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SPECTRAL ANALYSIS OF NONSYMMETRIC QUASI-TOEPLITZ MATRICES WITH APPLICATIONS TO PRECONDITIONED MULTISTEP FORMULAS*

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Abstract. The eigenvalue spectrum of a class of nonsymmetric preconditioned matrices arising in time-dependent partial differential equations is analyzed and discussed. The matrices generated by the underlying numerical integrators are small rank perturbations of block Toeplitz matrices; circulant-like preconditioners based on the former are considered. The eigenvalue distribution of the preconditioned matrix influences often crucially the convergence of Krylov iterative accelerators. Due to several reasons (lack of symmetry, band structure, and coefficients depending on the size) the classical approach based on smooth generating functions gives very little insight here. Therefore, to characterize the eigenvalues, a *difference equation* approach exploiting the band Toeplitz and circulant patterns generalizing the well-known results of Trench is proposed.

Key words. circulant preconditioners, nonsymmetric Toeplitz matrices, eigenvalues, difference equations, linear systems of time-step integrators, linear multistep formulas, boundary value problems

AMS subject classifications. 15A18, 65F10, 65F15, 65N22, 65Q05

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1. Introduction.

In this paper we focus on small rank perturbations of block nonsymmetric Toeplitz matrices preconditioned by circulant approximations introduced in [3, 4, 7].

An $n \times n$ matrix $A_n = (a_{j,k})$ is said to be *Toeplitz* if $a_{j,k} = a_{j-k}$, $j, k = 1, \ldots, n$, i.e., A_n is constant along its diagonals, and quasi-Toeplitz if it is a small rank perturbation of a Toeplitz matrix. $\breve{A}_n$ is *circulant* if it is Toeplitz and its diagonals satisfy $\breve{a}_{n-j} = \breve{a}_{-j}$. The circulant matrices $\breve{A}_n$ are diagonalized by the Fourier matrix $F = (F_{j,k})$, $F_{j,k} = e^{2\pi \mathbf{i} jk/n}/\sqrt{n}$, $j, k = 0, \ldots, n-1$, and $\mathbf{i}$ is the imaginary unit; see [19]. Circulant matrices are easily and efficiently invertible using the fast Fourier transform (FFT), as in [16].

Perturbations of block nonsymmetric Toeplitz matrices arise in the numerical approximation of time-dependent partial differential equations (PDEs) by generalizations of implicit multistep formulas used in boundary value form [20, 1, 14]. The techniques considered here could be adapted to other discretization schemes based on finite differences for PDEs.

Other circulant-like matrices used in the PDE context can be found in [8].

As explained in section 2.1, the matrices of the underlying linear systems can be written as follows:

$$M = A \otimes I - h\, B \otimes J, \tag{1.1}$$

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where A and B are $n \times n$ small rank perturbations of band Toeplitz matrices whose entries are given by the coefficients of the scheme involved, I is the identity, and J is an $m \times m$ matrix which can be large and sparse. More precisely, J is the Jacobian matrix of a system of equations discretized in space by finite differences; see [4] for details.

Unfortunately, when m and/or n are (even moderately) large, iterative solvers for (1.1), used without preconditioners or with general purpose preconditioners, such as those based on incomplete factorizations, often converge very slowly or not at all; see [4, section 5]. In general, direct methods cannot exploit the block structure of (1.1).

Preconditioners introduced in [4] take into account this structure. They are block-circulant and, in compact form, can be written as

$$P = \breve{A} \otimes I - h\,\breve{B} \otimes \tilde{J}, \tag{1.2}$$

where $\breve{A}$ and $\breve{B}$ are circulant-like approximations for A, B, respectively, and $\tilde{J}$ is a suitable approximation for J. Their performance has been tested in several papers [4, 5, 17].

The distribution of the eigenvalues of the matrices M and $P^{-1}M$ can influence the convergence of iterations of Krylov subspace methods. This is the case, e.g., if the condition number of the eigenvector matrix is moderate; see [22].

Tables of the condition number $\kappa_2(X)$ of the eigenvector matrix X for the (left) preconditioned matrix $P^{-1}M$ and related discussions can be found in [9], showing that eigenvalues can give reasonable information in our setting. Similar conclusions hold true for the nonpreconditioned case for most of the methods considered here. More details are reported in section 6.

A theoretical investigation of the eigenvalues is hard because, in general, P and M are nonsymmetric and nonsymmetrizable. Moreover, as explained in section 3 an analysis of the eigenvalues based on the generating function of the underlying Toeplitz matrices is not feasible here, although very meaningful for Hermitian matrices [16, 23].

These difficulties motivate us to a "direct" analysis, based on the generalized eigenvalue problem

$$M\,u = \lambda\,P\,u.$$

The tools used here are completely different from those in previous works such as [10], [7], or [25]. In particular, we cannot write $\breve{A}$, $\breve{B}$ as small rank perturbations of A, B.

By using instead linear difference equation theory and generalizing Trench's approach [33, 34], we derive closed formulas and first-order expansions for λ as a function of the time step h and of the eigenvalues of the Jacobian matrix J. This characterization involves the roots of a sparse polynomial whose degree is related to the size of A and B.

Our estimates are explicitly computed for some well-known 2-step integrators and compared with the "true" eigenvalues approximated by Matlab. The approach seems very useful for spectrum localization and is not too expensive provided that A and B have moderate size or an efficient rootfinder is associated with our technique.

The paper is organized as follows. Section 2 introduces the problem and the main circulant preconditioning techniques. In section 3 we discuss the relevant literature for spectral analysis, and we explain in more detail the motivation of our work. Section 4 is devoted to the spectral analysis, from the general case to the 2-step case study. In section 5 we describe two classical PDE examples, representing the test problems for our experiments of section 6.

2. Preliminaries. Let us consider a model problem based on a first-order initial-boundary value time-dependent partial differential equation

$$\begin{cases} \dfrac{\partial u}{\partial t} & = \mathcal{L}(u) + f, \quad x \in \mathbf{D}, \\ \mathcal{G}(u) & = g, \qquad\quad x \in \partial\mathbf{D}, \\ u & = u_0, \qquad\quad t = t_0, x \in \mathbf{D}, \end{cases} \tag{2.1}$$

where $\mathbf{D}$ is an open domain in $\mathbb{R}^N$, $N \geq 1$, and $\mathcal{L}$ is a differential operator, nonlinear in u in general. Equations (2.1) are *evolutionary* because they describe evolving phenomena and combine differentiation with respect to both space and time. For simplicity, we will focus on linear operators $\mathcal{L}$ and $\mathcal{G}$. However, most of the techniques considered here can be applied to a more general nonlinear framework by recalling that often numerical codes linearize the nonlinear algebraic equations by using a quasi-Newton step; see [21].

2.1. Linear multistep formulas in boundary value form. In the following, a brief description of a generalization of linear multistep formulas is given.

If the partial differential equation (2.1) is first discretized in space, we obtain a system of ordinary differential equations (ODEs). Such a system can be very large and is treated by means of a numerical method for ODEs.

Here we focus on linear multistep formulas applied in boundary value form (see [1, 14]), which generalize classical implicit linear multistep formulas by using both initial and boundary conditions even in the presence of an initial value problem. Such schemes have a relatively long history (see, e.g., [20, 1]) and can be very useful in some communities where "time" has no special orientation (see an example of these problems in the work by Shirley referred to in [26]).

More precisely, we suppose that (2.1), with solution $u(x,t)$, has been discretized in space on a certain grid Ω_τ, with mesh width $\tau > 0$, to yield a *semidiscrete* system

$$y'(t) = F(t, y(t)), \quad t_0 \leq t \leq t_s, \quad y(t_0) \text{ given}, \tag{2.2}$$

with $y(t) = (u_j(t))_{j=1}^m$, m being related to the number of grid points in space, and, for unidimensional spatial domain $\mathbf{D}$, i.e., $N = 1$ in (2.1), $u_j(t)$ approximates $u(x_j, t)$ at some x_j, $j = 1, \ldots, m$. The contribution of the discretized boundary conditions is enclosed in F. In order to approximate $u(x,t)$ on Ω_τ for $t = t_0, t_1, \ldots, t_s$, an appropriate temporal mesh, we apply an ODE method with step size $h > 0$.

Using the shortened notation $F_{n+i} = F(t_{n+i}, y_{n+i})$, $i = 0, \ldots, k$, if y_n approximates $y(t_n)$, linear multistep formulas in boundary value form are given by

$$\sum_{i=0}^{k} \alpha_i y_{n+i} = h \sum_{i=0}^{k} \beta_i F_{n+i}, \quad n = 0, \ldots, s-k, \tag{2.3}$$

where $y_0 = y(t_0)$ is provided by initial conditions of (2.1), while $y_1, \ldots, y_{\nu-1}$ and $y_{s-k+\nu+1}, \ldots, y_s$, computed at the mesh points $t_0, \ldots, t_{\nu-1}$, $t_{s-k+\nu+1}, \ldots, t_s$, are determined by using other difference formulas, usually of the same order of (2.3). In practical use, we couple three sets of formulas: $\nu - 1$ for $y_1, \ldots, y_{\nu-1}$, $s - k + 1$ with the coefficients as (2.3) and $k - \nu$ for $y_{s-k+\nu+1}, \ldots, y_s$. We note that the formulas of the first and third sets are still based on linear multistep finite differences expressions as (2.3), but each one has different coefficients (and is independent from those in (2.3)), while all formulas in the second set, based on (2.3), share the same coefficients $\alpha_0, \ldots, \alpha_k$, $\beta_0, \ldots, \beta_k$.

As announced, we simplify the notation; i.e., we suppose F linear, $F(t, y(t)) = J\,y(t) + g(t)$, where $J \in \mathbb{R}^{m\times m}$ and g is a vector-valued function of t. The underlying discrete boundary value problem can be solved by forming the following linear system:

$$\begin{aligned} &Mz = b, \quad M = A \otimes I_m - B \otimes (h\,J), \quad z^T = \left(y_0^T, y_1^T, \ldots, y_s^T\right), \\ &b = e_1 \otimes y_0 + h(B \otimes I_m)g, \quad g^T = (g(t_0)^T \ldots g(t_s)^T), \end{aligned} \tag{2.4}$$

where A, B are $(s+1)\times(s+1)$ real-valued quasi-Toeplitz nonsymmetric matrices and e_1 is the first column of the identity matrix. In practice, we accommodate the coefficients α_j, $\alpha_j^{(r)}$, $\quad j = 0, \ldots, k, \quad r = 1, \ldots, \nu-1, s-k+\nu+1, \ldots, s$ in A and β_j, $\beta_j^{(r)}$, $\quad j = 0, \ldots, k, \quad r = 1, \ldots, \nu-1, s-k+\nu+1, \ldots, s$ in B such that we can look at A as $\hat{A} + R_A$ and B as $\hat{B} + R_B$, $\hat{A}$ and $\hat{B}$ Toeplitz matrices with stencil

$$\left(0 \ldots 0\ \alpha_0 \ldots \underline{\alpha_\nu} \ldots \alpha_k 0 \ldots 0\right)$$

and

$$\left(0 \ldots 0\ \beta_0 \ldots \underline{\beta_\nu} \ldots \beta_k 0 \ldots 0\right),$$

respectively. The underlined element is the one on the main diagonal, and R_A and R_B have nonzero elements at most in their $\nu \times (k+1)$ upper left and $(k-\nu)\times(k+1)$ lower right corners.

The additional work needed for the solution of the discrete problems (2.4) with respect to those for the solution of implicit standard linear multistep formulas (i.e., used with only initial values) is justified by better stability and order properties; see [14, 4] for details and discussions.

More on the matrices A, B, and M generated by the schemes above can be found in [7, 6]. Examples of matrices A, B, and M for 2-step formulas will be given in what follows.

2.2. A review of block-circulant preconditioners. We noted in [4] that, in d dimensions, $d > 1$, when a fine enough spatial discretization is used in (2.1), direct methods are often not feasible to solve linear systems (2.4). Iterative methods are mandatory when the discrete problem is generated by a three-dimensional or even two-dimensional differential model (2.1). In [3, 4] Krylov subspace methods were proposed to solve (2.4). However, without preconditioning, the convergence can be very slow or iterations do not converge at all. Therefore, in [3, 4] a preconditioning strategy based on circulant matrices was introduced (see also [16]). Thus, other approximations were introduced in [5, 8]; see [8] for a more comprehensive bibliography. By left preconditioning we mean solving the equivalent nonsymmetric linear system

$$P^{-1}Mx = P^{-1}b \tag{2.5}$$

instead of $Mx = b$. Right preconditioning is obtained by considering

$$MP^{-1}y = b, \quad x = P^{-1}y.$$

Note that matrices MP^{-1} and $P^{-1}M$ are similar and hence share the same eigenvalues. Since we are interested in the eigenvalues of (2.5), our analysis is based entirely on left preconditioning.

In what follows, some block-circulant and block-circulant-like preconditioners for (2.4) are briefly reviewed.

Let us consider the following approximation of the matrix M:

$$P = \breve{A} \otimes I_m - h\breve{B} \otimes \tilde{J}, \tag{2.6}$$

where $\tilde{J}$ is a suitable approximation of the Jacobian matrix or the Jacobian itself. $\breve{A}$, $\breve{B}$ are circulant matrices whose entries are derived from the coefficients of the main method (2.3) as follows:

$$\begin{aligned} &\breve{A} = circ(\breve{a}),\ \breve{a}_j = c_{j,1}(s)\alpha_{j+\nu} + c_{j,2}(s)\alpha_{j+\nu-(s+1)}, \\ &\breve{B} = circ(\breve{b}),\ \breve{b}_j = c_{j,3}(s)\beta_{j+\nu} + c_{j,4}(s)\beta_{j+\nu-(s+1)}, j = 0, \ldots, s, \end{aligned} \tag{2.7}$$

where $circ(\cdot)$ denotes the circulant matrix having the first column specified in the argument, and the $c_{j,i}(s)$, $i = 1, \ldots, 4$, $j = 0, \ldots, s$, are linear in j. It is understood that α_j (β_j) is zero for $j < 0$ or $j > k$ in (2.7), so that the sparsity of A, B implies that of $\breve{A}$, $\breve{B}$. The coefficients $c_{i,j}(s)$ in (2.7) are chosen in such a way that $\breve{A}$, $\breve{B}$ are suitable approximations of A, B in (2.4), respectively.

The approximation of A, B with T. Chan's *optimal circulant preconditioner* (see [18]) requires that

$$c_{j,1}(s) = c_{j,3}(s) = 1 - \frac{j}{s+1},\ \text{and}\ c_{j,2}(s) = c_{j,4}(s) = \frac{j}{s+1}, j = 0, \ldots, s, \tag{2.8}$$

while for Strang's *natural (or simple) circulant preconditioner* (see [29])

$$\begin{aligned} &c_{j,1}(s) = c_{j,3}(s) = 1, \quad j = 0, \ldots, \left\lfloor \frac{s+1}{2} \right\rfloor, \\ &c_{j,2}(s) = c_{j,4}(s) = 1, \quad j = \left\lfloor \frac{s+1}{2} \right\rfloor + 1, \ldots, s, \quad c_{j,i}(s) = 0 \text{ otherwise.} \end{aligned}$$

On the other hand, if we consider, instead of (2.8), the following definition of the coefficients $c_{j,i}(s)$ for $\breve{A}$ and $\breve{B}$:

$$c_{j,1}(s) = c_{j,3}(s) = 1 + \frac{j}{s+1}, \quad c_{j,2}(s) = c_{j,4}(s) = \frac{j}{s+1}, \quad j = 0, \ldots, s, \tag{2.9}$$

we get the so-called P-circulant approximations which, used in (2.6), gives the P-circulant (block) preconditioner, introduced in [3, 4]. The latter definition avoids singularity problems which are sometimes typical of the former choices.

In [3, 4] and in [17] it was shown that both the P-circulant and generalized Strang preconditioned systems can be effective to accelerate the convergence. Unfortunately, when the Jacobian matrix J has some small (or zero) eigenvalues, the simple circulant or Strang preconditioner can be severely ill-conditioned or even singular (see [3, 4, 5]). An analysis of the spectrum for the preconditioned matrix based on simple circulant approximations can be found in [10]. However, we stress that the tools used here are completely different from those in the former. In particular, we cannot write anymore $\breve{A}$, $\breve{B}$ as small rank perturbations of A, B, respectively.

Therefore, we will focus on preconditioners (2.6) based on T. Chan's and the P-circulant approximations in the following discussions. Practical examples for the matrices A, B, $\breve{A}$, $\breve{B}$, M, and P can be found below.

Another approximation which was found effective (but is not considered here) is based on $\{\omega\}$-circulant approximations for matrices A and B in (2.4); see [8]. In

particular, $\breve{A}$, $\breve{B}$ are $\{\omega\}$-circulant matrices approximating A and B, respectively. The $\{\omega\}$-circulant matrices are Toeplitz matrices whose first entry of a row is given by multiplying the last entry of the preceding row by $\omega = \exp(\mathbf{i}\theta)$; see [19] for more details. Notice that the $\{1\}$-circulant matrices ($\theta = 0$) are just circulant matrices (and therefore generate simple or Strang's approximations for a given Toeplitz matrix), while $\{-1\}$-circulant matrices ($\theta = \pi$) are skew-circulant matrices.

We observe that various trigonometric approximations can be combined. For example, $\{\omega\}$-P-circulant preconditioners can be defined by using (2.9) to give the first row of the related $\{\omega\}$-circulant approximation. A similar combination can be made by using T. Chan's optimal circulant matrices. Moreover, it is straightforward to observe that P-circulant approximations can be seen as $\{\omega\}$-circulant preconditioners with $\theta = 0$, whose entries are defined as in (2.9). More comments on these generalizations can be found in [8].

2.3. Dahlquist's hypothesis. In the proposed eigenvalue analysis for the preconditioned linear systems (2.5), unless otherwise specified, we choose $J = \mu$ (i.e., a scalar) in (2.2), where $\mu \in \mathbb{C}^- := \{\lambda \in \mathbb{C} : \mathrm{Re}\lambda \leq 0\}$ ("Dahlquist's hypothesis"). It is customary to consider this scalar problem in the linear stability theory for ODEs. The parameter μ can be any eigenvalue of the Jacobian matrix J of the given PDE, supposed diagonalizable. Indeed, notice that, supposing J diagonalizable, we have

$$J = VDV^{-1}, \quad D = \mathrm{diag}(\mu_1, \ldots, \mu_m).$$

This framework is not restrictive for our analysis since

$$M = A \otimes I_m - hB \otimes \left(VDV^{-1}\right) = (I_{s+1} \otimes V)(A \otimes I_m - hB \otimes D)(I_{s+1} \otimes V^{-1}).$$

Assuming that the preconditioner is based on the exact Jacobian, a similar expression can be derived for P. Let us write

$$M(q) = A - qB, \quad P(q) = \breve{A} - q\breve{B}, \quad q = h\mu.$$

It is straightforward to observe that the eigenvalues of the preconditioned/transformed linear system (2.5) are given by the union of the eigenvalues of the finite sequence of matrices

$$\{P(q)^{-1}M(q)\}_q, \quad q = h\mu_i, \quad i = 1, \ldots, m.$$

Just to have an idea of the matrix structures, we sketch below the explicit expression of $M(q)$ and $P(q)$ for the particular example of a 2-step generalized Adams–Moulton method in connection to a P-circulant preconditioner, with an additional final condition given by the implicit Euler method:

$$M(q) = \begin{pmatrix} 1 & 0 & & & \\ -1 & 1 & 0 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 1 & 0 \\ & & & -1 & 1 \end{pmatrix} - q \cdot \begin{pmatrix} \frac{2}{3} & -\frac{1}{12} & & & \\ \frac{5}{12} & \frac{2}{3} & -\frac{1}{12} & & \\ & \ddots & \ddots & \ddots & \\ & & \frac{5}{12} & \frac{2}{3} & -\frac{1}{12} \\ & & & 0 & 1 \end{pmatrix},$$

$$P(q) = \begin{pmatrix} 1 & 0 & & & -\frac{s}{s+1} \\ -\frac{s}{s+1} & 1 & 0 & & \\ & \ddots & \ddots & \ddots & \\ & & -\frac{s}{s+1} & 1 & 0 \\ 0 & & & -\frac{s}{s+1} & 1 \end{pmatrix} - q \cdot \begin{pmatrix} \frac{2}{3} & \breve{b}_1 & & & \breve{b}_s \\ \breve{b}_s & \frac{2}{3} & \breve{b}_1 & & \\ & \ddots & \ddots & \ddots & \\ & & \breve{b}_s & \frac{2}{3} & \breve{b}_1 \\ \breve{b}_1 & & & \breve{b}_s & \frac{2}{3} \end{pmatrix},$$

where $\breve{b}_1 = -\frac{s+2}{12(s+1)}, \breve{b}_s = \frac{5s}{12(s+1)}$.

We recall that the underlying generalizations of Adams–Moulton formulas, which should be used only as implicit methods with one initial (given) and one final condition, are (i) A-stable not only for $k = 2$ but for arbitrarily high-order $k+1$ and (ii) all formulas preserve important properties such as the time reversal symmetry and the Hamiltonian function; see [14]. Note that if we use the usual 2-step Adams–Moulton formula, we should supply another starting value y_1.

3. Motivation of the work. From now on, we will assume Dahlquist's hypothesis (see section 2.3) in order to simplify the theoretical analysis.

Understanding the behavior of iterative solvers for (2.4) requires the knowledge of the following features:

1. How does the spectrum of M depend on the discretization parameters? For instance, for which values of q (both involving the time step and the Jacobian of the PDE) can we ensure that the spectrum lies in $\mathbb{C}^+ := \{\lambda \in \mathbb{C} : \mathrm{Re}\lambda > 0\}$? Can we exclude the pathological situation where M is singular?
2. When a suitable preconditioner is applied, we know that the spectrum of $P^{-1}M$ is clustered; see, e.g., [23]. But which localization of the cluster (and of the outliers, if present) should be expected? Again, how does that localization depend on q?

Concerning the first issue, the literature contains plenty of spectral results involving Toeplitz matrices (see, e.g., [12, 13]), even though the nonsymmetric case is more difficult to treat (surprisingly, smoothness of the generating function can be a disadvantage: see [32]). In particular, this difficulty arises in our setting, where generating functions are trigonometric polynomials, and the accurate localization results typical for Hermitian matrices are no longer applicable. Moreover, such results are of the asymptotic type and require a critical assumption: *the entries of M must not depend on the size*. In other words, as the size varies we obtain a finite section of a *fixed* infinite matrix. This is not our case, since varying s (the size of matrices A and B and $s = O(h^{-1})$) gives a different value of q in M.

The only known results we can apply concern mainly algorithms for computation of a few eigenvalues (in [2]) or a theoretical analysis of the "pencil" $A - qB$ (in the sense of generalized eigenvalues) in [14]: in the latter book we can find conditions on q for which M is nonsingular, that is, a partial answer to our questions raised above.

In summary, to the best of our knowledge, *a general theoretical characterization of the eigenvalues of $M = A - qB$ as functions of q is still lacking*. The underlying algebraic setting is the (standard) eigenvalue problem for nonsymmetric Toeplitz matrices with small rank corrections.

Concerning the second issue, some mathematical tools for the spectral analysis of $P^{-1}M$ have been proposed in the literature (see, e.g., [4, 10, 17, 25]), but they all assume that $M - P$ has small rank. This is true for some choices of P (such as Strang's preconditioner and a few extensions), but several other important instances (such as T. Chan's or P-circulant approximations) give rise to matrices $M - P$ whose rank is usually full.

Therefore, *appropriate tools for the analysis of the case where P differs from M by more than a matrix whose rank is small*[1] *are still unknown.* An exception is provided in the Hermitian case, not of interest in this context. The underlying algebraic setting is the *generalized* eigenvalue problem for nonsymmetric Toeplitz matrices with small rank corrections.

The following sections will attempt to give some answers to the open questions discussed so far.

4. Spectral analysis. From now on we focus on the generalized eigenvalue problem for nonsymmetric quasi-Toeplitz matrices:

$$M(q)u = \lambda P(q)u, \qquad u \neq 0. \tag{4.1}$$

The standard eigenproblem falls into this notation by making the formal assumption $P(q) = I$ (in this section we are interested just in the *structure* of the matrices involved).

The lack of symmetry and the band structure imply that the classical approach based on generating functions gives very little insight here (see the results presented in [32]). Therefore, the best way to characterize eigenvalues (and potentially eigenvectors) by exploiting the band Toeplitz pattern seems to be the *difference equation* approach, proposed by Trench [33] for the standard, pure Toeplitz case.

Let the $s+1$ equations of (4.1), as well as the entries of u, be indexed from 0 to s; the indices from ν to $s-k+\nu$ correspond to the rows of $M(q)$ and $P(q)$ not affected by the low rank correction and containing all of the coefficients of the main method. The resulting relations

$$\sum_{i=0}^{k}(\alpha_i - q\beta_i)u_{i+j} = \lambda\sum_{i=0}^{k}(\breve{a}_{i-\nu} - q\breve{b}_{i-\nu})u_{i+j}, \quad j = 0, \ldots, s-k$$

(where we assume a periodic pattern for $\breve{a}_i$ and $\breve{b}_i$, whenever a subscript is out of range), can be treated as linear k-order homogeneous difference equations with constant coefficients. The first and last rows of (4.1) will provide us with initial and final conditions.

The eigenvector u is a nonzero solution of the difference problem and therefore can be characterized in terms of the algebraic *characteristic equation* of degree k:

$$\pi(z) - \lambda\breve{\pi}(z) = 0, \quad \pi(z) := \sum_{i=0}^{k}(\alpha_i - q\beta_i)z^i, \ \breve{\pi}(z) := \sum_{i=0}^{k}(\breve{a}_{i-\nu} - q\breve{b}_{i-\nu})z^i \tag{4.2}$$

(notice that $\breve{\pi}(z)$ simplifies into z^ν in the standard problem).

From now on we assume that, for each eigenvalue λ, all of the roots $z_1(\lambda), \ldots, z_k(\lambda)$ of the characteristic equation are distinct (otherwise, λ is called *defective* [34], but this pathological situation occurs just in isolated cases and for specific values of s). In this case, each component of the solution of the difference equation has the form

$$u_j = \sum_{l=1}^{k} c_l z_l(\lambda)^j, \quad j = 0, \ldots, s, \tag{4.3}$$

for suitable coefficients $c_1, \ldots, c_k$ determined by the boundary conditions.

[1] In the sense that s is supposed large with respect to the band of the Toeplitz matrices involved, and the rank is not depending on s.

More specifically, the first ν and the last $k-\nu$ rows of (4.1) represent additional conditions on the sequence u_j. In the standard problem, we have ν *initial* and $k-\nu$ *final* conditions since just the first and last entries of u are involved, respectively. In the generalized problem, the circulant structure of $P(q)$ determines a mixing of initial and final entries in all of these k equations, but for simplicity we keep the same terminology.

Substituting (4.3) into the mentioned equations, we obtain k homogeneous relations involving the unknown coefficients $c_1, \dots, c_k$, which can be put in matrix form as follows:

$$\begin{aligned} K_{\text{in}}(z_1(\lambda), \dots, z_k(\lambda))c = 0, \\ K_{\text{fin}}(z_1(\lambda), \dots, z_k(\lambda))c = 0, \end{aligned} \tag{4.4}$$

where $K_{\text{in}} \in \mathbb{C}^{\nu \times k}, K_{\text{fin}} \in \mathbb{C}^{(k-\nu)\times k}$ and we have emphasized the dependence of these Vandermonde-like matrices on the roots of the characteristic equation. The trivial solution $c = 0$ would imply $u = 0$ and therefore must be discarded; hence the square matrix

$$K(z_1(\lambda), \dots, z_k(\lambda)) := \begin{pmatrix} K_{\text{in}} \\ K_{\text{fin}} \end{pmatrix} \tag{4.5}$$

must be singular. Its (vanishing) determinant can be regarded as a function of λ having the same zeros of the characteristic polynomial of (4.1).

An alternative parameterization with respect to the roots $z_j(\lambda)$ can be useful for a different characterization of λ.

Let ζ be one of the roots, say, $z_1(\lambda)$. From one point of view, ζ is a function of λ, but it is understood that λ can be retrieved as well from ζ by means of the characteristic equation

$$\lambda(\zeta) = \frac{\pi(\zeta)}{\breve{\pi}(\zeta)} \qquad (\lambda(\zeta) = \zeta^{-\nu}\pi(\zeta) \text{ in the standard case}); \tag{4.6}$$

we remark that *any* root gives the same value of λ. The other roots can be expressed in terms of λ by inverting some elementary symmetric functions. For example, in the generalized problem with $k = 2$ and $\nu = 1$, the easiest way is to consider the ratio between the constant term and the leading coefficient in (4.2)

$$\frac{\alpha_0 - q\beta_0 - \lambda(\breve{a}_s - q\breve{b}_s)}{\alpha_2 - q\beta_2 - \lambda(\breve{a}_1 - q\breve{b}_1)} = z_1(\lambda)z_2(\lambda),$$

whence, after the substitution $\lambda = \lambda(\zeta)$ given in (4.6),

$$z_2(\lambda) = \zeta^{-1}\frac{(\alpha_0 - q\beta_0)\breve{\pi}(\zeta) - (\breve{a}_s - q\breve{b}_s)\pi(\zeta)}{(\alpha_2 - q\beta_2)\breve{\pi}(\zeta) - (\breve{a}_1 - q\breve{b}_1)\pi(\zeta)} =: \zeta_2(\zeta). \tag{4.7}$$

In general, we can assume that we have explicit functions $\zeta_2(\zeta), \dots, \zeta_k(\zeta)$ that replace $z_2(\lambda), \dots, z_k(\lambda)$ in the matrix K of (4.5). Thus

$$\det K(\zeta, \zeta_2(\zeta), \dots, \zeta_k(\zeta)) =: \det(\zeta; q)$$

is a function of the single complex variable ζ, containing q as a parameter.

TABLE 4.1
Coefficients for some 2-step formulas.

Type	α_0	α_1	α_2	β_0	β_1	β_2
Midpoint (MP)	-1	0	1	0	2	0
Simpson (S)	-1	0	1	$\frac{1}{3}$	$\frac{4}{3}$	$\frac{1}{3}$
Adams–Moulton (AM)	-1	1	0	$\frac{5}{12}$	$\frac{2}{3}$	$-\frac{1}{12}$

As we will see in specific examples, the analysis of the function $\det(\zeta; q)$ can be sometimes reduced to the study of a sparse polynomial, which makes feasible a first-order analysis (perhaps a direct computation) of its roots $\zeta(q)$. Finally, the relation (4.6) allows us to obtain a knowledge of λ from that of $\zeta(q)$.

Remark 4.1. $\det(\zeta; q)$ has a number of redundant roots that should be discarded in order to simplify the analysis. Some of them are "spurious" values for which $\zeta = \zeta_j(\zeta)$ or $\zeta_j(\zeta) = \zeta_l(\zeta)$, with $j \neq l$ (the matrix K turns out to have two equal columns), violating the assumption of distinct roots. Furthermore, if ζ is a root of $\det(\zeta; q)$, then $\zeta_2(\zeta), \ldots, \zeta_k(\zeta)$ are roots as well, and they all give the same eigenvalue λ. In summary, since there are $s+1$ eigenvalues, we expect to find $k(s+1)$ roots of $\det(\zeta; q)$, plus the spurious roots (whose number cannot be estimated a priori, in general).

Remark 4.2. Once the behavior of $\zeta(q)$ has been obtained, in principle this can be used also for the study of eigenvectors: the key relation is (4.3), and the main issue would be the behavior (in terms of q) of the coefficients $c_1, \ldots, c_k$. This problem is not treated in the present paper, where we are interested only in the eigenvalues $\lambda(q)$.

4.1. A case study: 2-step formulas. In this paper, we focus on 2-step methods as the principal (or main) scheme (2.3) for a linear multistep formula in boundary value form, with one initial condition and one final condition provided by an implicit Euler scheme. For those methods, we have

$$k = 2, \nu = 1,$$

and Dahlquist's hypothesis of section 2.3 allows us to assume that

$$A = \begin{pmatrix} \alpha_1 & \alpha_2 & & & 0 \\ \alpha_0 & \alpha_1 & \alpha_2 & & \\ & \ddots & \ddots & \ddots & \\ & & \alpha_0 & \alpha_1 & \alpha_2 \\ & & & -1 & 1 \end{pmatrix}, \quad B = \begin{pmatrix} \beta_1 & \beta_2 & & & \\ \beta_0 & \beta_1 & \beta_2 & & \\ & \ddots & \ddots & \ddots & \\ & & \beta_0 & \beta_1 & \beta_2 \\ & & & 0 & 1 \end{pmatrix}, \tag{4.8}$$

where parameters are given in Table 4.1 for the most common cases.

Circulant approximations for A and B are given by

$$\breve{A} = \begin{pmatrix} \breve{a}_0 & \breve{a}_1 & & & \breve{a}_s \\ \breve{a}_s & \breve{a}_0 & \breve{a}_1 & & \\ & \ddots & \ddots & \ddots & \\ & & \breve{a}_s & \breve{a}_0 & \breve{a}_1 \\ \breve{a}_1 & & & \breve{a}_s & \breve{a}_0 \end{pmatrix}, \quad \breve{B} = \begin{pmatrix} \breve{b}_0 & \breve{b}_1 & & & \breve{b}_s \\ \breve{b}_s & \breve{b}_0 & \breve{b}_1 & & \\ & \ddots & \ddots & \ddots & \\ & & \breve{b}_s & \breve{b}_0 & \breve{b}_1 \\ \breve{b}_1 & & & \breve{b}_s & \breve{b}_0 \end{pmatrix}, \tag{4.9}$$

where the examples for its entries considered here are shown in Table 4.2.

TABLE 4.2
Entries for the preconditioner $P = P(q)$.

Type	$\breve{a}_0$	$\breve{a}_1$	$\breve{a}_s$	$\breve{b}_0$	$\breve{b}_1$	$\breve{b}_s$
MP, P-circ	0	$\frac{s+2}{s+1}$	$-\frac{s}{s+1}$	2	0	0
S, P-circ	0	$\frac{s+2}{s+1}$	$-\frac{s}{s+1}$	$\frac{4}{3}$	$\frac{s+2}{3(s+1)}$	$\frac{s}{3(s+1)}$
AM, Chan	1	0	$-\frac{s}{s+1}$	$\frac{2}{3}$	$-\frac{s}{12(s+1)}$	$\frac{5s}{12(s+1)}$
AM, P-circ	1	0	$-\frac{s}{s+1}$	$\frac{2}{3}$	$-\frac{s+2}{12(s+1)}$	$\frac{5s}{12(s+1)}$

We are not interested in T. Chan's approximation for the midpoint and Simpson methods, since it becomes singular in such cases [7, p. 1819].

The characteristic equation (4.2) has a quadratic form, with

$$\pi(z) = \gamma_0 + \gamma_1 z + \gamma_2 z^2 \qquad (\gamma_i := \alpha_i - q\beta_i),$$

$$\breve{\pi}(z) = \breve{g}_s + \breve{g}_0 z + \breve{g}_1 z^2 \qquad (\breve{g}_i := \breve{a}_i - q\breve{b}_i);$$

its roots ζ and ζ_2 are then related through (4.7), where we observe that the numerator vanishes for $\zeta = 0$, whereas the denominator loses its quadratic term. Hence we define

$$N(\zeta) := \frac{\gamma_0\breve{\pi}(\zeta) - \breve{g}_s\pi(\zeta)}{\zeta}, \quad D(\zeta) := \gamma_2\breve{\pi}(\zeta) - \breve{g}_1\pi(\zeta),$$

which are both linear polynomials such that

$$\zeta_2(\zeta) = \frac{N(\zeta)}{D(\zeta)}. \tag{4.10}$$

In light of Remark 4.1, we know that the function $\det(\zeta; q)$ has two spurious roots for which $\zeta = \zeta_2$, satisfying the quadratic equation $N(\zeta) - \zeta D(\zeta) = 0$; hence we know in advance that $N(\zeta) - \zeta D(\zeta)$ exactly divides $\det(\zeta; q)$.

In order to form the explicit expression of $\det(\zeta; q)$, first we must compute the 2×2 matrix

$$K(\zeta, \zeta_2) = \begin{pmatrix} \gamma_{\text{in}}(\zeta) & \gamma_{\text{in}}(\zeta_2) \\ \gamma_{\text{fin}}(\zeta) & \gamma_{\text{fin}}(\zeta_2) \end{pmatrix},$$

where $\gamma_{\text{in}}(\cdot)$ and $\gamma_{\text{fin}}(\cdot)$ are suitable polynomials obtained by imposing boundary conditions on the main difference equation.

More precisely, since $k = 2$ and $\nu = 1$, we have just one initial condition (the first equation in (4.1))

$$\gamma_1 u_0 + \gamma_2 u_1 = \lambda(\breve{g}_0 u_0 + \breve{g}_1 u_1 + \breve{g}_s u_s)$$

and one final condition (the last of (4.1))

$$-u_{s-1} + (1-q)u_s = \lambda(\breve{g}_1 u_0 + \breve{g}_s u_{s-1} + \breve{g}_0 u_s),$$

where u_j given by (4.3),

$$u_j = c_1\zeta^j + c_2\zeta_2^j,$$

should be substituted.

This way we obtain two homogeneous equations in the unknowns c_1, c_2, whose coefficients contribute to the matrix K. For instance, the coefficient of c_1 in the initial condition is

$$\gamma_{\text{in}}(\zeta) = \gamma_1 + \gamma_2\zeta - \lambda(\breve{g}_0 + \breve{g}_1\zeta + \breve{g}_s\zeta^s),$$

whereas that in the final condition is

$$\gamma_{\text{fin}}(\zeta) = -\zeta^{s-1} + (1-q)\zeta^s - \lambda(\breve{g}_1 + \breve{g}_s\zeta^{s-1} + \breve{g}_0\zeta^s).$$

The same holds for c_2 with ζ_2 in place of ζ; it must be remembered that

$$\lambda(\zeta) = \frac{\pi(\zeta)}{\breve{\pi}(\zeta)} = \frac{\pi(\zeta_2)}{\breve{\pi}(\zeta_2)}. \tag{4.11}$$

Some further algebraic manipulations give the following compact formulas:

$$\gamma_{\text{in}}(z) = \pi_0(z) - \frac{\pi(z)}{\breve{\pi}(z)}\mathcal{R}[z^s\breve{\pi}], \quad \gamma_{\text{fin}}(z) = z^{s-2}\pi_s(z) - \frac{\pi(z)}{\breve{\pi}(z)}\mathcal{R}[z^{s-1}\breve{\pi}],$$

where the notation $\mathcal{R}[P]$ means the s-degree remainder of P modulo $z^{s+1}-1$, and

$$\pi_0(z) := \frac{\pi(z) - \pi(0)}{z}, \quad \pi_s(z) := (1-q)z^2 - z.$$

A useful simplification arises by observing that in light of (4.11) λ needs not to be evaluated in ζ_2 when we form the second column of K. Therefore, the determinant is given by

$$\det(\zeta; q) = \gamma_{\text{in}}(\zeta)\gamma_{\text{fin}}(\zeta_2) - \gamma_{\text{in}}(\zeta_2)\gamma_{\text{fin}}(\zeta),$$

where

$$\gamma_{\text{in}}(\zeta_2) = \pi_0(\zeta_2) - \frac{\pi(\zeta)}{\breve{\pi}(\zeta)}Q_s(\zeta_2)$$

and

$$\gamma_{\text{fin}}(\zeta_2) = \zeta_2^{s-2}\pi_s(\zeta_2) - \frac{\pi(\zeta)}{\breve{\pi}(\zeta)}\tilde{Q}_s(\zeta_2),$$

with suitable s-degree polynomials Q_s and $\tilde{Q}_s$; the substitution (4.10) shows that $\det(\zeta; q)$ is a rational function whose denominator is $\breve{\pi}(\zeta)^2 D(\zeta)^s$. From the linearity of N and D, the function

$$d(\zeta; q) := \breve{\pi}(\zeta)^2 D(\zeta)^s \det(\zeta; q) \tag{4.12}$$

is a $(2s+4)$-degree polynomial in ζ, for which $N(\zeta) - \zeta D(\zeta)$ is a known exact divisor. Its significant roots occur in pairs $(\zeta(q), \zeta_2(q))$, each of them providing a unique value of $\lambda(q)$.

The formulas derived so far simplify very much if we are concerned with the nonpreconditioned case: it suffices to put formally $\breve{\pi}(z) := z$, so that

$$\zeta_2 = \frac{\gamma_0}{\gamma_2 \zeta}, \quad \gamma_{\text{in}}(z) := \pi_0(z) - \frac{\pi(z)}{z} = -\frac{\gamma_0}{z}, \quad \gamma_{\text{fin}}(z) := z^{s-2}(\pi_s(z) - z\pi(z)),$$

whence

$$\det(\zeta; q) = -\gamma_2 \zeta_2^{s-1}(\pi_s(\zeta_2) - \zeta_2 \pi(\zeta_2)) + \gamma_2 \zeta^{s-1}(\pi_s(\zeta) - \zeta\pi(\zeta));$$

here the denominator is just ζ^{s+2}, and the spurious roots of $d(\zeta; q) := \zeta^{s+2} \det(\zeta; q)$ are $\pm\sqrt{\gamma_0/\gamma_2}$.

It is important to observe that $d(\zeta; q)$ is a *sparse* polynomial, which makes a first-order analysis feasible.

We sketch below the essential formulas arising for the specific examples under consideration, which represent the individual instances of (4.10) for ζ_2, (4.12) for $d(\zeta; q)$, and (4.6) for $\lambda(q) := \lambda(\zeta(q))$. In the preconditioned cases, polynomials N and D have been scaled by a constant common factor σ which has been explicitly reported; hence the true expression of $d(\zeta; q)$ should be multiplied by σ^s, but obviously this correction has no influence on the roots and will not be considered in the subsequent analysis.

Nonpreconditioned matrices $M(q)$.

Midpoint (MP).

$$\zeta_2 = -\frac{1}{\zeta},$$
$$d(\zeta; q) = (-1)^s((1+q)\zeta + 1) + \zeta^{2s+3}(1 + q - \zeta),$$
$$\lambda(\zeta(q)) = \zeta(q) - 2q - \frac{1}{\zeta(q)}.$$

Simpson (S).

$$\zeta_2 = \frac{\gamma}{\zeta}, \quad \gamma := \frac{q/3 + 1}{q/3 - 1},$$
$$d(\zeta; q) = \gamma^{s+1}\left(\frac{q}{3} - 1\right)\left(1 + \frac{q}{3} + \left(1 + \frac{q}{3}\right)\zeta + \frac{q}{3\gamma}\zeta^2\right),$$
$$- \zeta^{2s+2}\left(\frac{q}{3} - 1\right)\left(\frac{q}{3} + \left(1 + \frac{q}{3}\right)\zeta + \left(\frac{q}{3} - 1\right)\zeta^2\right),$$
$$\lambda(\zeta(q)) = \left(1 - \frac{q}{3}\right)\zeta(q) - \frac{4}{3}q - \left(1 + \frac{q}{3}\right)/\zeta(q).$$

Adams–Moulton (AM).

$$\zeta_2 = \frac{\gamma}{\zeta}, \quad \gamma := -5 - \frac{12}{q},$$
$$d(\zeta; q) = \gamma^{s-1}\left(1 + \frac{5}{12}q\right)\left(\gamma\left(1 + \frac{5}{12}q\right) - \frac{1}{3}\gamma q\zeta + \frac{5}{12}q\zeta^2\right)$$
$$+ \zeta^{2s+2}\frac{q^2}{36}\left(\frac{5}{4} - \zeta - \frac{1}{4}\zeta^2\right),$$
$$\lambda(\zeta(q)) = \frac{q}{12}\zeta(q) + 1 - \frac{2}{3}q - \left(1 + \frac{5}{12}q\right)/\zeta(q).$$

Preconditioned matrices $P(q)^{-1}M(q)$.

MP, P-circulant.

$$\sigma = -\frac{s+1}{2}, \quad N(\zeta) = q - \zeta, \quad D(\zeta) = 1 + q\zeta, \quad \zeta_2 = \frac{N(\zeta)}{D(\zeta)},$$

$$\begin{aligned} d(\zeta;q) = {} & \frac{2\pi(\zeta)}{s+1}(N-\zeta D)\left[-\left(1-\frac{1}{s+1}\right)\zeta^s N^s + \left(1+\frac{1}{s+1}\right)D^s\right] \\ & + \left(1-\frac{1}{(s+1)^2}\right)\pi(\zeta)^2[N^s - (\zeta D)^s] \\ & - \frac{2(1+q)\breve{\pi}(\zeta)}{s+1}[N^{s+1} - (\zeta D)^{s+1}] + \frac{4}{(s+1)^2}[N^{s+2} - (\zeta D)^{s+2}], \end{aligned}$$

$$\pi(\zeta) = \zeta^2 - 2q\zeta - 1, \quad \breve{\pi}(\zeta) = \pi(\zeta) + \frac{1}{s+1}(\zeta^2+1), \quad \lambda(\zeta(q)) = \frac{\pi}{\breve{\pi}}.$$

S, P-circulant.

$$\sigma = -\frac{9(s+1)}{2}, \quad N(\zeta) = (3+q)(2q+(q-3)\zeta), \quad D(\zeta) = (3-q)(q+3+2q\zeta),$$

$$\begin{aligned} d(\zeta;q) = {} & \pi(\zeta)(N-\zeta D)(\breve{g}_1 D^{s-1}\phi_1 + \breve{g}_s(\zeta N)^{s-1}\psi_0) \\ & - \left(\breve{g}_1\breve{g}_s\pi(\zeta)^2 + \frac{2D\psi_0}{9(s+1)}\right)[N^s - (\zeta D)^s] - \frac{2\psi_1}{9(s+1)}[N^{s+1} - (\zeta D)^{s+1}] \end{aligned}$$

($\breve{g}_i := \breve{a}_i - q\breve{b}_i$, where $\breve{a}_i$ and $\breve{b}_i$ are given by Table 4.2),

$$\phi_1 := \frac{2D}{9(s+1)}, \quad \psi_0 := -\breve{\pi}(\zeta) + \frac{s}{s+1}\left(1+\frac{q}{3}\right)\pi(\zeta), \quad \psi_1 := (1-q)\breve{\pi}(\zeta) + \frac{4}{3}q\pi(\zeta),$$

$$\pi(\zeta) = \zeta^2 - 1 - \frac{q}{3}(\zeta^2 + 4\zeta + 1), \quad \breve{\pi}(\zeta) = \pi(\zeta) + \frac{1}{s+1}\left(1 + \zeta^2 + \frac{q}{3}(1-\zeta^2)\right).$$

AM, Chan.

$$\sigma = -\frac{12(s+1)}{2q/3 - 1}, \quad N(\zeta) = 5q + 12, \quad D(\zeta) = -q\zeta,$$

$$\begin{aligned} d(\zeta;q) = {} & \left(1-\frac{1}{s+1}\right)\pi(\zeta)(N-\zeta D)\left[\frac{q}{12}D^{s-1}\phi_1 - \left(1+\frac{5}{12}q\right)(\zeta N)^{s-1}\psi_0\right] \\ & + \zeta N D\phi_1\psi_0[N^{s-2} - (\zeta D)^{s-2}] + (\zeta N\phi_1\psi_1 + D\phi_0\psi_0)[N^{s-1} - (\zeta D)^{s-1}] \\ & + \left[\phi_0\psi_1 + \frac{q}{12}\left(1-\frac{1}{s+1}\right)^2\left(1+\frac{5}{12}q\right)\pi(\zeta)^2\right][N^s - (\zeta D)^s], \end{aligned}$$

$$\phi_0 := \left(1-\frac{2}{3}q\right)(\breve{\pi}(\zeta) - \pi(\zeta)), \quad \phi_1 := \frac{q}{12}\left[\breve{\pi}(\zeta) - \left(1-\frac{1}{s+1}\right)\pi(\zeta)\right],$$

$$\psi_0 := -\breve{\pi}(\zeta) + \left(1-\frac{1}{s+1}\right)\left(1+\frac{5}{12}q\right)\pi(\zeta), \quad \psi_1 := (1-q)\breve{\pi}(\zeta) - \left(1-\frac{2}{3}q\right)\pi(\zeta),$$

$$\pi(\zeta) = \zeta - 1 - \frac{q}{12}(\zeta^2 - 8\zeta - 5), \quad \breve{\pi}(\zeta) = \pi(\zeta) + \frac{1}{s+1}\left(-\frac{q}{12}\zeta^2 + 1 + \frac{5}{12}q\right).$$

AM, P-circulant.

$$\sigma = -(s{+}1),\ N(\zeta) = \left(1+\frac{5q}{12}\right)\left(1-\frac{2}{3}q+\frac{q\zeta}{6}\right),\ D(\zeta) = \frac{q}{12}\left[\left(1-\frac{2}{3}q\right)\zeta - 2 - \frac{5}{6}q\right],$$

$$d(\zeta;q) = \pi(\zeta)(N-\zeta D)(\breve{g}_1 D^{s-1}\phi_1 + \breve{g}_s(\zeta N)^{s-1}\psi_0) + \zeta N D\phi_1\psi_0[N^{s-2}-(\zeta D)^{s-2}]$$
$$+ (\zeta N\phi_1\psi_1 + D\phi_0\psi_0)[N^{s-1}-(\zeta D)^{s-1}] + (\phi_0\psi_1 - \breve{g}_1\breve{g}_s\pi(\zeta)^2)[N^s-(\zeta D)^s]$$

($\breve{g}_i := \breve{a}_i - q\breve{b}_i$, where $\breve{a}_i$ and $\breve{b}_i$ are given by Table 4.2),

$$\phi_0 := \left(1-\frac{2}{3}q\right)(\breve{\pi}(\zeta)-\pi(\zeta)), \quad \phi_1 := \frac{q}{12}\left[\breve{\pi}(\zeta) - \left(1+\frac{1}{s+1}\right)\pi(\zeta)\right],$$

$$\psi_0 := -\breve{\pi}(\zeta) + \left(1-\frac{1}{s+1}\right)\left(1+\frac{5}{12}q\right)\pi(\zeta), \quad \psi_1 := (1-q)\breve{\pi}(\zeta) - \left(1-\frac{2}{3}q\right)\pi(\zeta),$$

$$\pi(\zeta) = \zeta - 1 - \frac{q}{12}(\zeta^2 - 8\zeta - 5), \quad \breve{\pi}(\zeta) = \pi(\zeta) + \frac{1}{s+1}\left(\frac{q}{12}\zeta^2 + 1 + \frac{5}{12}q\right).$$

4.2. A first-order analysis. The parameterization of λ as a function of q obtained so far allows us to investigate the behavior of the eigenvalues for q small.

We recall that $q = h\mu$, where h is the time discretization step and μ represents any eigenvalue of the Jacobian matrix J in (2.4) related to the space discretization. Thus, a small value of q is a physically meaningful situation, occurring whenever, e.g., the Jacobian matrix has eigenvalues with a small modulus (as in the examples sketched in section 5) and/or a small time step is used. A particular care is required in the latter instance: we stress that $s \to \infty$ as $h \to 0$, so that the polynomial $d(\zeta;q)$ raises its degree, increasing the number of the roots $\zeta(q)$. However, the insights given by the first-order analysis are generally in good agreement with the localization of λ, as we will see in the numerical experiments of section 6.

In what follows, we present a first-order expansion of $\lambda(q)$ centered in zero for all of the three nonpreconditioned methods (MP, S, AM) and for two preconditioners (P-circulant approximations for MP and AM).

The starting point is the continuity of polynomial roots with respect to coefficients (provided that the degree remains constant). Hence $\zeta(q)$ is very close to $\zeta(0)$ for small q, and its first-order dependence on q can be made explicit.

In the MP method, $\zeta = \zeta(0)$ is a root of $d(\zeta;0) = (-1)^s(1+\zeta) + \zeta^{2s+3}(1-\zeta)$, and therefore

$$|\zeta|^{2s+3} = \left|\frac{1+\zeta}{1-\zeta}\right|.$$

Squaring both sides of the previous equation and letting $\zeta = \rho e^{\mathbf{i}\theta}$, after some algebraic manipulations, we get

$$\cos\theta = \frac{1+\rho^2}{2\rho}\cdot\frac{\rho^{4s+6}-1}{\rho^{4s+6}+1}. \tag{4.13}$$

(4.13) is the equation, in polar coordinates, of a curve containing all of the roots $\zeta(0)$ and lying in the following region of the complex plane:

$$\Omega = \left\{\theta \in \left(\frac{\pi}{2}, \frac{3}{2}\pi\right), \rho < 1\right\} \cup \left\{|\theta| < \frac{\pi}{2}, \rho > 1\right\} \cup \{\pm\mathbf{i}\},$$

where $\pm\mathbf{i}$ are exactly the spurious roots for which $\zeta = \zeta_2$.

Therefore, $\lambda(0)$ can be localized through the transformation $\lambda = \zeta - 1/\zeta$ of the previous curve. In particular, since $\mathrm{Re}\lambda = (\rho - 1/\rho)\cos\theta$, it is straightforward to observe that $\mathrm{Re}\lambda > 0$ whenever $\zeta \in \Omega$ (except for the spurious roots). By continuity, we have the useful result that the eigenvalues of M lie on $\mathbb{C}^+$ for q small enough. We recall that projection methods such as GMRES or BiCGstab show often a faster convergence behavior whenever the matrix of the linear systems we have to solve has all eigenvalues in one half-plane; see [22].

If we are interested in a deeper analysis, we can check that the roots $\zeta(0)$ are distinct and therefore

$$\zeta(q) \doteq \zeta(0) + \zeta'(0)q,$$

where $\doteq$ denotes a first-order approximation of the function on the left-hand side. Therefore,

$$\lambda(q) \doteq \zeta(0) - \frac{1}{\zeta(0)} + \left[\zeta'(0) + \frac{\zeta'(0)}{\zeta(0)^2} - 2\right] q;$$

the explicit expression of $\zeta'(0)$, if desired, can be retrieved from the classical theory on the conditioning of zeros of polynomials (see, e.g., [30, section 5.8]).

The Simpson method has a quite similar analysis. In addition, since the matrix A is the same as the previous case, the zero-order terms of $\zeta(q)$ and $\lambda(q)$ are exactly equal to the corresponding ones for MP. On the other hand, the first-order expansion for S has a different expression, which is reported below:

$$\lambda(q) \doteq \zeta(0) - \frac{1}{\zeta(0)} + \left[\zeta'(0) + \frac{\zeta'(0)}{\zeta(0)^2} - \frac{4}{3} - \frac{\zeta(0)}{3} - \frac{1}{3\zeta(0)}\right] q,$$

where $\zeta'(0)$ is different from the MP method.

The analysis of the AM method shows a further complication with respect to the previous cases. It is evident that $d(\zeta; q)$ loses several degrees when q goes to zero, so that many roots $\zeta(q)$ become infinite. Hence we are not able to predict the behavior of $\lambda(q)$, unless we apply an appropriate change of variable. For this purpose, let

$$\xi := q^{1/2}\zeta, \quad \beta := \gamma q,$$

and rewrite the polynomial d in terms of the new variable ξ. We obtain

$$\begin{aligned} q^s d(\xi; q) = \beta^{s-1}\left(1 + \frac{5}{12}q\right)\left(\beta\left(1 + \frac{5}{12}q\right) - \frac{1}{3}\beta q^{1/2}\xi + \frac{5}{12}q\xi^2\right) \\ + \xi^{2s+2}/36\left(\frac{5}{4}q - q^{1/2}\xi - \frac{1}{4}\xi^2\right), \end{aligned}$$

whence $\xi(q) \doteq \xi(0) + \xi'(0)q^{1/2}$, where $\xi(0)$ solves the equation

$$(-12)^s - \xi^{2s+4}/144 = 0,$$

that is, $\xi(0) = 2\sqrt{3}\exp(\mathbf{i}(\frac{l\pi}{s+2} + \frac{\pi}{2}))$, $l = 1, \ldots, s+1$. Other values of the index l would give spurious roots or already obtained values of λ. Taking into account the change of variable, the behaviors of ζ and λ are, respectively,

$$\zeta(q) \doteq \xi(0)q^{-1/2} + \xi'(0),$$

$$\lambda(q) \doteq 1 + \frac{\mathbf{i}}{\sqrt{3}}\cos\frac{l\pi}{s+2}q^{1/2} + \left[\frac{\xi'(0)}{12} + \frac{\xi'(0)}{\xi(0)^2} - \frac{2}{3}\right] q.$$

Hence, for small values of q, the eigenvalues of M are close to a vertical segment on $\mathbb{C}^+$ with the midpoint placed at 1.

The main difficulty arising in the preconditioned case is given by the presence of the spurious divisor $N - \zeta D$ in all instances of $d(\zeta; q)$. In order to perform the analysis, it is worth considering the quotient $\hat{d}(\zeta; q) := d(\zeta; q)/(N - \zeta D)$, studied for $q \approx 0$. Let

$$F_m(\zeta; q) := \frac{N^m - (\zeta D)^m}{N - \zeta D} = \sum_{j=0}^{m-1} N^j (\zeta D)^{m-j-1};$$

this expression appears in almost all of the terms of $\hat{d}(\zeta; q)$ and will determine the first-order behavior of the significant roots.

Concerning the P-circulant preconditioner for the MP method, for $q = 0$ we have $N(\zeta) = -\zeta$, $D(\zeta) = 1$. Therefore,

$$F_m(\zeta; 0) = \zeta^{m-1} \sum_{j=0}^{m-1} (-1)^j = \begin{cases} \zeta^{m-1} & \text{if } m \text{ is odd,} \\ 0 & \text{otherwise.} \end{cases}$$

Thus, the zero-order localization of the roots $\zeta(q)$ strictly depends on the parity of s: more specifically, when s is odd they solve the equation

$$\begin{aligned} &(\zeta^2 - 1)\zeta^{s+1} + \frac{2}{s+1}(\zeta^2 - 1)(\zeta^{2s} + 1) \\ &+ \frac{1}{(s+1)^2}[4\zeta^{s+1} - (\zeta^2 - 1)\zeta^{s-1} + 2(\zeta^2 - 1)(1 - \zeta^{2s})] = 0, \end{aligned}$$

and when s is even the equation becomes

$$(\zeta^2 - 1)(1 - \zeta^s - \zeta^{2s}) + \frac{1}{s+1}[(\zeta^2 - 1)(\zeta^{2s} + 1) - (\zeta^2 + 1)\zeta^s] = 0.$$

For q very small, the eigenvalues of $P^{-1}M$ can be estimated from the roots $\zeta = \zeta(0)$ through the relation

$$\lambda(0) = \frac{\zeta^2 - 1}{\zeta^2 - 1 + \dfrac{1}{s+1}(\zeta^2 + 1)}.$$

After more heavy computations we are able to obtain the first-order terms in the expansions of $\zeta(q)$ and $\lambda(q)$. In section 6 we will present explicit estimates based on the formulas derived so far and compare them with values obtained numerically.

The difficulties found in the analysis of the AM method arise in the P-circulant preconditioned case as well. Many ingredients of $d(\zeta; q)$ degenerate for $q = 0$: among others, polynomials $N(\zeta), D(\zeta), \pi(\zeta)$, and $\breve{\pi}(\zeta)$ drop their degree. This causes several roots $\zeta(q)$ to go to infinity: also here we need a suitable change of variable.

Let $\xi := q\zeta$, and rewrite all of the polynomials $N, D, \pi, \breve{\pi}, \phi_i, \psi_i (i = 0, 1)$ in terms of the new variable, in particular,

$$N(\xi) = \left(1 + \frac{5}{12}q\right)\left(1 - \frac{2}{3}q + \frac{1}{6}\xi\right), \quad D(\xi) = \frac{1}{12}\left[\left(1 - \frac{2}{3}q\right)\xi - q\left(2 + \frac{5}{6}q\right)\right].$$

The "clean" polynomial $\hat{d}$ takes the following expression after some algebra:

$$\hat{d}(\xi; q) = q^{-s-1}\check{d}(\xi; q),$$

where $\check{d}$ has constant degree $2s+2$ (independently on q) and its zero-order form is

$$\check{d}(\xi;0) = \left(-\frac{1}{s+1}\right)^s \xi^{s+1}\left\{-\frac{1}{12^{s+1}(s+1)}\left[\xi^{s-3}(12+2\xi)^2+\xi^{s+1}\right] - \left(1-\frac{1}{s+1}\right)\left(1+\frac{1}{12}\xi\right)\left(1+\frac{1}{6}\xi\right)^s\right\}.$$

Notice that $s+1$ roots of $\check{d}$ are distinct and behave as $\xi(q) \doteq \xi(0)+\xi'(0)q$, whence

$$\zeta(q) \doteq \xi(0)q^{-1}+\xi'(0).$$

These are the roots going to infinity, associated with the values of $\lambda(q)$ with

$$\lambda(0) = \frac{12+\xi(0)}{12+\xi(0)\left(1-\dfrac{1}{s+1}\right)};$$

the same eigenvalues are associated with the corresponding "dual" roots given by $\zeta_2 = N(\xi)/D(\xi)$ which are finite for $q=0$, as a direct look at N and D shows. Through the transformation $\xi = q\zeta_2$ we find the remaining $s+1$ roots of $\check{d}$, which collapse at the origin.

We will compare these results with numerical estimates for this setting as well; see section 6.

5. Model problems. As a first benchmark of our analysis, we consider two simple model problems which encompass two important types of spectra for their Jacobian matrices: real and negative and pure imaginary eigenvalues, respectively. Only one-dimensional (1D) problems are considered, but extensions to 2D and 3D cases are straightforward and not necessary in our setting.

Diffusion equation. As a typical example of a problem whose Jacobian matrix has negative (real) eigenvalues, we report the variable coefficient 1D diffusion equation with homogeneous Dirichlet boundary conditions at both ends. Let $a = a(x) \geq 0$ be a suitably smooth function.

$$\begin{cases} u_t - c(a\,u_x)_x = 0, & x \in [0, x_{\max}], t \in (0,T], \\ u(0,t) = u(x_{\max},t) = 0 & t \in (0,T], \\ u(x,0) = g(x), & x \in [0, x_{\max}]. \end{cases} \tag{5.1}$$

Discretizing the operator $\partial/\partial x$ in (5.1) with centered differences and step size $\Delta x = x_{\max}/(m+1)$ gives a sequence of systems of ODEs parameterized by Δx whose mth element is given by

$$\begin{cases} y'(t) = T_m y(t), & t \in [0,T], \\ y(0) = \eta, & \eta = (g(x_1)\dots g(x_m))^T, \end{cases} \tag{5.2}$$

where $x_j = j\Delta x$ and

$$T_m = \frac{c}{(\Delta x)^2}\begin{pmatrix} a_1 & b_1 & & \\ b_1 & \ddots & \ddots & \\ & \ddots & \ddots & b_{m-1} \\ & & b_{m-1} & a_m \end{pmatrix}, \tag{5.3}$$

where

$$a_j = -(a(x_{j-1/2}) + a(x_{j+1/2})), \quad b_j = a(x_{j+1/2}).$$

The Jacobian matrix T_m is $m \times m$ symmetric, tridiagonal, and weakly diagonally dominant with negative diagonal entries. From an extensive study performed in [15, 28] we get for each eigenvalue μ_j of T_m the bounds

$$-\frac{4c}{(\Delta x)^2} \max_x\{a(x)\} \le \mu_j \le -\frac{c\pi^2}{(x_{\max})^2} \min_x\{a(x)\}.$$

Note that, as Δx tends to zero, the systems of differential equations (5.2) become increasingly stiff, spreading the eigenvalues of the Jacobian matrix T_m along an interval in $(-4c \max_x\{a\}/(\Delta x)^2, 0)$ whose left boundary tends to $-\infty$ with $O((\Delta x)^{-2})$.

More precisely, the spectrum is equally distributed [31] as the values of the bivariate function $a(x)f(\theta)$, where

$$f(\theta) = \frac{2c}{(\Delta x)^2}(\cos(\theta) - 1), \quad \theta \in (-\pi, \pi),$$

is the so-called "generating function" related to the constant-coefficient version of the problem. As stated in [27, 24], if $a(x)$ has a zero at the origin of order α, the smallest eigenvalue shows an asymptotic behavior like $(\Delta x)^2/m^{\max(2,\alpha)}$.

Transport equation. The linear 1D transport equation with periodic boundary conditions and constant coefficient $c > 0$ in its simplest form reads:

$$\begin{cases} u_t + c\, u_x = 0, \\ u(x,0) = g(x), & x \in [0,\pi], \\ u(\pi,t) = u(0,t), & t \in [0,2\pi]. \end{cases} \tag{5.4}$$

Discretizing the partial derivative $\partial/\partial x$ with central differences and step size $\Delta x = \pi/m$, $x_j = j\Delta x$ gives a sequence of systems of ODEs parameterized by Δx whose mth element is given by

$$\begin{cases} y'(t) = C_m y(t), & t \in [0,2\pi], \\ y(0) = \eta, & \eta = (g(x_0) \dots\ g(x_{m-1}))^T, \end{cases} \tag{5.5}$$

with

$$C_m = \frac{c}{2\Delta x} \begin{pmatrix} 0 & -1 & & & 1 \\ 1 & \ddots & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & -1 \\ -1 & & & 1 & 0 \end{pmatrix}. \tag{5.6}$$

The matrix C_m is circulant $m \times m$ with generating function

$$\tilde{f}(\theta) = \frac{c}{2\Delta x}\left(e^{-\mathbf{i}\theta} - e^{\mathbf{i}\theta} - e^{-\mathbf{i}(m-1)\theta} + e^{\mathbf{i}(m-1)\theta}\right) = \frac{-\mathbf{i}c\,(\sin\theta - \sin(m-1)\theta)}{\Delta x}, \tag{5.7}$$

where $\theta \in (-\pi, \pi)$. Therefore, the eigenvalues of C_m are distributed as $\tilde{f}(\theta)$ in (5.7) and lie in the purely imaginary (closed) interval

$$[-2\mathbf{i}c/\Delta x, 2\mathbf{i}c/\Delta x],$$

which becomes wider as $O(1/\Delta x)$ as we refine the discretization. This implies that a finer mesh for the time-step integrator is required to resolve the (oscillatory) solution as Δx (the step for the discretization in space) decreases to zero.

An explicit expression of the spectrum of C_m can be obtained by observing that

$$C_m = F\Lambda F^*, \tag{5.8}$$

where Λ is a diagonal matrix containing the eigenvalues μ_j of C_m and F is the Fourier matrix; see, e.g., [19]. Thus, from the expression of the eigenvalues of a circulant matrix, we have

$$\mu_j = -\frac{2\mathbf{i}c}{\Delta x}\left(\sin\frac{2\pi j}{m}\right), \quad j = 0, \ldots, m-1,$$

i.e., the generating function computed in the points $\theta_j = 2\pi j/m$, $j = 0, \ldots, m-1$, as usual.

It is worth noting that the Jacobian matrices for both of the proposed model problems are normal and therefore can be diagonalized by unitary matrices. This feature is useful in order to use the bounds for the convergence of a Krylov accelerator which uses the preconditioners analyzed here; see [9, Theorems 3.1 and 3.2]. In particular, by applying the cited results, for the underlying problems we can predict convergence in at most $O(\log s)$ (preconditioned) iterations.

6. Numerical estimates and comparisons. We compare the results of zero- and of some first-order approximations presented in section 4.2 with the eigenvalues computed by Matlab's QR method for the model problems in section 5. We do not report plots generated by Simpson's formula because they are very similar to those related to the midpoint formula.

In all tests, unless specified otherwise, we consider $s = m = 100$, $c = 1$, $T = 2\pi$, $x_{\max} = \pi$, $t_0 = 0$. The Jacobian matrix J is taken, in light of Dahlquist's hypothesis, as the smallest eigenvalue (in modulus) for each one of the model problems considered in the previous section. In the variable diffusion model problem, the diffusion function is of the form $a(x) = x^k$, $k > 0$ integer; i.e., it has a zero in the origin of multiplicity k. However, a similar eigenvalue distribution of the preconditioned and nonpreconditioned problems has been observed even in the absence of zeros on the real axis for various functions such as $a(x) = x^k + \epsilon$, where $\epsilon > 0$ is a small constant, varying with $O(m^{-1})$. We stress that, in both cases, eigenvalues of the Jacobian matrix (5.3), are negative, but some of them go to zero as the space discretization gets refined. On the other hand, the same asymptotic behavior holds for some nonzero eigenvalues of the Jacobian matrix (5.6), although the transport equation has constant coefficients.

Results of some tests are reported in Figures 6.1 (nonpreconditioned case), 6.2, and 6.3 (preconditioned case). In all three cases, the condition number $\kappa_2(X)$ of the eigenvector matrix X is modest. Therefore GMRES' convergence is well described by the eigenvalues.

Note that in all tests we get that even just zero-order approximations can give reasonable information on the qualitative behavior of the eigenvalues related to the smallest eigenvalues (in modulus) of the Jacobian matrix of the differential problem both in the nonpreconditioned and in the preconditioned cases, for variable and constant coefficient equations, provided that the mesh for the discretization in space is fine enough.

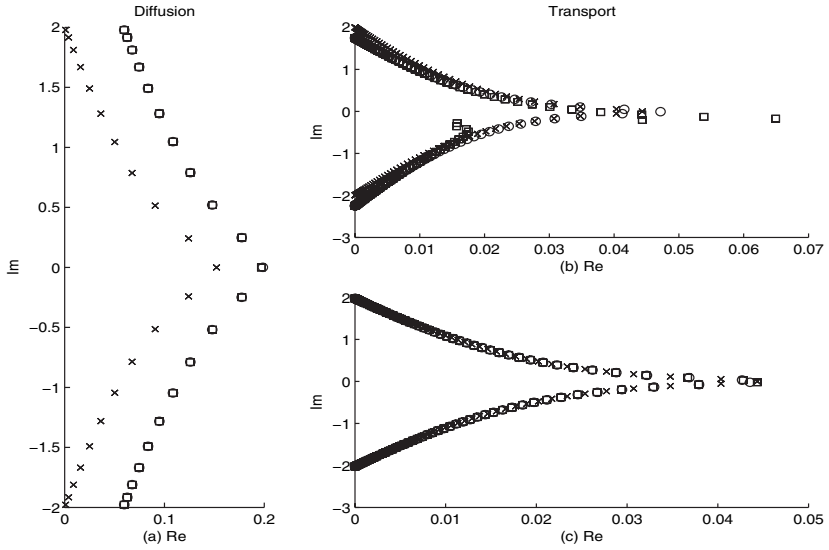

FIG. 6.1. *MP method, smallest eigenvalue (in modulus) for* (a) *the diffusion equation with* $a(x) = x^4$, $s = 20$, $m = 20$ *giving* $\kappa_2(X) \approx 7$, (b) *the transport equation,* $s = 100$, $m = 100$, $c = 1$ *giving* $\kappa_2(X) \approx 28$, *and* (c) *the same equation with* $c = 0.1$ *giving* $\kappa_2(X) \approx 28$; *x=order* 0, *o=eig*(M), $\square$*=order* 1 *approximations.*

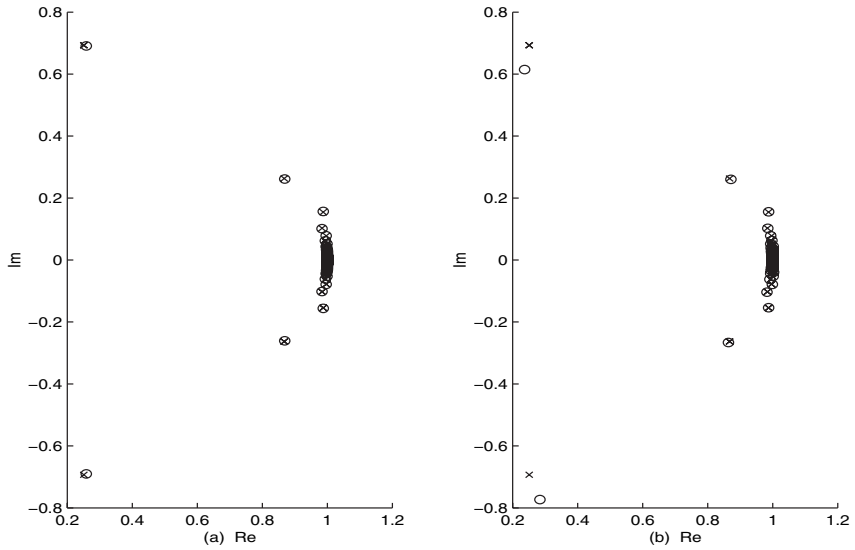

FIG. 6.2. *MP method with* P*-circulant preconditioning, smallest eigenvalue (in modulus) for* (a) *the diffusion equation with* $a(x) = x^4$, $s = 100$, $m = 100$ *and* (b) *the transport equation,* $s = 100$, $m = 100$; *+=order 0, o=eig*$(P^{-1}M)$ *approximations.*

In order to emphasize the effect of the first-order approximations with respect to zero order, just in Figure 6.1 (left) we use a rougher mesh with $s = m = 20$ for the midpoint formula without using preconditioning.

It is surprising that, for the transport equation (upper right plot in Figure 6.1), the order 1 approximation gives worse approximations than order 0 for some eigen-

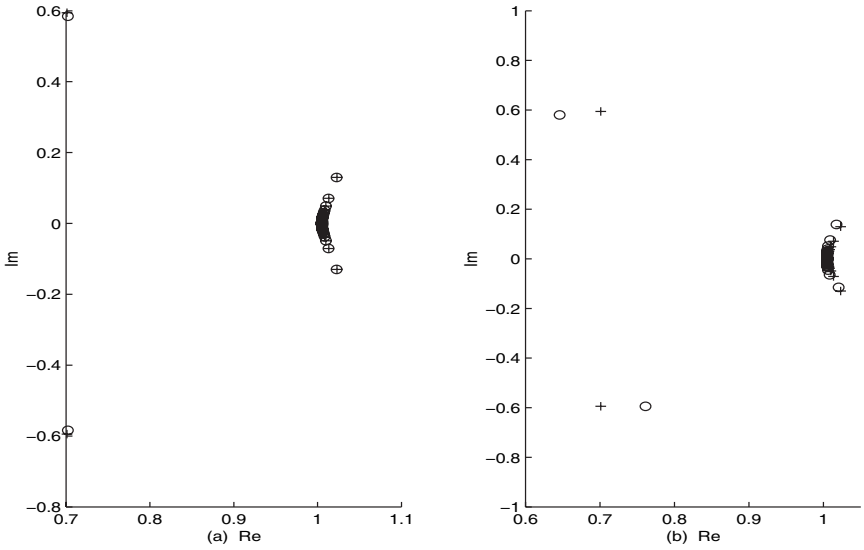

FIG. 6.3. *Adams–Moulton with* P*-circulant preconditioning, smallest eigenvalue (in modulus) for* (a) *the diffusion equation with* $a(x) = x^4$, $s = 100$, $m = 100$ *and* (b) *the transport equation,* $s = 100$, $m = 100$*; +=order 0, o=eig*$(P^{-1}M)$ *approximations.*

values: the "wrong" values come from roots $\zeta(0)$ very close to the real axis (the same occurs for the derivatives $\zeta'(0)$, $\zeta''(0)$, etc.). This phenomenon is probably explained by observing that q is pure imaginary in this setting, so that in the power series $\sum_{j=0}^{+\infty} \zeta^{(j)}(0)q^j$ just the even terms contribute to refine the real part, as well as the odd terms are related only to the imaginary part; this way the convergence radius of the series could be reduced, and the actual value of q could fall outside the region of analyticity. On the other hand, continuity still holds so that order 0 is always meaningful.

Our conjecture is confirmed by the lower right plot in Figure 6.1, where we have simply set $c = 0.1$: q has been divided by a factor of 10, and order 1 estimates become again more accurate than order 0.

For these moderate dimensions, every $\zeta(0)$ has been computed through the Matlab function `roots`. If one is interested in locating the spectrum of much larger matrices, we suggest the use of more efficient rootfinders specifically designed for sparse polynomials, such as MPSolve proposed in [11].

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