i=0}^{2} |\gamma_i|\tilde\lambda(t^{n+i}) \le 7\tilde\lambda(t^{n+j}) + \widehat{C}k, \quad j = 1,2,3.$$

Therefore, the above estimate for J_{n+3} yields

$$\begin{aligned} J_{n+3} \le \frac12 \cdot \frac{14}{13} \sum_{i=0}^{2} |\gamma_i|\tilde\lambda(t^{n+i})\|\vartheta^{n+i}\|^2 + \frac12 7 \sum_{j=1}^{3} \mu_{3-j}\tilde\lambda(t^{n+j})\|\vartheta^{n+j}\|^2 \\ + \widehat{C}k \sum_{j=1}^{3} \mu_{3-j}\|\vartheta^{n+j}\|^2. \end{aligned} \tag{5.21}$$

In view of the stability assumption (5.13), from (5.19), (5.20) and (5.21) we infer that

$$\begin{aligned} |\Theta^{n+3}|_G^2 - |\Theta^{n+2}|_G^2 + \rho k\|\vartheta^{n+3}\|^2 + \frac12 k\nu(t^{n+3}) \sum_{i=1}^{2} \mu_{3-i}\big(\|\vartheta^{n+3}\|^2 - \|\vartheta^{n+i}\|^2\big) \\ + 7\big(\frac{14}{13} - \frac12\big)k\tilde\lambda(t^{n+3})\|\vartheta^{n+3}\|^2 \le \frac12 \cdot \frac{14}{13} k \sum_{i=0}^{2} |\gamma_i|\tilde\lambda(t^{n+i})\|\vartheta^{n+i}\|^2 \\ + \frac12 7k \sum_{i=1}^{2} \mu_{3-i}\tilde\lambda(t^{n+i})\|\vartheta^{n+i}\|^2 + \widehat{C}k^2 \sum_{i=1}^{3} \mu_{3-i}\|\vartheta^{n+3}\|^i. \end{aligned} \tag{5.22}$$

Estimating the coefficient $\nu(t^{n+3})$ of $\|\vartheta^{n+i}\|^2$ on the left-hand side of (5.22) as in (5.10), proceeding as in the proof of Proposition 5.1, and using the fact that $|\gamma_0|+|\gamma_1|+|\gamma_2| = 7$, we easily arrive at the desired stability estimate (5.14), provided k is sufficiently small. □

The sufficient stability condition (5.13) can also be written in the form (1.21) with $q = 3$. We already mentioned in (1.17) how much the coefficient of $\nu(t)$ and $\tilde\lambda(t)$ in (1.21) with $q = 3$ could be possibly decreased.

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