AN ANALOGUE TO THE A(ϑ)-STABILITY CONCEPT FOR IMPLICIT–EXPLICIT BDF METHODS*

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Dedicated to Professor Christian Lubich on the occasion of his 60^{th} *birthday, July 29, 2019.*

Abstract. For implicit–explicit multistep schemes, using a suitable form of Dahlquist's test equation, we introduce an analogue to the A(ϑ)-stability concept, valid for implicit methods, and formulate a stability criterion in terms of an auxiliary function that plays a key role in our analysis. Furthermore, for implicit–explicit backward difference formula methods, we either evaluate the auxiliary function or establish very good estimates of it; as a result, we derive a sharp or very good, respectively, unconditional stability condition, the analogue of the determination of the exact angle ϑ for implicit methods or of a good approximation thereof. A comparison with the corresponding necessary stability condition provides evidence of the quality of the sufficient stability condition. In addition, we verify our analysis with results of a series of numerical experiments.

Key words. Test equation, implicit–explicit multistep methods, BDF methods, A(ϑ)-stability, unconditional stability, stability conditions.

AMS subject classifications. Primary 65L06, 65L20; Secondary 65L04

1. Introduction.

We consider Dahlquist's first test problem in the form

$$\begin{cases} y'(t) + (1 + \mathrm{i}\lambda)y(t) = \mu y(t), & t \geqslant 0, \\ y(0) = 1, \end{cases} \tag{1.1}$$

with λ and μ *real* and *complex* constants, respectively; cf. [14]. Let us note already at this point that in this paper we are interested in the *unconditional* stability of numerical methods for (1.1); therefore, the zero-order terms of the test differential equation in (1.1) could have been multiplied by a positive constant a; the fact that we fixed the real part of the coefficient $1+\mathrm{i}\lambda$ equal to 1 is just a matter of normalization. An advantage of the present form of the test equation is that it allows a slight reinterpretation of the A(ϑ)-stability concept for implicit methods, which can be straightforwardly extended to implicit–explicit multistep schemes. Obviously, $|y(t)| = \mathrm{e}^{(\operatorname{Re}\mu-1)t}$ remains bounded if $\operatorname{Re}\mu \leqslant 1$.

Let (α, β) and (α, γ) be the implicit and explicit q-step backward difference (or differen-

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tiation) formula (BDF) methods, respectively, generated by the polynomials α, β and γ,

$$\begin{cases} \alpha(\zeta) = \sum_{j=1}^{q} \frac{1}{j} \zeta^{q-j}(\zeta-1)^j = \sum_{i=0}^{q} \alpha_i \zeta^i, \quad \beta(\zeta) = \zeta^q, \\ \gamma(\zeta) = \zeta^q - (\zeta-1)^q = \sum_{i=0}^{q-1} \gamma_i \zeta^i, \end{cases} \tag{1.2}$$

$q = 1, \dots, 6$. The implicit q-step BDF methods are strongly A(ϑ_q)-stable with $\vartheta_1 = \vartheta_2 = 90°$, $\vartheta_3 \approx 86.03°$, $\vartheta_4 \approx 73.35°$, $\vartheta_5 \approx 51.84°$, and $\vartheta_6 \approx 17.84°$; see [21, Section V.2]. Exact values of $\vartheta_3, \vartheta_4, \vartheta_5, \vartheta_6$ are given in [7]; see also [24] and [18]. The order of method (α, β) is $p = q$. For a given α, method (α, γ) is the unique explicit q-step scheme of order $p = q$. The one-step implicit and explicit schemes, respectively, are the implicit and the explicit Euler methods.

Let $h > 0$ be an arbitrary constant time step, $t^n := nh, n \in \mathbb{N}_0$, and $y^0, \dots, y^{q-1} \in \mathbb{C}$ be arbitrary starting approximations to the initial value 1. We consider the discretization of the initial value problem (1.1) by the implicit–explicit q-step BDF scheme (α, β, γ); more precisely, we discretize the left-hand side of the differential equation in (1.1) by the implicit scheme (α, β) and the term on the right-hand side by the explicit scheme (α, γ), i.e., we recursively define approximations $y^n, n \geqslant q$, to the nodal values $y(t^n)$ as follows:

$$\sum_{i=0}^{q} \alpha_i y^{n+i} + h(1 + \mathrm{i}\lambda) y^{n+q} = h\mu \sum_{i=0}^{q-1} \gamma_i y^{n+i}, \quad n \in \mathbb{N}_0. \tag{1.3}$$

Since α_q is positive, given starting approximations $y^0, \dots, y^{q-1} \in \mathbb{C}$, the approximations $y^n, n \geqslant q$, are well defined by (1.3).

It is well known that the multistep scheme (1.3) is *unconditionally stable*, i.e., stable for all positive h, that is, the numerical approximations remain bounded for all positive h, if and only if the family of polynomials $\rho(\cdot; h)$,

$$\rho(\zeta; h) := \alpha(\zeta) + h(1 + \mathrm{i}\lambda)\beta(\zeta) - h\mu\gamma(\zeta), \quad h > 0, \tag{1.4}$$

satisfy the root condition; see, e.g., [20, Section III.3], [12, pp. 113–115].

1.1. Main problem. Here, we focus on the following problem, which may be viewed as an attempt to extend the well-known A(ϑ)-stability concept for implicit methods, introduced by Olof Widlund, cf. [32], to implicit–explicit multistep schemes.

Problem 1.1. *Under what conditions on given nonnegative constants $\hat{\lambda}$ and $\hat{\mu}$ is the implicit–explicit BDF scheme* (1.3) *unconditionally stable for all real λ and complex μ of modulus not exceeding $\hat{\lambda}$ and $\hat{\mu}$, respectively?*

The motivation for considering this problem is completely analogous to the motivation for the A(ϑ)-stability for implicit methods; for instance, it leads to *necessary* stability conditions of implicit–explicit BDF schemes for parabolic equations, thus enabling us to study the discrepancy between sufficient and necessary stability conditions; cf., e.g., [3]. For $\hat{\mu} = 0$, i.e., for the implicit method (α, β), the answer to Problem 1.1 is an immediate consequence of the

A(ϑ_q)-stability: the implicit method is unconditionally stable for (1.1) if $|\lambda| \leqslant \hat{\lambda} \leqslant \tan\vartheta_q$. This condition is sharp: if $\hat{\lambda} > \tan\vartheta_q$, then the method is, in general, not unconditionally stable. The case that the term on the right-hand side, $\mu y(t)$, is also discretized implicitly, i.e., in the form $h\mu y^{n+q}$, is also easy: for $(\cos\vartheta_q)\hat{\lambda} + \hat{\mu} \leqslant \sin\vartheta_q$, the points $(1 + \mathrm{i}\lambda) - \mu$ lie in the stability sector $S_{\vartheta_q} := \{z \in \mathbb{C} : z = \rho e^{\mathrm{i}\varphi}, \rho \geqslant 0, |\varphi| \leqslant \vartheta_q\}$ of the implicit method (α, β), and the scheme is unconditionally stable; this is also a sharp condition in the sense that if $(\cos\vartheta_q)|\lambda| + |\mu| > \sin\vartheta_q$, the scheme is, in general, not unconditionally stable; notice that $\sin\vartheta_q - (\cos\vartheta_q)|\lambda|$ is the distance of the point $1 + \mathrm{i}\lambda$ from the boundary of the stability sector S_{ϑ_q} of the method; cf. [3, Figure 1].

1.2. Main results. First, we shall formulate in Proposition 1.2 an *unconditional stability criterion* for (1.3) in terms of the auxiliary function

$$K_{(\alpha,\beta,\gamma)}(y) := \sup_{s>0} \max_{\zeta\in\mathscr{K}} \frac{|s\gamma(\zeta)|}{|\alpha(\zeta) + s(1 + \mathrm{i}y)\beta(\zeta)|}, \quad -\tan\vartheta_q < y < \tan\vartheta_q; \tag{1.5}$$

here, $\mathscr{K}$ is the unit circle in the complex plane, $\mathscr{K} := \{z \in \mathbb{C} : |z| = 1\}$. Notice that in the denominator and in the numerator we have the modulus of the characteristic polynomials of the terms on the left- and the right-hand side of (1.3), respectively, with the time step h replaced by s and λ replaced by y; the factor μ is not included since this would simply result in the multiplication of $K_{(\alpha,\beta,\gamma)}(y)$ by $|\mu|$. We take the supremum over all positive s because we are interested in the unconditional stability of the method, for all positive h; the maximum on the unit circle will enable us to check the root condition. It is easily seen that $K_{(\alpha,\beta,\gamma)}$ is an even function of y.

As we shall see, for $q > 1$, function $K_{(\alpha,\beta,\gamma)}$ is not increasing in $(0, \tan\vartheta_q)$. Therefore, the modification $\widetilde{K}_{(\alpha,\beta,\gamma)}$ of $K_{(\alpha,\beta,\gamma)}$,

$$\widetilde{K}_{(\alpha,\beta,\gamma)}(y) := \sup_{0\leqslant\tau\leqslant y} K_{(\alpha,\beta,\gamma)}(\tau), \quad 0 \leqslant y < \tan\vartheta_q, \tag{1.6}$$

is important for our purposes. For $-\tan\vartheta_q < y < 0$, we let $\widetilde{K}_{(\alpha,\beta,\gamma)}(y) := \widetilde{K}_{(\alpha,\beta,\gamma)}(-y)$.

The unconditional stability criterion for (1.3) is:

Proposition 1.2 (Unconditional stability criterion). *The following conditions*

$$\hat{\mu} \leqslant 1/\widetilde{K}_{(\alpha,\beta,\gamma)}(\hat{\lambda}) =: b_{q,o}(\hat{\lambda}) \tag{1.7}$$

and

$$\hat{\mu} < 1/\widetilde{K}_{(\alpha,\beta,\gamma)}(\hat{\lambda}) = b_{q,o}(\hat{\lambda}) \tag{1.8}$$

are necessary and sufficient, respectively, for the unconditional stability of the implicit–explicit q-step BDF scheme, $q = 1, \dots, 6$, for (1.1) for all real λ and complex μ of modulus not exceeding $\hat{\lambda}$ and $\hat{\mu}$, respectively.

The interpretation of (1.7) and (1.8) is that the roots of all polynomials $\rho(\cdot; h)$ of (1.4) lie in the closed and open unit disk, respectively, in the complex plane for these λ and μ. In particular, (1.7) is necessary for these polynomials to satisfy the root condition.

Our approach up to this point, Problem 1.1 and Proposition 1.2, corresponding to the A(ϑ)-stability concept and the A(ϑ)-stability criterion, respectively, applies to all implicit–explicit multistep methods (α,β,γ), provided the implicit method (α,β) is strongly A(ϑ)-stable; this condition ensures boundedness of the function $K_{(\alpha,\beta,\gamma)}$ in compact subsets of the interval $(-\tan\vartheta,\tan\vartheta)$.

The last, crucial step, the evaluation of the optimal bound $b_{q,o}(\hat\lambda)$ or the determination of a good lower bound thereof, is the analogue of the actual determination of the maximum angle ϑ. In this paper, we carry this out for the popular implicit–explicit BDF methods.

First, as expected, due to the A-stability of the implicit Euler and two-step BDF methods, $\hat\lambda$ does not enter into the stability conditions (1.7) and (1.8) in the case of the corresponding implicit–explicit methods; in other words, the bounds $b_{q,o}(y), q=1,2$, are constant. More precisely, $b_{q,o}(y)=1/(2^q-1), y\geqslant 0$. Actually, it turns out that the strict inequality in the sufficient stability condition (1.8) can be relaxed to a nonstrict inequality. Therefore, these two methods are unconditionally stable for (1.1), if and only if

$$\hat\mu\leqslant 1 \quad\text{and}\quad \hat\mu\leqslant\frac{1}{3}, \tag{1.9}$$

respectively.

The case of high order methods is considerably more involved. To give a somewhat simplified form of the optimal bound $b_{q,o}$ in Proposition 1.2, we need suitable notation. For $\zeta\in\mathscr{K},\zeta=\mathrm{e}^{\mathrm{i}t}=\cos t+\mathrm{i}\sin t$, let $x:=\cos t$. For $q=3,4,5,6$, with $d(\zeta)=\alpha(\zeta)/\beta(\zeta)$, it is convenient to introduce the functions φ and ψ by

$$d(\zeta)=c_q\Big[-\psi(x)\sqrt{1-x}+\mathrm{i}\frac{\varphi(x)}{\sqrt{1+x}}\sin t\Big],\quad\text{with}\quad c_3=c_4=\frac{1}{3},\quad c_5=c_6=\frac{1}{15}, \tag{1.10}$$

as well as the corresponding polynomials $p,r\in\mathbb{P}_{q-1}$ and the function f_q,

$$p(x):=[\varphi(x)]^2+[\psi(x)]^2,\quad r(x):=|\gamma(\zeta)|^2,\quad f_q(x):=p(x)/[\varphi(x)]^2. \tag{1.11}$$

Let $x_1<x_2$ be the roots of ψ such that ψ is positive in the interval (x_1,x_2). The relation $\max_{x_1<x<x_2}f_q(x)=1/\sin^2\vartheta_q$, see [7, (10) and (5)], yields

$$\varphi(x)\geqslant(\tan\vartheta_q)\psi(x)\quad\text{for}\quad x_1<x<x_2. \tag{1.12}$$

The geometric interpretation of (1.12) is that no point $-d(\zeta),\zeta\in\mathscr{K}$, lies in the interior of the sector S_{ϑ_q}.

Theorem 1.3 (Simplified form of the optimal bound $b_{q,o}$). *For $q=3,4,5,6$, the optimal bound $b_{q,o}$ in Proposition 1.2 takes the form*

$$b_{q,o}(y)=\begin{cases}\dfrac{1}{2^q-1} & \text{for}\ \ 0\leqslant y\leqslant y_q^\star,\\[2ex] \displaystyle\min_{x_1<x<x_2}\frac{\varphi(x)-y\psi(x)}{\sqrt{p(x)r(x)}} & \text{for}\ \ y_q^\star<y<\tan\vartheta_q,\end{cases} \tag{1.13}$$

with

$$\begin{cases}y_3^\star:=10.747771218818176, & y_4^\star:=2.465496414280889,\\ y_5^\star:=0.899586281651322, & y_6^\star:=0.141292221298238.\end{cases} \tag{1.14}$$

Let us recall from [7] that

$$\begin{cases} \tan\vartheta_3 = 14.417705545479805, & \tan\vartheta_4 = 3.344127598057502, \\ \tan\vartheta_5 = 1.272589304065916, & \tan\vartheta_6 = 0.321830865317692. \end{cases} \tag{1.15}$$

In view of (1.13), the sharp sufficient stability condition (1.8) is very simple in the interval $[0, y_q^\star]$ but not particularly convenient in the interval $(y_q^\star, \tan\vartheta_q)$ since the evaluation of the optimal bound $b_{q,o}(y)$ requires some effort. As we shall see, the optimal bound $b_{q,o}$ is nonlinear in $(y_q^\star, \tan\vartheta_q)$. It turns out that replacing $b_{q,o}$ in (1.8) by its linear interpolant $b_{q,s}$ at the endpoints $y_q^\star$ and $\tan\vartheta_q$ results in a very convenient and good (but nonsharp) linear sufficient stability condition for $y_q^\star < y < \tan\vartheta_q$; we prove that $b_{q,s}(y)$ is a lower bound of $b_{q,o}(y)$ and provide convincing evidence that it is a good approximation thereof.

Summarizing, our main result for high-order implicit–explicit BDF methods is as follows.

Theorem 1.4 (Sufficient stability conditions). *The implicit–explicit q-step BDF scheme, $q = 3, 4, 5, 6$, is unconditionally stable for (1.1) for all real λ and complex μ of modulus not exceeding $\hat\lambda$ and $\hat\mu$, respectively, provided*

$$\begin{cases} \hat\mu < \dfrac{1}{2^q - 1} =: b_{q,s}(\hat\lambda) = b_{q,o}(\hat\lambda) & \text{for } \ 0 \leqslant \hat\lambda \leqslant y_q^\star, \\[2ex] \hat\mu < \dfrac{1}{2^q - 1}\dfrac{\tan\vartheta_q - \hat\lambda}{\tan\vartheta_q - y_q^\star} =: b_{q,s}(\hat\lambda) & \text{for } \ y_q^\star < \hat\lambda < \tan\vartheta_q. \end{cases} \tag{1.16}$$

The bound in the first line of the sufficient stability condition (1.16) coincides with the optimal bound $b_{q,o}$. In contrast, the *linear* bound $b_{q,s}$ in the second line of (1.16) is not sharp; the optimal bound $b_{q,o}$ is *nonlinear* in the interval $(y_q^\star, \tan\vartheta_q)$. Fortunately, the sufficient stability condition in (1.16) is very good also in $(y_q^\star, \tan\vartheta_q)$ since the discrepancy between the bounds $b_{q,o}$ and $b_{q,s}$ is very small there; the graphs in Figure 1.1, with the nonlinearity being almost invisible in $(y_q^\star, \tan\vartheta_q)$, and the data in Table 1.1 as well as our numerical results in section 7 provide convincing evidence for this claim. The geometric interpretation of the sufficient stability condition (1.16) is that $(\hat\lambda, \hat\mu)$ lie in the corresponding trapezoids in Figure 1.1.

Discrepancy between the sufficient stability conditions (1.16) *and* (1.8). In the intervals $[0, y_q^\star]$, the sufficient stability condition (1.16) is sharp since $b_{q,s}$ and $b_{q,o}$ coincide. Let us now consider the discrepancy $d_q(y) := b_{q,o}(y) - b_{q,s}(y)$ and the relative discrepancy $d_{q,r}(y) := \frac{b_{q,o}(y)}{b_{q,s}(y)} - 1$ between the bounds of the convenient linear sufficient stability condition (1.16) and the sharp nonlinear sufficient stability condition (1.8) in the interval $(y_q^\star, \tan\vartheta_q)$. For uniform partitions $y_q^\star = y_0 < \cdots < y_{100} = \tan\vartheta_q$, we evaluated d_q and $d_{q,r}$ at the interior nodes $y_1, \dots, y_{99}$. In contrast to the discrepancy, the relative discrepancy increases as y approached $\tan\vartheta_q$ since both bounds become very small; therefore, in Table 1.1 we present the results separately for the first two quarters, from left to right, and for the third and fourth quarters,

$$d_q := \max_{1\leqslant i\leqslant 99} d(y_i), d_{q,r}^{1,2} := \max_{1\leqslant i\leqslant 50} d_{q,r}(y_i), d_{q,r}^{3} := \max_{50\leqslant i\leqslant 75} d_{q,r}(y_i), d_{q,r}^{4} := \max_{75\leqslant i\leqslant 99} d_{q,r}(y_i). \tag{1.17}$$

Table 1.1

Maximal discrete discrepancy d_q and relative discrepancies $d_{q,r}$ in $[y_q^\star, \tan\vartheta_q)$; see (1.17).

q	d_q	$d_{q,r}^{1,2}$ (1st & 2nd quarters)	$d_{q,r}^{3}$ (3rd quarter)	$d_{q,r}^{4}$ (4th quarter)
3	$1.009081 \cdot 10^{-3}$	$1.3942108 \cdot 10^{-2}$	$1.9737417 \cdot 10^{-2}$	$2.4656523 \cdot 10^{-2}$
4	$1.440568 \cdot 10^{-3}$	$4.2710986 \cdot 10^{-2}$	$6.1319520 \cdot 10^{-2}$	$7.7559374 \cdot 10^{-2}$
5	$9.104154 \cdot 10^{-4}$	$5.5818262 \cdot 10^{-2}$	$8.0739529 \cdot 10^{-2}$	$10.284578 \cdot 10^{-2}$
6	$3.017380 \cdot 10^{-4}$	$3.7625951 \cdot 10^{-2}$	$5.5255248 \cdot 10^{-2}$	$7.1345866 \cdot 10^{-2}$

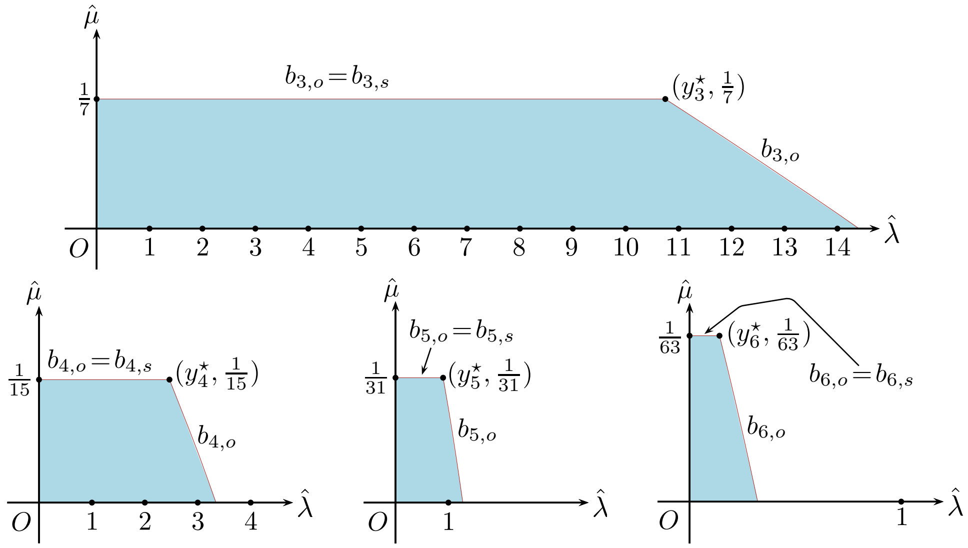

Figure 1.1. *The graphs of the optimal bounds $b_{q,o}, q = 3, 4, 5, 6$, for the implicit–explicit q-step BDF method; the graph is not a linear segment in $[y_q^\star, \tan\vartheta_q)$. The sufficient stability condition (1.16) means that $(\hat\lambda, \hat\mu)$ lie in the blue trapezoids. The graph of the piecewise linear bounds $b_{q,s}$ of the sufficient stability condition coincides with the graph of $b_{q,o}$ in $[0, y_q^\star]$. The graph of $b_{q,s}$ in $[y_q^\star, \tan\vartheta_q)$, a side of the trapezoid (not shown here), is the linear interpolant of the graph of $b_{q,o}$; the discrepancy between the two graphs would be almost invisible.*

1.3. Related work. The analysis of multistep methods for parabolic equations originated in [33]; see also [34]. Low-order linearized schemes for nonlinear parabolic equations were used already in the early 1970s; see, for instance, [15], [16]. High-order implicit–explicit multistep schemes, including the implicit–explicit BDF methods (1.2), for linear parabolic equations, were introduced and analyzed by M. Crouzeix, [13]; see also [4] and [1] for the application to nonlinear equations. Implicit–explicit two-step schemes were considered in [31].

Multistep methods for stiff differential equations are analyzed in [25] and for parabolic equations also in [2, 6, 8, 10, 19, 23, 26, 28, 30].

The *stability region* $S \subset \mathbb{C}^2$ of the implicit–explicit (α, β, γ)-method consists of the points $(\lambda h, \mu h) \in \mathbb{C}^2, h > 0$, such that the scheme

$$\sum_{i=0}^{q} \alpha_i y^{n+i} + h\lambda y^{n+q} = h\mu \sum_{i=0}^{q-1} \gamma_i y^{n+i}, \quad n \in \mathbb{N}_0, \tag{1.18}$$

for the test equation $y' + \lambda y = \mu y$, with $\lambda, \mu \in \mathbb{C}$, is stable. For low-order methods, with the implicit method being A-stable, this problem was addressed in [17], where subdomains of the stability regions were determined. In [11] and [22], the behavior of implicit–explicit methods of order up to 5, including the corresponding methods considered here, was studied, for a special class of test equations, namely, with real λ and imaginary μ, and stability contours in $\mathbb{C}$ were determined. In [29] the test equation $y' + \lambda y = \lambda\mu y$, with $\lambda > 0$ and $\mu \in \mathbb{C}$, is discretized by q-step implicit–explicit methods of order q, with $q = 1, \dots, 5$; the methods depend on a parameter $0 < \delta \leqslant 1$ and reduce to (1.2) for $\delta = 1$. For each method, under a numerically verified positivity condition of a quantity $G(\delta)$, cf. [29, (24)], the stability region consisting of all $\mu \in \mathbb{C}$ such that the method is stable for all $0 < \lambda \leqslant \infty$ is determined.

Here, we focus on the easier Problem 1.1.

An outline of the paper is as follows. In Section 2, we prove Proposition 1.2 and discuss some properties of the auxiliary function $K_{(\alpha,\beta,\gamma)}$. In Section 3, we treat the easy case of low-order methods. Sections 4 and 6 constitute the hard kernel of the paper, a detailed study of the auxiliary function; in the former we prove Theorem 1.3 and the part of Theorem 1.4 concerning stability under the sufficient stability condition in the first line of (1.16), and in the latter we establish the remaining part of Theorem 1.4; the analysis is elementary but quite involved. In Section 5 we present the graphs of the auxiliary function. In Section 7, we provide computational evidence of the sharpness of our theoretical results.

2. Proof of Proposition 1.2 and some properties of the auxiliary function. In this section we prove the unconditional stability criterion of Proposition 1.2 and discuss some properties of the auxiliary function $K_{(\alpha,\beta,\gamma)}$ of (1.5).

2.1. Proof of Proposition 1.2. First, for a given $\lambda \in (-\tan\vartheta_q, \tan\vartheta_q)$, it is easily seen that

$$K_{(\alpha,\beta,\gamma)}(\lambda)\hat{\mu} \leqslant 1 \tag{2.1}$$

is a necessary stability condition for the implicit–explicit scheme (1.3) for all equations (1.1) with $|\mu| = \hat{\mu}$. Indeed, assume that (2.1) is not satisfied. Then, for the function k,

$$k(\tau, \zeta) := \frac{\hat{\mu}\tau\gamma(\zeta)}{\alpha(\zeta) + \tau(1 + \mathrm{i}\lambda)\beta(\zeta)}, \quad \tau > 0, \ |\zeta| \geqslant 1, \tag{2.2}$$

we have

$$\exists z \in \mathscr{K}, \ s > 0 \quad |k(s, z)| > 1. \tag{2.3}$$

Since $\lim_{|\zeta|\to\infty} |k(s, \zeta)| = 0$, we infer that there exists a $\zeta^\star \in \mathbb{C}$ with $|\zeta^\star| > 1$ such that $|k(s, \zeta^\star)| = 1$, i.e.,

$$\frac{\hat{\mu}s\gamma(\zeta^\star)}{\alpha(\zeta^\star) + s(1 + \mathrm{i}\lambda)\beta(\zeta^\star)} = \mathrm{e}^{-\mathrm{i}t},$$

for a $t \in [0, 2\pi)$. Therefore, with $\mu := \hat{\mu}\mathrm{e}^{\mathrm{i}t}$,

$$\alpha(\zeta^\star) + s(1 + \mathrm{i}\lambda)\beta(\zeta^\star) - s\mu\gamma(\zeta^\star) = 0. \tag{2.4}$$

Thus, for $h = s$, the root condition is not satisfied, whence the scheme (1.3) is unstable. The interpretation of (2.1) is that the roots of the polynomials $\rho(\zeta; h) := \alpha(\zeta) + h(1 + \mathrm{i}\lambda)\beta(\zeta) - h\mu\gamma(\zeta), h > 0$, with $|\mu| = \hat{\mu}$, lie in the closed unit disk in the complex plane.

We immediately infer from (2.1) and the definition of $\widetilde{K}_{(\alpha,\beta,\gamma)}$ that (1.7) is a necessary condition for the unconditional stability of the implicit–explicit scheme (1.3) *for all* λ and μ considered in Proposition 1.2.

Similarly, the analogue of (2.1) with the nonstrict inequality replaced by a strict inequality ensures that the roots of the polynomials $\rho(\zeta; h) := \alpha(\zeta) + h(1 + \mathrm{i}\lambda)\beta(\zeta) - h\mu\gamma(\zeta), h > 0$, with $|\mu| = \hat{\mu}$, lie in the open unit disk in the complex plane, and we infer that (1.3) is stable. As before, we see that (1.8) is a sufficient condition for the unconditional stability of the implicit–explicit scheme (1.3) for all λ and μ considered in Proposition 1.2

2.2. Properties of the auxiliary function. For $q > 1$, function $K_{(\alpha,\beta,\gamma)}$ is not increasing in $(0, \tan\vartheta_q)$; cf. the graph of $K_{(\alpha,\beta,\gamma)}$ for the implicit–explicit two-step BDF method, for nonnegative y, in Figure 2.1, as well as the graphs of the reciprocals of $K_{(\alpha,\beta,\gamma)}$ for the implicit–explicit high-order BDF methods in Figures 5.1–5.2. This is the motivation for the introduction of the modification $\widetilde{K}_{(\alpha,\beta,\gamma)}$ of $K_{(\alpha,\beta,\gamma)}$ in (1.6).

The constant $K_{(\alpha,\beta,\gamma)} := K_{(\alpha,\beta,\gamma)}(0)$ was introduced in [4] and is explicitly known, namely,

$$K_{(\alpha,\beta,\gamma)}(0) = |\gamma(-1)| = 2^q - 1; \tag{2.5}$$

see [4]. In this paper we bypass the minor computational part of the verification of (2.5) in [4].

Let $d(\zeta) := \alpha(\zeta)/\beta(\zeta)$ for ζ on $\mathscr{K}$ represent the points of the *root locus curve* of the implicit method (α, β). The points $-d(\zeta), \zeta \in \mathscr{K}$, do not lie in the interior of the stability sector S_{ϑ_q}. We introduce the parts $\mathscr{K}_y^+$ and $\mathscr{K}_y^-$ of the unit circle $\mathscr{K}$ according to the sign of $\operatorname{Re}\big((1 - \mathrm{i}y)d(\zeta)\big)$,

$$\mathscr{K}_y^+ := \{\zeta \in \mathscr{K} : \operatorname{Re}\big((1 - \mathrm{i}y)d(\zeta)\big) \geqslant 0\}, \quad \mathscr{K}_y^- := \{\zeta \in \mathscr{K} : \operatorname{Re}\big((1 - \mathrm{i}y)d(\zeta)\big) < 0\}.$$

For a fixed $\zeta \in \mathscr{K}$, the determination of the supremum over s in (1.5) reduces to the minimization of a quadratic polynomial; we obtain

$$K_{(\alpha,\beta,\gamma)}(y) = \max\Big\{\frac{1}{\sqrt{1 + y^2}} \max_{\zeta \in \mathscr{K}_y^+} |\gamma(\zeta)|, \sup_{\zeta \in \mathscr{K}_y^-} \frac{|d(\zeta)|}{|\operatorname{Im}\big((1 - \mathrm{i}y)d(\zeta)\big)|}|\gamma(\zeta)|\Big\} \tag{2.6}$$

for $-\tan\vartheta_q < y < \tan\vartheta_q$; see [3, (3.17)], and notice that $|\beta(\zeta)| = 1$ for $\zeta \in \mathscr{K}$.

A simple representation of $K_{(\alpha,\beta,\gamma)}$ is unfortunately not available. Letting s tend to infinity, it follows immediately from (1.5) that

$$K_{(\alpha,\beta,\gamma)}(y) \geqslant \frac{1}{\sqrt{1 + y^2}} \max_{\zeta \in \mathscr{K}} |\gamma(\zeta)|. \tag{2.7}$$

Furthermore, an obvious consequence of the definition (1.5) is that

$$K_{(\alpha,\beta)}(y) \min_{\zeta \in \mathscr{K}} |\gamma(\zeta)| \leqslant K_{(\alpha,\beta,\gamma)}(y) \leqslant K_{(\alpha,\beta)}(y) \max_{\zeta \in \mathscr{K}} |\gamma(\zeta)|, \tag{2.8}$$

with $K_{(\alpha,\beta)}(y)$ given by the analogue to (1.5) with $\gamma(\zeta)$ replaced by $\beta(\zeta)$; a simple representation of $K_{(\alpha,\beta)}(y)$ is given in [3, (3.9)].

In particular, for A-stable methods (α,β), $K_{(\alpha,\beta)}(y)=1$; see [3, (3.9)]. In the simplest case of the implicit–explicit one-step BDF method, i.e., of the implicit–explicit Euler method, we have $|\gamma(\zeta)|=1$, and infer from (2.8) that $K_{(\alpha,\beta,\gamma)}(y)$ is constant,

$$K_{(\alpha,\beta,\gamma)}(y)=1,\quad y\in\mathbb{R}. \tag{2.9}$$

This is an exception. For the implicit–explicit two-step BDF method, $\alpha(\zeta)=\frac{3}{2}\zeta^2-2\zeta+\frac{1}{2},\beta(\zeta)=\zeta^2,\gamma(\zeta)=2\zeta-1$, we have $1=|\gamma(1)|\leqslant|\gamma(\zeta)|\leqslant|\gamma(-1)|=3$ for $\zeta\in\mathscr{K}$ and infer from (2.8) that

$$1\leqslant K_{(\alpha,\beta,\gamma)}(y)\leqslant K_{(\alpha,\beta,\gamma)}(0)=3,\quad y\in\mathbb{R}; \tag{2.10}$$

cf. (2.5). Let us now show that $K_{(\alpha,\beta,\gamma)}(y)$ tends to 1 as y tends to infinity, and thus the lower bound in (2.10) cannot be improved; see also the graph of $K_{(\alpha,\beta,\gamma)}$ in Figure 2.1. First, since the first term on the right-hand side of (2.6) does not exceed 1 for $y\geqslant 2\sqrt{2}$, it suffices to consider the second term. Now, for $\zeta\in\mathscr{K},\zeta=\mathrm{e}^{\mathrm{i}t}=\cos t+\mathrm{i}\sin t$, with $x:=\cos t$, we have $d(\zeta)=(1-x)^2+\mathrm{i}(2-x)\sin t$ and $\gamma(\zeta)=2x-1+2\mathrm{i}\sin t$, whence

$$|d(\zeta)\gamma(\zeta)|^2=(1-x)(5-3x)(5-4x); \tag{2.11}$$

furthermore,

$$\begin{cases}\operatorname{Re}\big((1-\mathrm{i}y)d(\zeta)\big)=(1-x)^2+y(2-x)\sin t,\\ \operatorname{Im}\big((1-\mathrm{i}y)d(\zeta)\big)=(2-x)\sin t-y(1-x)^2.\end{cases} \tag{2.12}$$

Now, $\zeta\in\mathscr{K}_y^-$ if and only if $(1-x)^2+y(2-x)\sin t<0$; in particular, we must have $y>0,x\neq\pm1$ and $\sin t<0$, in which case the condition reads

$$\sqrt{(1-x)^3}<y(2-x)\sqrt{1+x}. \tag{2.13}$$

Notice that, for any fixed $x\in(-1,1)$, condition (2.13) is satisfied for sufficiently large y. For $\sin t<0$, we have

$$|\operatorname{Im}\big((1-\mathrm{i}y)d(\zeta)\big)|=(2-x)\sqrt{1-x^2}+y(1-x)^2,$$

and, in view also of (2.11),

$$\frac{|d(\zeta)|}{|\operatorname{Im}\big((1-\mathrm{i}y)d(\zeta)\big)|}|\gamma(\zeta)|=\frac{\sqrt{(5-3x)(5-4x)}}{(2-x)\sqrt{1+x}+y\sqrt{(1-x)^3}}; \tag{2.14}$$

cf. the second term on the right-hand side of (2.6). Obviously, for fixed $x\in(-1,1)$, the expression on the right-hand side of (2.14) tends to 0 as y tends to ∞, while, for fixed $y>0$, it tends to 1 as x increases to 1; this yields the desired property, namely, $K_{(\alpha,\beta,\gamma)}(y)\to1$ as $y\to\infty$.

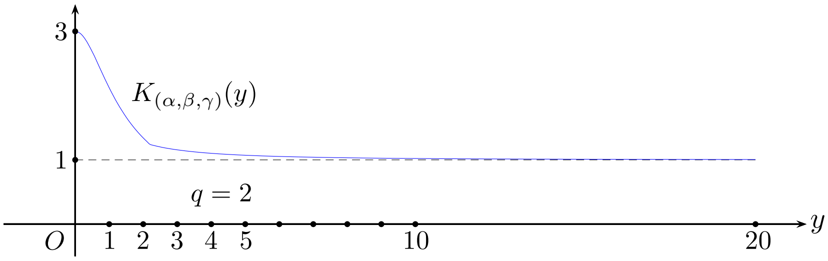

Figure 2.1. *The graph of $K_{(\alpha,\beta,\gamma)}$ for the implicit–explicit two-step BDF method, for nonnegative y.*

Let us now slightly simplify the representation of $\widetilde{K}_{(\alpha,\beta,\gamma)}(y)$ for $q = 3,4,5,6$. The first term in brackets on the right-hand side of (2.6) is not really useful since it does not exceed $K_{(\alpha,\beta,\gamma)}(0) = 2^q - 1$ and it attains $2^q - 1$ for $y = 0$; see (2.5): indeed, $|\gamma(\zeta)| \leqslant |\gamma(-1)|$ for $\zeta \in \mathscr{K}$. Therefore, $\widetilde{K}_{(\alpha,\beta,\gamma)}(y)$ takes the form

$$\widetilde{K}_{(\alpha,\beta,\gamma)}(y) = \max\big\{2^q - 1, \sup_{0\leqslant\tau\leqslant y} \varPhi(\tau)\big\} \tag{2.15}$$

with

$$\varPhi(\tau) := \sup_{\zeta\in\mathscr{K}_\tau^-} \frac{|d(\zeta)|}{|\operatorname{Im}\big((1-\mathrm{i}\tau)d(\zeta)\big)|}|\gamma(\zeta)|; \tag{2.16}$$

see Figures 2.2–2.3 for the graphs of the reciprocal f of $\varPhi$, $f(\tau) := 1/\varPhi(\tau), 0 \leqslant \tau < \tan\vartheta_q$, for $q = 3,4,5,6$. Precise values of $f(0)$ are given in Remark 4.2.

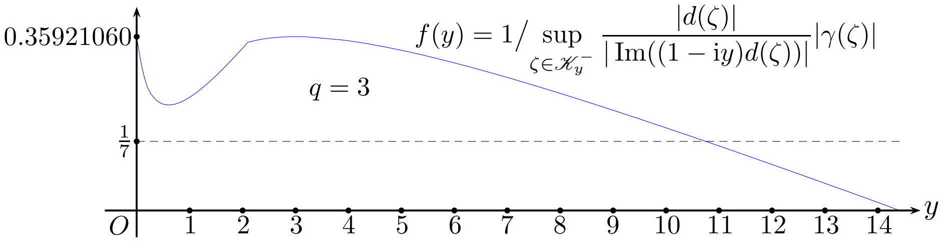

Figure 2.2. *The reciprocal f of the function $\varPhi$ of (2.16) for the implicit–explicit three-step BDF scheme; see also the second term in brackets on the right-hand side of (2.15).*

3. Unconditional stability of the implicit–explicit one- and two-step BDF methods.

The sufficiency and sharpness of the stability conditions (1.9) for the one- and two-step methods, respectively, with the nonstrict inequality replaced by a strict inequality follow from the sharp sufficient stability condition (1.8) in combination with (2.9) and (2.10), respectively. Stability under the nonstrict inequality follows from the fact that, in addition, for the one-step method, polynomial $\rho, \rho(\zeta;h) = \zeta - 1 + h(1+\mathrm{i}\lambda)\zeta - h\mu$, see (1.4), has one single root; for the two-step method, $\rho(\zeta;h) = \big[\frac{3}{2} + h(1+\mathrm{i}\lambda)\big]\zeta^2 - 2(1+h\mu)\zeta + \frac{1}{2} + h\mu$, and, obviously, for $|\mu| \leqslant 1$, we have $|1/2+\mu h| < |3/2+(1+\mathrm{i}\lambda)h|$, whence the product of the roots of ρ is strictly

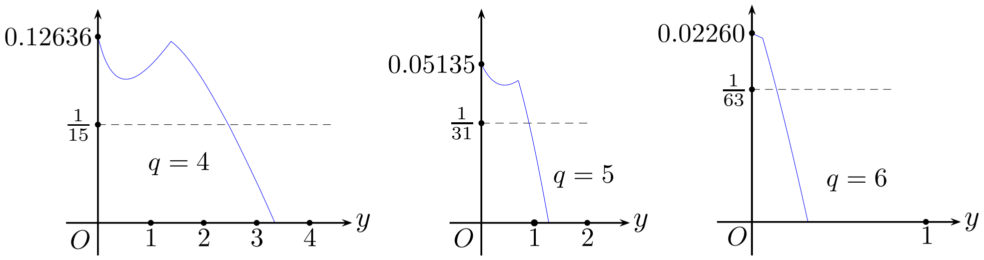

Figure 2.3. *The reciprocal f of the function Φ of (2.16) for the implicit–explicit four-, five- and six-step BDF schemes; see also the second term in brackets on the right-hand side of (2.15).*

less than 1 in modulus. In particular, ρ cannot have a unimodular double root for $|\mu| = 1/3$. Let us also note that for the second order *modified* implicit–explicit two-step BDF scheme $(\alpha, \tilde\beta, \gamma)$, with $\tilde\beta(\zeta) = 3\zeta^2/2 - \zeta + 1/2$, the corresponding stability condition is $\hat\mu < 1/2$; see [5].

The unconditional stability of these two methods can also be easily established by the energy technique, i.e., by multiplying with $\overline{y^{n+q}}$ and taking real parts. The basic property is again the A-stability of the corresponding implicit schemes. The following two relations, reflecting the G-stability property of the BDF methods, are crucial

$$\operatorname{Re}\big((y^{n+1} - y^n)\overline{y^{n+1}}\big) = \frac{1}{2}\big(|y^{n+1}|^2 - |y^n|^2 + |y^{n+1} - y^n|^2\big),$$

$$\begin{aligned}\operatorname{Re}\Big(\big(\frac{3}{2}y^{n+2} - 2y^{n+1} + \frac{1}{2}y^n\big)\overline{y^{n+2}}\Big) &= \frac{5}{4}|y^{n+2}|^2 - |y^{n+1}|^2 - \frac{1}{4}|y^n|^2\\ &- \operatorname{Re}(y^{n+2}\overline{y^{n+1}} - y^{n+1}\overline{y^n}) + \frac{1}{4}|y^{n+2} - 2y^{n+1} + y^n|^2;\end{aligned}$$

see [21, Example 6.5, pp. 308–309].

4. Proof of Theorem 1.3.

In this section we simplify the form of $\widetilde K_{(\alpha,\beta,\gamma)}(y)$ and prove Theorem 1.3; this immediately yields stability under the sufficient stability condition in the first line of (1.16). Theorem 1.3 is an immediate consequence of the following result.

Proposition 4.1 (Simplified representation of $\widetilde K_{(\alpha,\beta,\gamma)}$). *The function $\widetilde K_{(\alpha,\beta,\gamma)}$ for the implicit–explicit q-step BDF method can be written in the form*

$$\widetilde K_{(\alpha,\beta,\gamma)}(y) = \begin{cases} 2^q - 1, & 0 \leqslant y \leqslant y_q^\star,\\ K_{(\alpha,\beta,\gamma)}(y) = \displaystyle\max_{x_1<x<x_2} \frac{\sqrt{p(x)r(x)}}{\varphi(x) - y\psi(x)}, & y_q^\star < y < \tan\vartheta_q. \end{cases} \tag{4.1}$$

Assume, for the time being, that the equality on the right-hand side in the second line of (4.1) holds true. Then $K_{(\alpha,\beta,\gamma)}$ is strictly increasing in the interval $(y_q^\star, \tan\vartheta_q)$, and, consequently, it coincides with $\widetilde K_{(\alpha,\beta,\gamma)}$. Indeed, if $y_1 < y_2$ and the maximum for y_1 is attained at a point $\tilde x$, then, in view of (1.12),

$$K_{(\alpha,\beta,\gamma)}(y_1) = \frac{\sqrt{p(\tilde x)r(\tilde x)}}{\varphi(\tilde x) - y_1\psi(\tilde x)} < \frac{\sqrt{p(\tilde x)r(\tilde x)}}{\varphi(\tilde x) - y_2\psi(\tilde x)} \leqslant K_{(\alpha,\beta,\gamma)}(y_2)$$

since $\psi(\tilde{x}) > 0$. Thus, in the interval $(y_q^\star, \tan\vartheta_q)$, it suffices to show the equality on the right-hand side in the second line of (4.1).

We shall prove Proposition 4.1 separately for each $q = 3, 4, 5, 6$ in the following four subsections. Our point of departure are relations (2.15) and (2.16). To avoid repetitions, we introduce notation and make some preliminary remarks.

An obvious consequence of (1.10) and (1.11) is

$$|d(\zeta)|^2 = c_q^2(1-x)p(x) \quad \text{and} \quad |d(\zeta)\gamma(\zeta)| = c_q\sqrt{(1-x)p(x)r(x)}. \tag{4.2}$$

Furthermore, in view of (1.10), we have

$$\begin{cases} \operatorname{Re}\big((1-\mathrm{i}y)d(\zeta)\big) = c_q\Big[-\psi(x)\sqrt{1-x} + y\dfrac{\varphi(x)}{\sqrt{1+x}}\sin t\Big], \\ \operatorname{Im}\big((1-\mathrm{i}y)d(\zeta)\big) = c_q\Big[y\psi(x)\sqrt{1-x} + \dfrac{\varphi(x)}{\sqrt{1+x}}\sin t\Big]. \end{cases} \tag{4.3}$$

Thus,

$$\zeta \in \mathscr{K}_y^- \iff -\psi(x)\sqrt{1-x} + y\frac{\varphi(x)}{\sqrt{1+x}}\sin t < 0. \tag{4.4}$$

It turns out that $\psi(-1) < 0$; hence, the case $\sin t = 0$ (whence $x = \pm 1$) is excluded. Therefore, in the following we assume that $-1 < x < 1$.

Finally, we recall the function f_q of (1.11),

$$f_q(x) = 1 + \frac{[\psi(x)]^2}{[\varphi(x)]^2} = \frac{p(x)}{[\varphi(x)]^2} = 1 + \frac{|\operatorname{Re} d(\zeta)|^2}{|\operatorname{Im} d(\zeta)|^2} \quad \text{for} \quad -1 < x < 1, \tag{4.5}$$

and introduce the function g_q by

$$g_q(x) := \frac{(2^q-1)\varphi(x) - \sqrt{p(x)r(x)}}{(2^q-1)\psi(x)} \quad \text{for} \quad x_1 < x < x_2. \tag{4.6}$$

4.1. Three-step method. Here, we prove Proposition 4.1 in the case of the three-step method, i.e., for $q = 3$.

Let us recall from [7] that, for $q = 3, \varphi(x) = (4x^2 - 9x + 8)\sqrt{1+x}$ and $\psi(x) = (4x - 1)\sqrt{(1-x)^3}$; consequently, $p(x) = [\varphi(x)]^2 + [\psi(x)]^2 = 44x^2 - 91x + 65$. It is also easily seen that $r(x) = 12x^2 - 24x + 13 = |\gamma(\zeta)|^2$.

Notice that $\operatorname{Re} d(\zeta) < 0$ if and only if $\psi(x) > 0$, i.e., if and only if $1/4 < x < 1$; in this case, $x_1 = 1/4$ and $x_2 = 1$.

We also recall from [7] that the derivative f_3' of f_3 can be written in the form

$$f_3'(x) = 6\frac{(1-x)^2(1-4x)(22x-13)}{[\varphi(x)]^3\sqrt{1+x}}. \tag{4.7}$$

Let us now return to (4.4). The term $\varphi(x)/\sqrt{1+x} = 4x^2 - 9x + 8$ is positive for all real x, whence, for $x \leqslant 1/4$, $\sin t$ must be negative. For $1/4 < x < 1$, the term $-\psi(x)\sqrt{1-x} =$

$(1-x)^2(1-4x)$ is negative, and $\sin t$ may also be positive. Therefore, we distinguish two subcases: $\sin t < 0$ and $\sin t > 0$.

Before we proceed, let us note that

$$7\varphi(x) - \sqrt{p(x)r(x)} > 0 \quad \forall x \in [-1/2, 1]. \tag{4.8}$$

Indeed, this inequality is equivalent to $p(x)r(x) < 49[\varphi(x)]^2$, whence equivalent to $f_3(x)r(x) < 49$; cf. (4.5). Since r is decreasing in the interval $[-1/2, 1]$, in view also of (4.7), we infer that

$$f_3(x)r(x) \leqslant \max\Big\{f_3\big(-\frac{1}{2}\big), f_3\big(\frac{13}{22}\big)\Big\} r\big(-\frac{1}{2}\big) = f_3\big(-\frac{1}{2}\big)\cdot 28 = \frac{4}{3}\cdot 28 < 49.$$

First case: $-1 < x \leqslant 1/4$. Then, $\sin t < 0$, whence $\sin t = -\sqrt{1-x^2}$, and, according to the second relations in (4.2) and (4.3),

$$\frac{|d(\zeta)\gamma(\zeta)|}{|\operatorname{Im}\big((1-\mathrm{i}y)d(\zeta)\big)|} = \frac{\sqrt{p(x)r(x)}}{|\varphi(x) - y\psi(x)|} = \frac{\sqrt{p(x)r(x)}}{\varphi(x) - y\psi(x)} \tag{4.9}$$

since $\psi(x)$ is nonpositive in the interval $(-1, 1/4]$; cf. (2.16). We shall see that the quantity in (4.9) does not exceed 7 for $0 \leqslant y < \tan\vartheta_3$. We distinguish two subcases: $-1 < x < -1/2$ and $-1/2 \leqslant x \leqslant 1/4$.

i) For $-1 < x < -1/2$, we first note that

$$\operatorname{Re}\big((1-\mathrm{i}y)d(\zeta)\big) < 0 \iff (1-x)^2(1-4x) < -y(4x^2 - 9x + 8)\sin t,$$

and thus, since $\sin t$ is negative,

$$\operatorname{Re}\big((1-\mathrm{i}y)d(\zeta)\big) < 0 \iff (1-x)^2(1-4x) < y\sqrt{1-x^2}(4x^2 - 9x + 8);$$

thus, y is positive and

$$\varphi(x) > -\frac{1}{y}\psi(x). \tag{4.10}$$

In view of (4.10) and (4.9), estimate

$$\frac{|d(\zeta)\gamma(\zeta)|}{|\operatorname{Im}\big((1-\mathrm{i}y)d(\zeta)\big)|} \geqslant 7 \tag{4.11}$$

yields

$$-7\big(y + \frac{1}{y}\big)\psi(x) < \sqrt{p(x)r(x)}. \tag{4.12}$$

It is easily seen that p, r and $-\psi$ are decreasing functions in the interval $[-1, -1/2]$. Thus,

$$\sqrt{p(x)r(x)} \leqslant \sqrt{p(-1)r(-1)} = 70\sqrt{2} < 90.44\sqrt{1.7} = -14\psi(-0.7) \leqslant -14\psi(x)$$

for $-1 \leqslant x \leqslant -0.7$ and

$$\sqrt{p(x)r(x)} \leqslant \sqrt{p(-0.7)r(-0.7)} < 63\sqrt{1.5} = -14\psi(-0.5) \leqslant -14\psi(x)$$

for $-0.7 \leqslant x \leqslant -0.5$. Hence, (4.12) leads to the contradiction, for positive y,

$$y + \frac{1}{y} < 2.$$

ii) For $-1/2 \leqslant x \leqslant 1/4$, relations (4.11) and (4.9) yield

$$7\varphi(x) - \sqrt{p(x)r(x)} \leqslant 7y\psi(x),$$

a contradiction to (4.8) since ψ is nonpositive in $[-1/2, 1/4]$.

Second case: $1/4 < x < 1$. In this case ψ is positive, and we distinguish two subcases: $\sin t > 0$ and $\sin t < 0$.

i) $\sin t > 0$. Then $\sin t = \sqrt{1-x^2}$. Now, according to the second relations in (4.2) and (4.3),

$$\frac{|d(\zeta)\gamma(\zeta)|}{|\operatorname{Im}\big((1-\mathrm{i}y)d(\zeta)\big)|} = \frac{\sqrt{p(x)r(x)}}{\varphi(x) + y\psi(x)}; \tag{4.13}$$

therefore, in this case, condition (4.11) can be equivalently written as

$$7y\psi(x) \leqslant \sqrt{p(x)r(x)} - 7\varphi(x). \tag{4.14}$$

This inequality is not valid since the term on its left-hand side is obviously nonnegative, while the term on its right-hand side is negative; cf. (4.8).

ii) $\sin t < 0$. First, for $0 \leqslant y < \tan\vartheta_3$, in view of (1.12) we have

$$\varphi(x) > y\psi(x), \tag{4.15}$$

whence (4.9) is valid also in this case. From (4.9) and (4.15) we infer that (4.11) is valid for some $\zeta \in \mathscr{K}_y^-$ if and only if

$$\exists x \in (1/4, 1) \quad y \geqslant g_3(x) \tag{4.16}$$

with the function g_3 of (4.6) and $x_1 = 1/4, x_2 = 1$. Now, g_3 tends to ∞ as x decreases to $1/4$ or increases to 1. From (4.8) and the fact that ψ is positive in the interval $(1/4, 1)$, we infer that g_3 possesses a positive minimum $y_3^\star$ in $(1/4, 1)$. The minimum $y_3^\star$ is attained at $x_3^\star \approx 0.5604664$ and is

$$y_3^\star \approx g_3(0.5604664) \approx 10.747771218818176; \tag{4.17}$$

see also Figure 4.1.

The proof is complete.

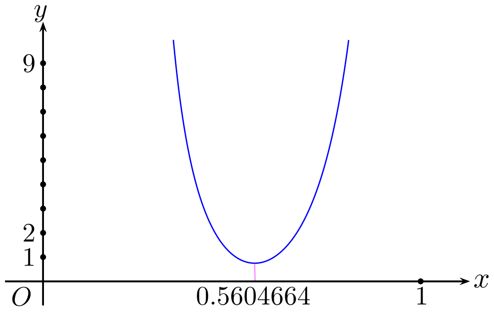

Figure 4.1. *The graph of* $g, g(x) := g_3(x) - 10$, *with* g_3 *the function of* (4.6) *in the interval* $[0.345, 0.8093]$. *The vertical segment connects the points* $(0.5604664, 0)$ *and* $(0.5604664, 0.747771219)$.

4.2. Four-step method. Here, we prove Proposition 4.1 in the case of the four-step method, i.e., for $q = 4$.

We recall from [7] that, for $q = 4$, $\varphi(x) = (8 - 15x + 16x^2 - 6x^3)\sqrt{1+x}$ and $\psi(x) = 2(3x+1)\sqrt{(1-x)^5}$; consequently, $p(x) = [\varphi(x)]^2 + [\psi(x)]^2 = 68 - 172x + 197x^2 - 73x^3$. It is also easily seen that $r(x) = 25 - 80x + 88x^2 - 32x^3 = |\gamma(\zeta)|^2$.

With $\sigma(x) := 8 - 15x + 16x^2 - 6x^3$, which is positive in $[-1, 1]$, the derivative f_4' of f_4 can be written in the form

$$f_4'(x) = \frac{120(1-x)^4(3x+1)(1-5x)}{(1+x)\big[\sigma(x)\big]^3}; \tag{4.18}$$

see [7, f_4' and positivity of p_4].

Let us now return to (4.4). As already mentioned, $\varphi(x)/\sqrt{1+x} = \sigma(x) = 8 - 15x + 16x^2 - 6x^3$ is positive in the interval $[-1, 1]$. Therefore, we infer that, for $x \leqslant -1/3$, $\sin t$ must be negative. For $-1/3 < x < 1$, the term $-\psi(x)\sqrt{1-x} = 2(x-1)^3(3x+1)$ is negative, and $\sin t$ may also be positive. Therefore, we distinguish two subcases: $\sin t < 0$ and $\sin t > 0$.

Before we proceed, let us note that

$$15\varphi(x) - \sqrt{p(x)r(x)} > 0 \quad \forall x \in [-0.7, 1]. \tag{4.19}$$

Indeed, this inequality is equivalent to $p(x)r(x) < [15\varphi(x)]^2$, whence equivalent to $f_4(x)r(x) < 225$; cf. (4.5). In view of (4.18) and $r'(x) = -96x^2 + 176x - 80 = 16(1-x)(6x-5)$, we have

$$f_4(x)r(x) \leqslant \max\Big\{f_4(-0.7), f_4\big(\frac{1}{5}\big)\Big\} \max\big\{r(-0.7), r(1)\big\} = f_4(-0.7)r(-0.7) < 225.$$

First case: $-1 < x \leqslant -1/3$. Then $\sin t < 0, \sin t = -\sqrt{1-x^2}$, and, according to the second relations in (4.2) and (4.3),

$$\frac{|d(\zeta)\gamma(\zeta)|}{|\operatorname{Im}\big((1-\mathrm{i}y)d(\zeta)\big)|} = \frac{\sqrt{p(x)r(x)}}{|\varphi(x) - y\psi(x)|} = \frac{\sqrt{p(x)r(x)}}{\varphi(x) - y\psi(x)} \tag{4.20}$$

since $\psi(x)$ is nonpositive in the interval $(-1, -1/3]$; cf. (2.16). We shall see that the right-hand side of (4.20) does not exceed 15 for $0 \leqslant y < \tan\vartheta_4$. We distinguish two subcases: $-1 < x < -0.7$ and $-0.7 \leqslant x \leqslant -1/3$.

i) For $-1 < x < -0.7$, from $\operatorname{Re}\big((1-\mathrm{i}y)d(\zeta)\big) < 0$, we obtain

$$y\varphi(x) > -\psi(x); \tag{4.21}$$

in particular, y is positive. Now the quantities in (4.20) are larger than or equal to 15 if and only if $\sqrt{p(x)r(x)} \geqslant 15\big[\varphi(x) - y\psi(x)\big]$. Using here (4.21), we infer that

$$-15\Big(y + \frac{1}{y}\Big)\psi(x) < \sqrt{p(x)r(x)}.$$

This leads to the contradiction $y + \frac{1}{y} < 2$, for positive y. Indeed, we have

$$\sqrt{p(x)r(x)} < -30\psi(x) \quad \forall x \in [-1, -0.7]. \tag{4.22}$$

To see this, we first notice that p, r and $-\psi$ are decreasing in $[-1, -0.7]$. Therefore,

$$\sqrt{p(x)r(x)} \leqslant \sqrt{p(-1)r(-1)} = 240\sqrt{2} < -30\psi(-0.8) \leqslant -30\psi(x)$$

for $x \in [-1, -0.8]$ and

$$\sqrt{p(x)r(x)} \leqslant \sqrt{p(-0.8)r(-0.8)} < 245 < -30\psi(-0.7) \leqslant -30\psi(x)$$

for $x \in [-0.8, -0.7]$, which lead to the desired inequality (4.22).

ii) For $-0.7 \leqslant x \leqslant -1/3$, the quantities in (4.20) are larger than or equal to 15 if and only if

$$15y\psi(x) \geqslant 15\varphi(x) - \sqrt{p(x)r(x)}.$$

This is a contradiction to (4.19) since the quantity on the left-hand side is nonpositive, while on the right-hand side we have a positive term.

Second case: For $-1/3 < x < 1$, $\sin t$ may be both positive and negative. We consider these two subcases separately. Notice that ψ is positive in this case.

i) If $\sin t > 0$, then $\sin t = \sqrt{1-x^2}$ and, according to the second relations in (4.2) and (4.3),

$$\frac{|d(\zeta)\gamma(\zeta)|}{|\operatorname{Im}\big((1-\mathrm{i}y)d(\zeta)\big)|} = \frac{\sqrt{p(x)r(x)}}{\varphi(x) + y\psi(x)}. \tag{4.23}$$

The quantities in this relation are larger than or equal to 15 if and only if

$$\sqrt{p(x)r(x)} - 15\varphi(x) \geqslant 15y\psi(x).$$

This is a contradiction to (4.19) since the term on the right-hand side is nonnegative, while on the left-hand side we have a negative quantity.

ii) If $\sin t < 0$, then $\sin t = -\sqrt{1-x^2}$ and, according to the second relations in (4.2) and (4.3),

$$\frac{|d(\zeta)\gamma(\zeta)|}{|\operatorname{Im}\big((1-\mathrm{i}y)d(\zeta)\big)|} = \frac{\sqrt{p(x)r(x)}}{|\varphi(x) - y\psi(x)|}. \tag{4.24}$$

First, for $-1/3 < x < 1$ and $0 \leqslant y < \tan\vartheta_4$, in view of (1.12) we have

$$\varphi(x) > y\psi(x), \tag{4.25}$$

and the absolute value in the denominator of the right-hand side of (4.24) can be dropped. Therefore, in view of (4.24) and (4.25), we infer that the quantities in (4.24) are larger than or equal to 15 for some $\zeta \in \mathscr{K}_y^-$ if and only if $\sqrt{p(x)r(x)} \geqslant 15\varphi(x) - 15y\psi(x)$ for some $-1/3 < x < 1$, which can be equivalently written in the form

$$\exists x \in (-1/3, 1) \quad y \geqslant g_4(x) \tag{4.26}$$

with the function g_4 of (4.6) and $x_1 = -1/3, x_2 = 1$. Now, g_4 tends to ∞ as x decreases to $-1/3$ or increases to 1. From (4.19) and the fact that ψ is positive in the interval $(-1/3, 1)$, we infer that g_4 possesses a positive minimum $y_4^\star$ in $(-1/3, 1)$. The minimum $y_4^\star$ is attained at $x_4^\star \approx 0.1203494$ and is

$$y_4^\star \approx g_4(0.1203494) \approx 2.465496414280889; \tag{4.27}$$

see also Figure 4.2.

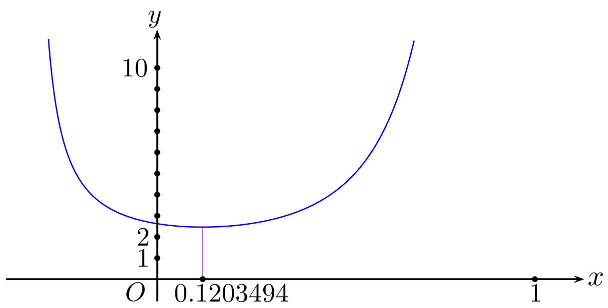

Figure 4.2. *The graph of the function* g_4 *of* (4.6) *in the interval* $[-0.288, 0.68]$. *The vertical segment connects the points* $(0.1203494, 0)$ *and* $(0.1203494, 2.46549641428)$.

4.3. Five-step method.

Here, we prove Proposition 4.1 in the case of the five-step method, i.e., for $q = 5$.

Let us recall from [7] that, for $q = 5$, $\varphi(x) = \sigma(x)\sqrt{1+x}$, with $\sigma(x) := 48x^4 - 150x^3 + 164x^2 - 75x + 28$, and $\psi(x) = 2(11 + 3x - 24x^2)\sqrt{(1-x)^5}$; consequently, $p(x) = [\varphi(x)]^2 + [\psi(x)]^2 = 3288x^4 - 10587x^3 + 12053x^2 - 5572x + 1268$. It is also easily seen that $r(x) = 80x^4 - 280x^3 + 360x^2 - 200x + 41 = |\gamma(\zeta)|^2$.

Now, $\operatorname{Re} d(\zeta) < 0$ if and only if $\psi(x) > 0$, i.e., if and only if

$$x_1 := \frac{3 - \sqrt{1065}}{48} < x < \frac{3 + \sqrt{1065}}{48} =: x_2; \tag{4.28}$$

we have $-1 < x_1 < 0 < x_2 < 1$.

We also recall from [7, f_5' and positivity of p_5] that the derivative f_5' of f_5 can be written in the form

$$f_5'(x) = -120\frac{(1-x)^4(24x^2 - 3x - 11)(274x^2 - 223x - 1)}{(1+x)^2\big[\sigma(x)\big]^3} \tag{4.29}$$

and that σ is positive in the interval $[-1,1]$. The roots of f_5' are $1, x_1, x_2$, and

$$x_3 := \frac{223-\sqrt{50825}}{548} \quad \text{and} \quad x_4 := \frac{223+\sqrt{50825}}{548};$$

notice that $-1 < x_1 < x_3 < 0 < x_2 < x_4 < 1$.

Let us now return to (4.4). The roots x_1 and x_2 of $24x^2-3x-11$ are given in (4.28), and, as already mentioned, $\varphi(x)/\sqrt{1+x} = \sigma(x)$ is positive; therefore, $\sin t$ must be negative for $-1 < x \leqslant x_1$ and for $x_2 \leqslant x < 1$. For $x_1 < x < x_2$, $\sin t$ may also be positive. Therefore, we distinguish two subcases: $\sin t < 0$ and $\sin t > 0$.

Before we proceed, let us note that

$$31\varphi(x) - \sqrt{p(x)r(x)} > 0 \quad \forall x \in [-0.825, 1]. \tag{4.30}$$

Indeed, this inequality is equivalent to $p(x)r(x) < 31^2[\varphi(x)]^2$, whence equivalent to $f_5(x)r(x) < 961$; cf. (4.5). Now, $r'(x) = 320x^3 - 840x^2 + 720x - 200 = 40(x-1)^2(8x-5)$. Therefore, in view also of (4.29), we obtain

$$f_5(x)r(x) \leqslant \max\big\{f_5(-0.825), f_5(-0.2)\big\}r(-0.825) = f_5(-0.2)r(-0.825) < 1.43\cdot 646 < 961$$

for $-0.825 \leqslant x \leqslant -0.2$ and

$$f_5(x)r(x) \leqslant \max\big\{f_5(x_3), f_5(x_4)\big\}r(-0.2) = f_5(x_3)r(-0.2) < 1.62\cdot 98 < 961$$

for $-0.2 \leqslant x \leqslant 1$, and the desired inequality (4.30) follows.

First case: $-1 < x \leqslant x_1$ or $x_2 \leqslant x < 1$. Then, $\sin t < 0$, whence $\sin t = -\sqrt{1-x^2}$, and, according to the second relations in (4.2) and (4.3),

$$\frac{|d(\zeta)\gamma(\zeta)|}{|\operatorname{Im}\big((1-\mathrm{i}y)d(\zeta)\big)|} = \frac{\sqrt{p(x)r(x)}}{|-\varphi(x)+y\psi(x)|} = \frac{\sqrt{p(x)r(x)}}{\varphi(x)-y\psi(x)} \tag{4.31}$$

since $\psi(x)$ is nonpositive in these intervals; cf. (2.16). We shall see that the quantity in (4.31) does not exceed 31 for $0 \leqslant y < \tan\vartheta_5$. If this were the case, then we would have

$$\sqrt{p(x)r(x)} \geqslant 31\big[\varphi(x) - y\psi(x)\big]. \tag{4.32}$$

We distinguish two subcases: $-1 < x < -0.825$, and $-0.825 \leqslant x \leqslant x_1$ or $x_2 \leqslant x < 1$.

i) For $-1 < x < -0.825$, we note that $\operatorname{Re}\big((1-\mathrm{i}y)d(\zeta)\big) < 0$ if and only if $\psi(x) > -y\varphi(x)$, and thus y is positive since $\psi(x)$ is negative for $x < x_1$; then (4.32) yields

$$\sqrt{p(x)r(x)} > -31\Big(\frac{1}{y}+y\Big)\psi(x). \tag{4.33}$$

As we already saw, r is decreasing for negative x; p is also decreasing since $p'(x) = 13152x^3 - 31761x^2 + 24106x - 5572 < 0$ for $x < 0$. Furthermore, ψ is increasing for $x < x_1$. Thus, we have

$$\sqrt{p(x)r(x)} \leqslant \sqrt{p(-1)r(-1)} < -62\psi(-0.88) \leqslant -62\psi(x) \quad \forall x \in [-1, -0.88]$$

and

$$\sqrt{p(x)r(x)} \leqslant \sqrt{p(-0.88)r(-0.88)} < -62\psi(-0.825) \leqslant -62\psi(x) \quad \forall x \in [-0.88, -0.825].$$

Hence, (4.33) leads to the contradiction, for positive y,

$$y + \frac{1}{y} < 2.$$

ii) For $-0.825 \leqslant x \leqslant x_1$ or $x_2 \leqslant x < 1$, the quantity in (4.31) exceeds 31 if and only if

$$31\varphi(x) - \sqrt{p(x)r(x)} \leqslant 31y\psi(x),$$

a contradiction to (4.30) since ψ is nonpositive.

Second case: $x_1 < x < x_2$. We distinguish two subcases: $\sin t > 0$ and $\sin t < 0$.

i) $\sin t > 0$. Then $\sin t = \sqrt{1-x^2}$. Since in this case ψ is positive, we have, according to the second relations in (4.2) and (4.3),

$$\frac{|d(\zeta)\gamma(\zeta)|}{|\operatorname{Im}\big((1-\mathrm{i}y)d(\zeta)\big)|} = \frac{\sqrt{p(x)r(x)}}{\varphi(x) + y\psi(x)}; \tag{4.34}$$

these quantities exceed 31 if and only if

$$31y\psi(x) \leqslant \sqrt{p(x)r(x)} - 31\varphi(x), \tag{4.35}$$

a contradiction since the term on its left-hand side is obviously nonnegative, while the term on its right-hand side is negative; cf. (4.30).

ii) $\sin t < 0$. First, for $0 \leqslant y < \tan\vartheta_5$, in view of (1.12) we have

$$\varphi(x) - y\psi(x) > 0 \quad \forall x \in (x_1, x_2),$$

whence (4.31) is valid also in this case. Therefore, in view of (4.34), we infer that

$$\frac{|d(\zeta)\gamma(\zeta)|}{|\operatorname{Im}\big((1-\mathrm{i}y)d(\zeta)\big)|} \geqslant 31$$

is valid for some $\zeta \in \mathscr{K}_y^-$ if and only if

$$\exists x \in (x_1, x_2) \quad y \geqslant g_5(x) \tag{4.36}$$

with the function g_5 of (4.6) and x_1 and x_2 given in (4.28). Now, g_5 tends to ∞ as x decreases to x_1 or increases to x_2. From (4.30) and the fact that ψ is positive in the interval (x_1, x_2), we infer that g_5 possesses a positive minimum $y_5^\star$ in (x_1, x_2). The minimum $y_5^\star$ is attained at $x_5^\star \approx -0.09394996$ and is

$$y_5^\star \approx g_5(-0.09394996) \approx 0.899586281651322; \tag{4.37}$$

see also Figure 4.3.

The proof is complete.

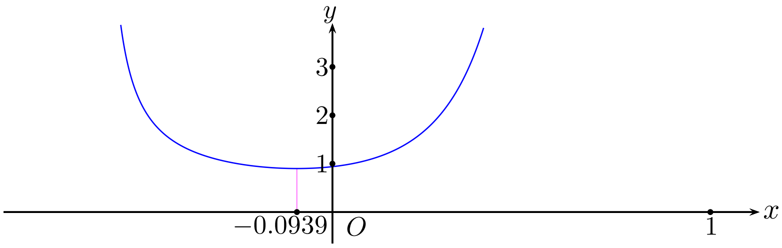

Figure 4.3. *The graph of the function g_5 of (4.6) in the interval $[-0.56, 0.4]$. The vertical segment connects the points $(-0.0939, 0)$ and $(-0.0939, 0.89959)$.*

4.4. Six-step method. Here, we prove Proposition 4.1 in the case of the six-step method, i.e., for $q = 6$.

Let us recall from [7] that, for $q = 6$, $\varphi(x) = \sigma(x)\sqrt{1+x}$, with $\sigma(x) := 8 - 15x + 184x^2 - 370x^3 + 288x^4 - 80x^5$, and $\psi(x) = 2(11 - 16x - 40x^2)\sqrt{(1-x)^7}$; consequently, $p(x) = [\varphi(x)]^2 + [\psi(x)]^2 = 548 - 4972x + 20453x^2 - 32187x^3 + 22488x^4 - 5880x^5$. It is also easily seen that $r(x) := 65 - 432x + 1104x^2 - 1360x^3 + 816x^4 - 192x^5 = |\gamma(\zeta)|^2$.

Now $\operatorname{Re} d(\zeta) < 0$ if and only if $\psi(x) > 0$, i.e., if and only if

$$x_1 := \frac{-4 - 3\sqrt{14}}{20} < x < \frac{-4 + 3\sqrt{14}}{20} =: x_2. \tag{4.38}$$

We also recall from [7, f_6' and positivity of p_6] that the derivative f_6' of the function f_6 can be written in the form

$$f_6'(x) = -2520(1-x)^6 \frac{(40x^2 + 16x - 11)(28x^2 - 12x - 1)}{(1+x)^2\big[\sigma(x)\big]^3} \tag{4.39}$$

and that σ is positive in the interval $[-1, 1]$. The roots of the quadratic polynomial $28x^2 - 12x - 1$ are $x_3 := -1/14$ and $x_4 := 1/2$; we have $-1 < x_1 < x_3 < 0 < x_2 < x_4 < 1$.

Let us now return to (4.4). The roots x_1 and x_2 of $40x^2 + 16x - 11$ are given in (4.38), and, as already mentioned, $\varphi(x)/\sqrt{1+x} = \sigma(x)$ is positive; therefore, $\sin t$ must be negative for $-1 < x \leqslant x_1$ and for $x_2 \leqslant x < 1$. For $x_1 < x < x_2$, $\sin t$ may also be positive. Therefore, we distinguish two subcases: $\sin t < 0$ and $\sin t > 0$.

Before we proceed, let us note that

$$63\varphi(x) - \sqrt{p(x)r(x)} > 0 \quad \forall x \in [-0.89, 1]. \tag{4.40}$$

Indeed, this inequality is equivalent to $p(x)r(x) < 63^2[\varphi(x)]^2$, whence equivalent to $f_6(x)r(x) < 3969$; cf. (4.5). Now, $r'(x) = -48(2x-1)(10x-9)(x-1)^2$. Therefore, in view also of (4.39), we obtain

$$\begin{aligned}
f_6(x)r(x) &\leqslant \max\big\{f_6(-0.89), f_6(-0.6)\big\} r(-0.89)\\
&= f_6(-0.89)r(-0.89) < 1.305 \cdot 2902 < 3969 \quad \forall x \in [-0.89, -0.6],\\
f_6(x)r(x) &\leqslant f_6(-0.4)r(-0.6) < 2.5 \cdot 1137 < 3969 \quad \forall x \in [-0.6, -0.4],\\
f_6(x)r(x) &\leqslant f_6(-0.2)r(-0.4) < 7 \cdot 525 < 3969 \quad \forall x \in [-0.4, -0.2],\\
f_6(x)r(x) &\leqslant \max\big\{f_6(x_3), f_6(x_4)\big\} \max\big\{r(-0.2), r(0.9)\big\}\\
&= f_6(x_3)r(-0.2) < 11 \cdot 208 < 3969 \quad \forall x \in [-0.2, 1].
\end{aligned}$$

First case: $-1 < x \leqslant x_1$ or $x_2 \leqslant x < 1$. Then, $\sin t < 0$, whence $\sin t = -\sqrt{1-x^2}$, and, according to the second relations in (4.2) and (4.3),

$$\frac{|d(\zeta)\gamma(\zeta)|}{|\operatorname{Im}\big((1-\mathrm{i}y)d(\zeta)\big)|} = \frac{\sqrt{p(x)r(x)}}{|-\varphi(x)+y\psi(x)|} = \frac{\sqrt{p(x)r(x)}}{\varphi(x)-y\psi(x)} \tag{4.41}$$

since $\psi(x)$ is nonpositive in these intervals; cf. (2.16). We shall see that the quantity in (4.41) does not exceed 63 for $0 \leqslant y < \tan\vartheta_6$. If this were the case, then we would have

$$\sqrt{p(x)r(x)} \geqslant 63\big[\varphi(x) - y\psi(x)\big]. \tag{4.42}$$

We distinguish two subcases: $-1 < x < -0.89$, and $-0.89 \leqslant x \leqslant x_1$ or $x_2 \leqslant x < 1$.

i) For $-1 < x < -0.89$, we note that $\operatorname{Re}\big((1-\mathrm{i}y)d(\zeta)\big) < 0$ if and only if $\psi(x) > -y\varphi(x)$, and thus y is positive since $\psi(x)$ is negative for $x < x_1$; then (4.42) yields

$$\sqrt{p(x)r(x)} > -63\big(\frac{1}{y}+y\big)\psi(x). \tag{4.43}$$

As we already saw, r is decreasing for negative x; p is also decreasing, since $p'(x) = -29400x^4 + 89952x^3 - 96561x^2 + 40906x - 4972 < 0$ for $x < 0$. Furthermore, ψ is increasing for $x < x_1$. Thus, we have

$$\sqrt{p(x)r(x)} \leqslant \sqrt{p(-1)r(-1)} < -126\psi(-0.92) \leqslant -126\psi(x) \quad \forall x \in [-1,-0.92]$$

and

$$\sqrt{p(x)r(x)} \leqslant \sqrt{p(-0.92)r(-0.92)} < -126\psi(-0.89) \leqslant -126\psi(x) \quad \forall x \in [-0.92,-0.89].$$

Hence, (4.43) leads to the contradiction, for positive y,

$$y + \frac{1}{y} < 2.$$

ii) For $-0.89 \leqslant x \leqslant x_1$ or $x_2 \leqslant x < 1$, the quantity in (4.41) exceeds 63 if and only if

$$63\varphi(x) - \sqrt{p(x)r(x)} \leqslant 63y\psi(x),$$

a contradiction to (4.40) since ψ is nonpositive.

Second case: $x_1 < x < x_2$. We distinguish two subcases: $\sin t > 0$ and $\sin t < 0$.

i) $\sin t > 0$. Then $\sin t = \sqrt{1-x^2}$. Since in this case ψ is positive, we have, according to the second relations in (4.2) and (4.3),

$$\frac{|d(\zeta)\gamma(\zeta)|}{|\operatorname{Im}\big((1-\mathrm{i}y)d(\zeta)\big)|} = \frac{\sqrt{p(x)r(x)}}{|\varphi(x)+y\psi(x)|} = \frac{\sqrt{p(x)r(x)}}{\varphi(x)+y\psi(x)}; \tag{4.44}$$

these quantities exceed 63 if and only if

$$63y\psi(x) \leqslant \sqrt{p(x)r(x)} - 63\varphi(x),$$

a contradiction since the term on its left-hand side is obviously nonnegative, while the term on its right-hand side is negative; cf. (4.40).

ii) $\sin t < 0$. First, for $0 \leqslant y < \tan\vartheta_6$, in view of (1.12) we have

$$\varphi(x) - y\psi(x) > 0 \quad \forall x \in (x_1, x_2), \tag{4.45}$$

whence

$$\frac{|d(\zeta)\gamma(\zeta)|}{|\operatorname{Im}\big((1-\mathrm{i}y)d(\zeta)\big)|} = \frac{\sqrt{p(x)r(x)}}{|-\varphi(x)+y\psi(x)|} = \frac{\sqrt{p(x)r(x)}}{\varphi(x)-y\psi(x)}. \tag{4.46}$$

Therefore, we infer that

$$\frac{|d(\zeta)\gamma(\zeta)|}{|\operatorname{Im}\big((1-\mathrm{i}y)d(\zeta)\big)|} \geqslant 63$$

is valid for some $\zeta \in \mathscr{K}_y^-$ if and only if

$$\exists x \in (x_1, x_2) \quad y \geqslant g_6(x) \tag{4.47}$$

with the function g_6 of (4.6) and x_1 and x_2 given in (4.38). Now, g_6 tends to ∞ as x decreases to x_1 or increases to x_2. From (4.40) and the fact that ψ is positive in the interval (x_1, x_2), we infer that g_6 possesses a positive minimum $y_6^\star$ in (x_1, x_2). The minimum $y_6^\star$ is attained at $x_6^\star \approx -0.1228462$ and is

$$y_6^\star \approx g_6(-0.1228462) \approx 0.141292221298238; \tag{4.48}$$

see also Figure 4.4.

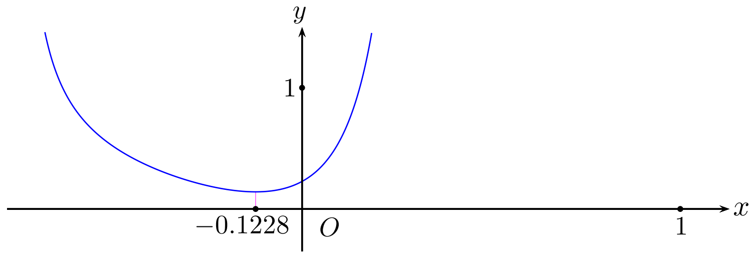

Figure 4.4. *The graph of the function* g_6 *of* (4.6) *in the interval* $[-0.68, 0.184]$. *The vertical segment connects the points* $(-0.1228, 0)$ *and* $(-0.1228, 0.14129)$.

Remark 4.2 (On the precise values $f(0)$ in Figures 2.2–2.3). As we have seen, for $q = 3, 4, 5, 6$, with the corresponding functions p, r, φ, ψ and points x_1, x_2, the following representation of function Φ of (2.16) holds true:

$$\Phi(y) = \sup_{x_1<x<x_2} \frac{\sqrt{p(x)r(x)}}{\varphi(x)-y\psi(x)}, \quad 0 \leqslant y < \tan\vartheta_q. \tag{4.49}$$

Consequently,

$$\Phi(0) = \sup_{x_1<x<x_2} \sqrt{\frac{p(x)}{[\varphi(x)]^2} r(x)} = \sup_{x_1<x<x_2} \sqrt{f_q(x)r(x)} \tag{4.50}$$

due to (4.5); notice, furthermore, that, since $\psi(x_1) = 0$, this relation yields $f_q(x_1) = 1$. It is of some interest to note that, as can be shown, the supremum in (4.50) is attained at x_1, i.e.,

$$\Phi(0) = \sqrt{r(x_1)}. \tag{4.51}$$

Therefore, the values $f(0)$ of the functions in Figures 2.2–2.3 are $f(0) = 1/\Phi(0) = 1/\sqrt{r(x_1)}$. For instance, for $q = 3, 4$, we have

$$f(0) = \frac{1}{\sqrt{r(1/4)}} = \frac{2}{\sqrt{31}} \quad \text{and} \quad f(0) = \frac{1}{\sqrt{r(-1/3)}} = \frac{3\sqrt{3}}{\sqrt{1691}}, \tag{4.52}$$

respectively.

5. The reciprocals of the functions $K_{(\alpha,\beta,\gamma)}$. In this section we present the graphs of the reciprocals of the functions $K_{(\alpha,\beta,\gamma)}$.

The reciprocals of the functions $\widetilde{K}_{(\alpha,\beta,\gamma)}$ for the implicit–explicit q-step BDF method, $q = 3, 4, 5, 6$, are equal to $1/(2^q - 1)$ in the interval $[0, y_q^\star]$; as we have seen, in the interval $[y_q^\star, \tan\vartheta_q)$ we have $\widetilde{K}_{(\alpha,\beta,\gamma)}(y) = K_{(\alpha,\beta,\gamma)}(y)$; the graphs of the reciprocals of these functions in the interval $[y_q^\star, \tan\vartheta_q)$ coincide with the corresponding graphs of the function f in Figures 2.2, 2.3, respectively. In Figures 5.1–5.2, we give the graphs of the reciprocals of the functions $K_{(\alpha,\beta,\gamma)}$.

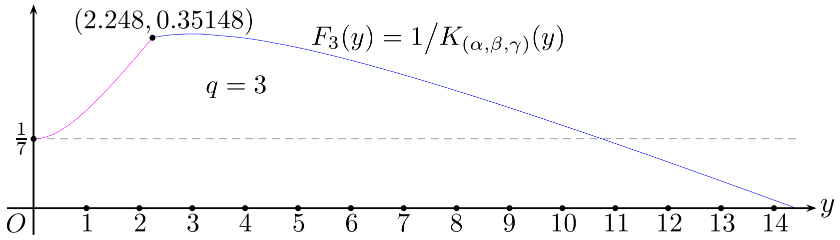

Figure 5.1. *The reciprocal of the function $K_{(\alpha,\beta,\gamma)}$ for the implicit–explicit three-step BDF method. In the interval $[0, 2.248]$, this is the reciprocal of the first term in brackets on the right-hand side of (2.6), while in the interval $[2.248, \tan\vartheta_3)$ it is the reciprocal of the second term in brackets on the right-hand side of (2.6).*

6. Proof of the remaining part of Theorem 1.4. We proved the part of Theorem 1.4 concerning stability under the condition in the first line of (1.16) in Section 4. In this section we prove the remaining part of Theorem 1.4, namely, stability under the sufficient stability condition in the second line of (1.16); see (6.1) and (1.8). We also show that the corresponding optimal bound $b_{q,o}$ is indeed nonlinear for $\hat{\lambda} \in (y_q^\star, \tan\vartheta_q)$; cf. the strict inequality in (6.1).

For the reader's convenience, we first recall the polynomials p and r and the functions φ and ψ, as well as the parameters x_1 and x_2, introduced in Section 4, corresponding to each implicit–explicit q-step method, $q = 3, 4, 5, 6$.

1. For the three-step BDF method, we have $x_1 = 1/4, x_2 = 1$,

$$p(x) = 44x^2 - 91x + 65, \quad r(x) = 12x^2 - 24x + 13,$$
$$\varphi(x) = (4x^2 - 9x + 8)\sqrt{1+x}, \quad \psi(x) = (4x - 1)\sqrt{(1-x)^3}.$$

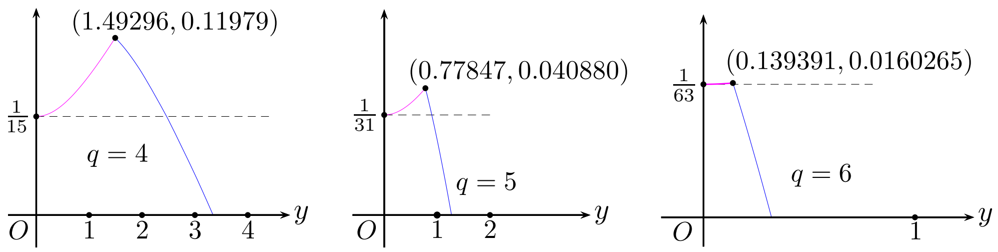

Figure 5.2. *The reciprocals $F_q, q = 4,5,6$, of the function $K_{(\alpha,\beta,\gamma)}$ for the implicit–explicit four-, five- and six-step BDF methods. In the intervals $[0, 1.49296]$, $[0, 0.77847]$ and $[0, 0.139391]$, respectively, F_q is the reciprocal of the first term in brackets on the right-hand side of (2.6), $q = 4,5,6$, while in the intervals $[1.49296, \tan\vartheta_4)$, $[0.77847, \tan\vartheta_5)$ and $[0.139391, \tan\vartheta_6)$, respectively, it is the reciprocal of the second term in brackets on the right-hand side of (2.6).*

2. For the four-step BDF method, we have $x_1 = -1/3, x_2 = 1$,

$$p(x) = 68 - 172x + 197x^2 - 75x^3, \quad r(x) = 25 - 80x + 88x^2 - 32x^3,$$
$$\varphi(x) = (8 - 15x + 16x^2 - 6x^3)\sqrt{1+x}, \quad \psi(x) = 2(3x+1)\sqrt{(1-x)^5}.$$

3. For the five-step BDF method, we have

$$x_1 = \frac{3-\sqrt{1065}}{48} \approx -0.617382036336697, \quad x_2 = \frac{3+\sqrt{1065}}{48} \approx 0.742382036336697,$$

$$p(x) = 3288x^4 - 10587x^3 + 12053x^2 - 5572x + 1268,$$
$$r(x) = 80x^4 - 280x^3 + 360x^2 - 200x + 41,$$
$$\varphi(x) = (48x^4 - 150x^3 + 164x^2 - 75x + 28)\sqrt{1+x},$$
$$\psi(x) = 2(11 + 3x - 24x^2)\sqrt{(1-x)^5}.$$

4. For the six-step BDF method, we have

$$x_1 = \frac{-4-3\sqrt{14}}{20} \approx -0.761248608016091, \quad x_2 = \frac{-4+3\sqrt{14}}{20} \approx 0.361248608016091,$$

$$p(x) = 548 - 4972x + 20453x^2 - 32187x^3 + 22488x^4 - 5880x^5,$$
$$r(x) = 65 - 432x + 1104x^2 - 1360x^3 + 816x^4 - 192x^5,$$
$$\varphi(x) = (8 - 15x + 184x^2 - 370x^3 + 288x^4 - 80x^5)\sqrt{1+x},$$
$$\psi(x) = 2(11 - 16x - 40x^2)\sqrt{(1-x)^7}.$$

Lemma 6.1 (On the sufficient stability condition in the second line of (1.16)). *For the implicit–explicit q-step BDF method, we have the estimate*

$$K_{(\alpha,\beta,\gamma)}(y) < (2^q - 1)\frac{\tan\vartheta_q - y_q^\star}{\tan\vartheta_q - y} \quad \forall y \in (y_q^\star, \tan\vartheta_q). \tag{6.1}$$

Proof. We first rewrite the desired estimate (6.1) in the form

$$(\tan\vartheta_q - y)K_{(\alpha,\beta,\gamma)}(y) < (2^q-1)(\tan\vartheta_q - y_q^\star) \quad \forall y \in I_q, \tag{6.2}$$

with $I_q := (y_q^\star, \tan\vartheta_q)$. We recall from (4.1) that $K_{(\alpha,\beta,\gamma)}$ and $\widetilde{K}_{(\alpha,\beta,\gamma)}$ coincide in I_q and

$$K_{(\alpha,\beta,\gamma)}(y) = \max_{x_1<x<x_2} \frac{\sqrt{p(x)r(x)}}{\varphi(x) - y\psi(x)}, \quad y \in I_q, \quad q = 3,4,5,6. \tag{6.3}$$

Therefore, it suffices to prove that

$$(\tan\vartheta_q - y)\frac{\sqrt{p(x)r(x)}}{\varphi(x) - y\psi(x)} < (2^q-1)(\tan\vartheta_q - y_q^\star) \quad \forall y \in I_q, \quad q = 3,4,5,6, \tag{6.4}$$

for $x \in (x_1, x_2), x \neq x_q^\star$; we recall that, at $x_q^\star$, we have $K_{(\alpha,\beta,\gamma)}(y_q^\star) = 2^q - 1$, but $y_q^\star \notin I_q$. We write (6.4) as $A_q(x) < yB_q(x)$, $x \in (x_1,x_2), x \neq x_q^\star$, with

$$A_q(x) := \tan\vartheta_q\sqrt{p(x)r(x)} - (2^q-1)(\tan\vartheta_q - y_q^\star)\varphi(x), \quad x \in (x_1,x_2), \tag{6.5}$$

and

$$B_q(x) := \sqrt{p(x)r(x)} - (2^q-1)(\tan\vartheta_q - y_q^\star)\psi(x), \quad x \in (x_1,x_2), \tag{6.6}$$

$q = 3,4,5,6$. We shall need information about the roots of A_q and B_q in the interval (x_1, x_2).

First, concerning A_q, we observe that equation $A_q(x) = 0$ is equivalent to

$$\tan^2\vartheta_q p(x)r(x) = (2^q-1)^2(\tan\vartheta_q - y_q^\star)^2\big[\varphi(x)\big]^2;$$

in view of (4.5), the last equation can in turn be equivalently rewritten as $\varGamma_q(x) = 0$ with

$$\varGamma_q(x) := f_q(x)r(x) - C_q, \quad x \in (x_1,x_2), \tag{6.7}$$

with

$$C_q := (2^q-1)^2\Big(1 - \frac{y_q^\star}{\tan\vartheta_q}\Big)^2, \quad q = 3,4,5,6. \tag{6.8}$$

Let us now consider the four cases $q = 3,4,5,6$ separately.

i) For $q = 3$, we have $C_3 = 3.174829179, x_1 = 1/4$ and $x_2 = 1$. In view of (4.7) and the fact that r is decreasing in $(1/4, 1)$, we have

$$f_3(x)r(x) \geqslant f_3(\frac{1}{4})r(0.574) = r(0.574) > C_3 \quad \forall x \in (1/4, 0.574]$$

and

$$f_3(x)r(x) \leqslant f_3(\frac{13}{22})r(0.576) < C_3 \quad \forall x \in [0.576, 1);$$

therefore, $\varGamma_3$ is positive in $(1/4, 0.574]$ and negative in $[0.576, 1)$. We easily infer that A_3 has a root x_A in the interval $(0.574, 0.576)$; A_3 is positive in $(1/4, x_A)$ and negative in $(x_A, 1)$. Furthermore, $x_A > x_3^\star = 0.5604664$; see also Figure 6.1.

ii) For $q = 4$, we have $C_4 = 15.53209593, x_1 = -1/3$ and $x_2 = 1$. As in the case $q = 3$, we see that Γ_4 is positive in $(-1/3, 0.13]$ and negative in $[0.162, 1)$. We easily infer that A_4 has a root x_A in the interval $(0.13, 0.162)$; A_4 is positive in $(-1/3, x_A)$ and negative in $(x_A, 1)$. Furthermore, $x_A > x_4^\star = 0.1203494$; see also Figure 6.2.

iii) For $q = 5$, we have $C_5 = 82.56035532, x_{1,2} = (3 \mp \sqrt{1065})/48$. In view of (4.29) and the monotonicity properties of polynomial r in (x_1, x_2) (recall that $r'(x) = 40(x-1)^2(8x-5)$), we have

$$f_5(x)r(x) \geqslant f_5(x_1)r(-0.2) = r(-0.2) > C_5 \quad \forall x \in (x_1, -0.2]$$

and

$$f_5(x)r(x) \geqslant f_5(-0.2)r(-0.08) > C_5 \quad \forall x \in (-0.2, -0.08],$$

i.e., $f_5(x)r(x) > C_5$ for $x \in (x_1, -0.08]$. Furthermore,

$$f_5(x)r(x) \leqslant f_5(\tilde{x}_5)r(-0.045) < C_5 \quad \forall x \in [-0.045, x_2).$$

Therefore, Γ_5 is positive in $(x_1, -0.08]$ and negative in $[-0.045, x_2)$. We easily infer that A_5 has a root x_A in the interval $(-0.08, -0.045)$; A_5 is positive in (x_1, x_A) and negative in (x_A, x_2). Furthermore, $x_A > x_5^\star = -0.09394996$; see also Figure 6.3.

iv) For $q = 6$, we have $C_6 = 1249.010379, x_{1,2} = (-4 \mp 3\sqrt{14})/20$. As in the case $q = 5$, distinguishing more subcases this time, we see that Γ_6 is positive in $(x_1, -0.1]$. In $[-0.0947, x_2)$, Γ_6 is negative since

$$f_6(x)r(x) \leqslant f_6(\tilde{x}_6)r(-0.0947) < C_6 \quad \forall x \in [-0.0947, x_2).$$

We easily infer that A_6 has a root x_A in the interval $(-0.1, -0.0947)$; A_6 is positive in (x_1, x_A) and negative in (x_A, x_2). Furthermore, $x_A > x_6^\star = -0.1228462$; see also Figure 6.4.

We next turn our attention to B_q, and observe that equation $B_q(x) = 0$ is equivalent to $\Delta_q(x) = 0$ with

$$\Delta_q(x) := \frac{\sqrt{p(x)r(x)}}{\psi(x)} - (2^q - 1)(\tan\vartheta_q - y_q^\star), \quad x \in (x_1, x_2),$$

$q = 3, 4, 5, 6$. Since x_1 and x_2 are roots of ψ, we easily see that Δ_q tends to ∞ as x decreases to x_1 or increases to x_2. Consequently, Δ_q can only have an even number of roots in the interval (x_1, x_2), counting also their multiplicities. For instance, for $q = 3$, we have $\Delta_3(0.7) < 0$, and infer that Δ_3, and consequently also B_3, possesses at least one root $\hat{x}_1 < 0.7$ and at least one root $\hat{x}_2 > 0.7$. Actually, $\hat{x}_1$ and $\hat{x}_2$ are the only roots of B_3 in $(1/4, 1)$; see also Figure 6.1. Furthermore, since $\Delta_3(0.576) > 0$, we have $\hat{x}_1 > 0.576 > x_A$; see also the discussion in *i)* concerning the roots of A_3. Summarizing, we have the following ordering

$$1/4 < x_3^\star < x_A < \hat{x}_1 < \hat{x}_2 < 1.$$

This is the case also for $q = 4, 5, 6$, i.e., Δ_q, and consequently also B_q, possesses exactly two roots $\hat{x}_1$ and $\hat{x}_2$ in the corresponding intervals (x_1, x_2), see also Figures 6.2, 6.3, 6.4, and we have the ordering

$$x_1 < x_q^\star < x_A < \hat{x}_1 < \hat{x}_2 < x_2.$$

From this information concerning A_q and B_q, we easily infer that

$$A_q(x) < yB_q(x) \quad \forall x \in [x_A, \hat{x}_1] \cup [\hat{x}_2, x_2] \qquad \forall y \in I_q; \tag{6.9}$$

actually, $A_q(x) \leqslant 0$ and $B_q(x) \geqslant 0$, while, for every x, at least one of these inequalities holds as a strict inequality.

Furthermore:

1. For $x \in (x_1, x_q^\star) \cup (x_q^\star, x_A)$, $B_q(x)$ is positive, and relation $A_q(x) < yB_q(x)$ reads $\frac{A_q(x)}{B_q(x)} < y$. Since $y > y_q^\star$, it suffices to show that $\frac{A_q(x)}{B_q(x)} \leqslant y_q^\star$. But

$$\frac{A_q(x)}{B_q(x)} - y_q^\star = \frac{(\tan\vartheta_q - y_q^\star)\big[\sqrt{p(x)r(x)} - (2^q-1)\varphi(x) + (2^q-1)y_q^\star\psi(x)\big]}{B_q(x)},$$

whence $\frac{A(x)}{B(x)} - y_q^\star \leqslant 0$ if and only if

$$\sqrt{p(x)r(x)} - (2^q-1)\varphi(x) + (2^q-1)y_q^\star\psi(x) \leqslant 0.$$

The last inequality reads $g_q(x) \geqslant y_q^\star$, cf. (4.6), and we already know that it holds true for $x \in (x_1, x_2)$.

2. For $x \in (\hat{x}_1, \hat{x}_2)$, $B_q(x)$ is negative, and relation $A_q(x) < yB_q(x)$ reads $\frac{A_q(x)}{B_q(x)} > y$. Since $y < \tan\vartheta_q$, it suffices to show that $\frac{A_q(x)}{B_q(x)} \geqslant \tan\vartheta_q$. But

$$\frac{A_q(x)}{B_q(x)} - \tan\vartheta_q = \frac{(2^q-1)(\tan\vartheta_q - y_q^\star)\big[\varphi(x) - \tan\vartheta_q\psi(x)\big]}{-B_q(x)}.$$

Therefore, $\frac{A_q(x)}{B_q(x)} - \tan\vartheta_q \geqslant 0$ if and only if $\varphi(x) \geqslant (\tan\vartheta_q)\psi(x)$; the last inequality holds true for all $x \in (x_1, x_2)$ in view of (1.12).

The proof is complete. ■

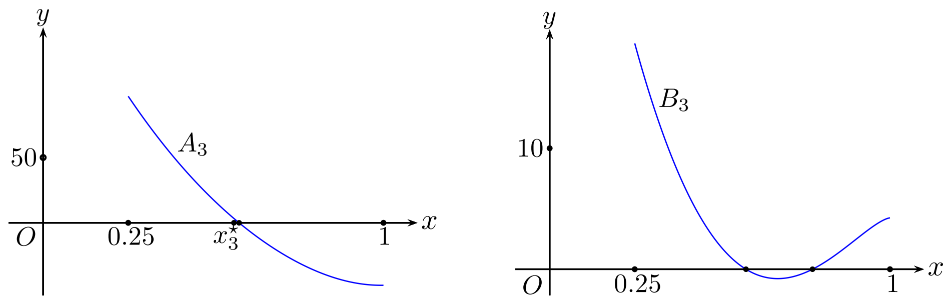

Figure 6.1. *The graphs of A_3 and B_3, see (6.5) and (6.6), in the interval $[0.25, 1]$ for the implicit–explicit three-step BDF method. The root of A_3 is $x_A \approx 0.575766 > x_3^\star \approx 0.5604664$. The roots of B_3 are $\hat{x}_1 \approx 0.57688145572238$ and $\hat{x}_2 \approx 0.7722924766936324$.*

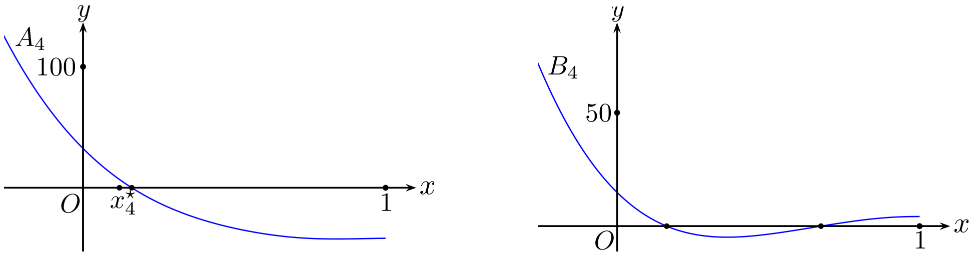

Figure 6.2. *The graph of A_4 and B_4, see (6.5) and (6.6), in the interval $[-0.32, 1]$ for the implicit–explicit four-step BDF method. The root of A_4 is $x_A \approx 0.1609042 > x_4^\star \approx 0.1203494$. The roots of B_4 are $\hat{x}_1 \approx 0.16392482721$ and $\hat{x}_2 \approx 0.673783681332$.*

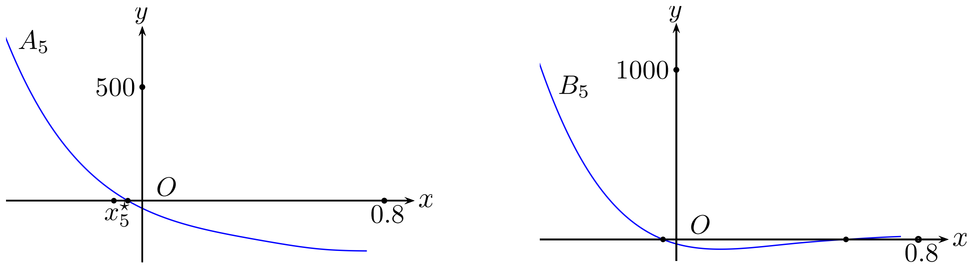

Figure 6.3. *The graph of A_5 and B_5, see (6.5) and (6.6), in the interval $[-0.5, 0.74238]$ for the implicit–explicit five-step BDF method. The root of A_5 is $x_A \approx -0.047857230139 > x_5^\star \approx -0.09394996$. The roots of B_5 are $\hat{x}_1 \approx -0.044010720715$ and $\hat{x}_2 \approx 0.5608143692$.*

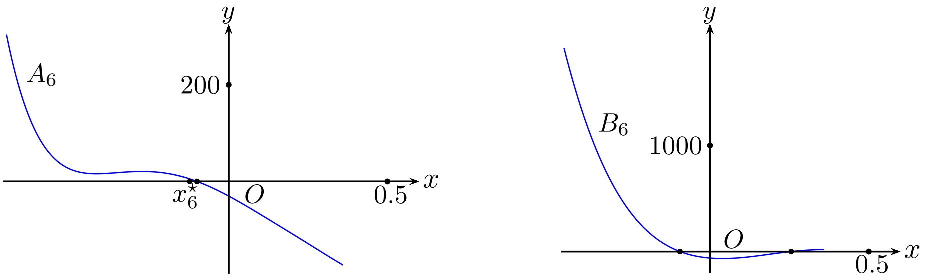

Figure 6.4. *The graph of A_6 and B_6, see (6.5) and (6.6), in the intervals $[-0.7, 0.36]$ and $[-0.46, 0.36]$, respectively, for the implicit–explicit six-step BDF method. The root of A_6 is $x_A \approx -0.09989611608648 > x_6^\star \approx -0.1228462$. The roots of B_6 are $\hat{x}_1 \approx -0.09463549647219$ and $\hat{x}_2 \approx 0.2559357891275995$.*

7. Numerical verification. Our goal here is the numerical assessment of the convenient sufficient unconditional stability conditions (1.9) and (1.16). We present numerical results to illustrate the discrepancy between the sufficient stability condition (1.16) in Theorem 1.4 and the necessary stability condition (1.7). We used the starting values $y^i = 1, i = 0, \dots, q-1$. Also, for simplicity, since real μ yield satisfactory results, we only considered this case; complex μ could lead to instability even for smaller $|\mu|$.

We recall that we are interested in the unconditional stability of the methods; we could obtain the same numerical results for time steps h/a with the zeroth order terms in the test equation of (1.1) multiplied by a positive constant a.

If the sharp stability condition (1.9) is not satisfied for the implicit–explicit Euler method, then we could use μ with $\operatorname{Re}\mu > 1$. This case is not of interest to us, since even the modulus of the solution y of (1.1), $|y(t)| = \mathrm{e}^{(\operatorname{Re}\mu-1)t}$, tends to ∞ as $t \to \infty$; this is why we do not present relevant numerical results in Table 7.1.

The constants $\lambda \in (y_q^\star, \tan\vartheta_q), q = 3,\dots,6$, in Table 7.1 are good approximations to the midpoints of these intervals. For $|\lambda| \in (y_q^\star, \tan\vartheta_q)$, to obtain instability for small $|\mu|$, one needs to carefully choose the time step h. It follows from our analysis that if, for a given $y \in (y_q^\star, \tan\vartheta_q)$, the maximum in (4.1) is attained at a point $x^\star(y) \in (x_1, x_2)$, then the supremum over s in (1.5) is attained at

$$s^\star(y) = -\frac{|d(\zeta^\star(y))|^2}{\operatorname{Re}\big((1-\mathrm{i}y)d(\zeta^\star(y))\big)} \quad \text{with} \quad \zeta^\star(y) := x^\star(y) - \mathrm{i}\sqrt{1-(x^\star(y))^2},$$

where $d(\zeta) = \alpha(\zeta)/\beta(\zeta)$. The time steps h in Table 7.1 are very good approximations to $s^\star(|\lambda|)$. In contrast, for $\lambda \leqslant y_q^\star$, good results are obtained for various time steps h; in these cases, we did not make any attempt to optimize h.

Table 7.1
Numerical assessment of the sufficient stability conditions (1.9) and (1.16).

q	μ	λ	h	$\lvert y^{42000}\rvert$	conditions (1.9)–(1.16)
1	1	0.5	0.1	$1.50 \cdot 10^{-19}$	satisfied
2	−0.3333	0	10000	$7.22 \cdot 10^{-8}$	satisfied
2	−0.3336	0	10000	$1.47 \cdot 10^{5}$	violated
3	−0.14285	0	10000	$7.90 \cdot 10^{-9}$	satisfied
3	−0.14314	0	10000	$3.05 \cdot 10^{13}$	violated
3	0.0714	12.582738	0.0893334	$1.44 \cdot 10^{-2}$	satisfied
3	0.0737	12.582738	0.0893334	$7.78 \cdot 10^{1}$	violated
4	−0.066666	0	10000	$1.56 \cdot 10^{-10}$	satisfied
4	−0.066840	0	10000	$3.12 \cdot 10^{12}$	violated
4	0.0333	2.904812	0.6619035	$1.09 \cdot 10^{-18}$	satisfied
4	0.0351	2.904812	0.6619035	$1.25 \cdot 10^{3}$	violated
5	−0.032258	0	10000	$1.67 \cdot 10^{-13}$	satisfied
5	−0.032372	0	10000	$1.53 \cdot 10^{12}$	violated
5	0.01612	1.0860879	1.8059204	$5.56 \cdot 10^{-31}$	satisfied
5	0.01720	1.0860879	1.8059204	$1.37 \cdot 10^{3}$	violated
6	−0.015873	0	10000	$4.09 \cdot 10^{-18}$	satisfied
6	−0.015955	0	10000	$3.23 \cdot 10^{13}$	violated
6	0.0079365	0.23156154	2.3852828	$1.57 \cdot 10^{-14}$	satisfied
6	0.0083200	0.23156154	2.3852828	$1.03 \cdot 10^{2}$	violated

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