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# SOME COMPUTATIONAL ASPECTS OF THE CONSISTENT MASS FINITE ELEMENT METHOD FOR A (SEMI-)PERIODIC EIGENVALUE PROBLEM

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ABSTRACT. We consider a model eigenvalue problem (EVP) in 1D, with periodic or semi–periodic boundary conditions (BCs). The discretization of this type of EVP by consistent mass finite element methods (FEMs) leads to the generalized matrix EVP  $Kc = \lambda Mc$ , where K and M are real, symmetric matrices, with a certain (skew–)circulant structure. In this paper we fix our attention to the use of a quadratic FE–mesh. Explicit expressions for the eigenvalues of the resulting algebraic EVP are established. This leads to an explicit form for the approximation error in terms of the mesh parameter, which confirms the theoretical error estimates, obtained in [2].

1. Introduction and problem setting. Elliptic EVPs on a bounded interval in  $\mathbb{R}$  with (semi-)periodic BCs may occur in the context of various physical and engineering problems on periodic structures. In particular, they are closely related to EVPs in  $\mathbb{R}$  with periodic coefficient functions, see e.g. [3] and [5], the latter class containing the 1D–Schrödinger equation for an electron in a crystalline medium. The error analysis of FEMs for this type of EVPs has been dealt with in [2].

In this paper we consider the following model problem. Let  $\alpha=1$  or  $\alpha=-1$ . Find  $\lambda\in\mathbb{R}$  and a corresponding smooth (nonzero) function y on [0,1] such that

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(1.1) 
$$-y''(x) = \lambda y(x), \ 0 < x < 1; \quad y(0) = \alpha y(1), \ y'(0) = \alpha y'(1).$$

Choosing

$$V^{\alpha} = \left\{ v \in H^{1}(\Omega) \mid v(0) = \alpha v(1) \right\},\,$$

as the space of trial— and test functions, the formally equivalent variational EVP reads

$$(1.2) (P_{var}) : \text{Find } [\lambda, u] \in \mathbb{R} \times V^{\alpha} : \int_0^1 y'v' \, dx = \lambda \int_0^1 yv \, dx, \ \forall v \in V^{\alpha}.$$

The discretization of this variational EVP by a consistent mass finite element method leads to the generalized matrix EVP

$$(1.3) Kc = \lambda Mc,$$

where the "stiffness matrix" K and the "mass matrix" M take a certain (skew–) circulant structure, depending on the type of FE–meshes used. In particular, the use of a uniform linear FE–mesh for the discretization of (1.1) leads to stiffness and mass matrices of ordinary (skew–)circulant form. Closed expressions for the eigenvalues of the latter types of matrices – and hence also for those of the corresponding generalized EVP (1.3) – have been established e.g. in [1].

However, when using a uniform quadratic FE-mesh for the approximation of the EVP (1.1), the matrices M and K will take a more general circulant form, which, to the author's knowledge, has not been dealt with so far. In the next section we first introduce the notion of a doubly (skew-)circulant matrix and we establish closed expressions for its eigenvalues. Next, we apply the general results obtained to the specific algebraic EVP (1.3), encountered in the FE-approximation of (1.2) with piecewise quadratic polynomials.

Section 3 contains some results on the approximation of the eigenvalues of (1.1). In particular, we give an explicit form for the approximation error, confirming the theoretical order of convergence of the FEM, proven in [2].

Throughout the paper,  $A^*$  will denote the Hermitean conjugate of the matrix A, while  $\overline{A}$  will denote its complex conjugate. Analogously,  $\overline{z}$  is the complex conjugate of the complex number z.

2. Doubly (skew-)circulant matrices. In the first subsection we give the precise definition of a doubly (skew-)circulant matrix, and we derive a few basic results concerning its spectrum. In the second subsection, we apply these results to the specific algebraic EVP (1.3), resulting from the use of a uniform quadratic FE-mesh for the consistent mass approximation of (1.2).

### 2.1. General results.

**Definition 2.1.** Let  $n \in \mathbb{N}_0$ . A doubly circulant, respectively a doubly skew-circulant matrix of order 2n is a matrix of the form

$$\mathcal{D}_{s} = \begin{pmatrix}
a_{0} & a_{1} & a_{2} & \cdots & a_{2n-2} & a_{2n-1} \\
b_{0} & b_{1} & b_{2} & \cdots & b_{2n-2} & b_{2n-1} \\
sa_{2n-2} & sa_{2n-1} & a_{0} & \cdots & a_{2n-4} & a_{2n-3} \\
sb_{2n-2} & sb_{2n-1} & b_{0} & \cdots & b_{2n-4} & b_{2n-3} \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
sa_{2} & sa_{3} & sa_{4} & \cdots & a_{0} & a_{1} \\
sb_{2} & sb_{3} & sb_{4} & \cdots & b_{0} & b_{1}
\end{pmatrix},$$

where s = 1 or s = -1, respectively.

In what follows these matrices will also be denoted as

(2.2) 
$$\mathcal{D}_1 = \operatorname{dcirc} \begin{pmatrix} a_0 & \cdots & a_{2n-1} \\ b_0 & \cdots & b_{2n-1} \end{pmatrix}$$
 and  $\mathcal{D}_{-1} = \operatorname{dscirc} \begin{pmatrix} a_0 & \cdots & a_{2n-1} \\ b_0 & \cdots & b_{2n-1} \end{pmatrix}$ .

Now, put

$$\sigma_k = e^{\frac{\pi}{k}i}$$
 and  $\omega_k = \sigma_k^2$ ,

and consider the unitary Fourier matrix  $F_k$  of order k, defined by

(2.3) 
$$(F_k)_{rs} = \frac{1}{\sqrt{k}} \cdot \overline{\omega}_k^{(r-1)(s-1)}, \quad r, s = 1, \dots, k.$$

Moreover, introduce the diagonal matrix  $\Omega_k$  of order k,

(2.4) 
$$\Omega_k = \operatorname{diag}(1, \sigma_k, \sigma_k^2, \dots, \sigma_k^{k-1}).$$

Our aim is to examine the effect of the unitary reduction of  $\mathcal{D}_1$  by  $F_{2n}$ . We obtain

**Proposition 2.1.** The matrix  $\mathcal{D}_1$ , (2.1), shows the following property:

(2.5) 
$$(E F_{2n}) \mathcal{D}_1 (E F_{2n})^* = \begin{pmatrix} D_0 & & & \\ & D_1 & & \\ & & \ddots & \\ & & & D_{n-1} \end{pmatrix}.$$

Here E is a suitable permutation matrix of order 2n (in the terminology of [1, p.25]), while  $F_{2n}$  is the Fourier matrix of order 2n, defined by (2.3). The right

hand side is a block diagonal matrix, with blocks of order 2, given by

(2.6) 
$$D_{k} = \begin{pmatrix} \frac{S_{k} + \overline{\omega}_{2n}^{k} T_{k}}{2} & \frac{S_{k+n} + \overline{\omega}_{2n}^{k} T_{k+n}}{2} \\ \frac{S_{k} - \overline{\omega}_{2n}^{k} T_{k}}{2} & \frac{S_{k+n} - \overline{\omega}_{2n}^{k} T_{k+n}}{2} \end{pmatrix}, \qquad k = 0, \dots, n-1,$$

where

(2.7) 
$$S_l = \sum_{i=0}^{2n-1} a_i (\omega_{2n}^l)^i$$
 and  $T_l = \sum_{i=0}^{2n-1} b_i (\omega_{2n}^l)^i$ ,  $l = 0, \dots, 2n-1$ .

Proof. For the matrix  $F_{2n} \mathcal{D}_1 F_{2n}^*$ , we readily find

$$(F_{2n}\mathcal{D}_1 F_{2n}^*)_{rs} = \frac{1}{2n} \left( S_{s-1} + \overline{\omega}_{2n}^{r-1} T_{s-1} \right) \begin{cases} \kappa_{s-r}, & \text{when } r \leq s, \\ \overline{\kappa}_{r-s}, & \text{when } r > s, \end{cases} r, s = 1, \dots, 2n,$$

where

$$\kappa_j = \sum_{i=0}^{n-1} (\omega_{2n}^{2i})^j, \quad j = 0, \dots, 2n-1.$$

Next, noting that

$$\kappa_j = \left\{ \begin{array}{ll} n, & \text{when } j = 0 \text{ or } j = n, \\ 0, & \text{otherwise,} \end{array} \right.$$

we get

$$\begin{array}{lll} (F_{2n}\mathcal{D}_{1}F_{2n}^{*})_{rr} & = & \frac{1}{2}\left(S_{r-1} + \overline{\omega}_{2n}^{r-1}T_{r-1}\right), & r = 1, \dots, 2n, \\ (F_{2n}\mathcal{D}_{1}F_{2n}^{*})_{r\,r+n} & = & \frac{1}{2}\left(S_{r+n-1} + \overline{\omega}_{2n}^{r-1}T_{r+n-1}\right), & r = 1, \dots, n, \\ (F_{2n}\mathcal{D}_{1}F_{2n}^{*})_{r+n\,r} & = & \frac{1}{2}\left(S_{r-1} + \overline{\omega}_{2n}^{r+n-1}T_{r-1}\right), & r = 1, \dots, n, \\ (F_{2n}\mathcal{D}_{1}F_{2n}^{*})_{rs} & = & 0, & r \neq s \text{ and } |r-s| \neq n, \\ \text{nally a suitable rearrangement of rows and colums of the matrix } F_{2n}\mathcal{D}_{1}F_{2n}^{*} \\ \text{nally a suitable rearrangement of rows and column of the matrix } F_{2n}\mathcal{D}_{1}F_{2n}^{*} \\ \text{nally a suitable rearrangement.} \end{array}$$

Finally, a suitable rearrangement of rows and column of the matrix  $F_{2n} \mathcal{D}_1 F_{2n}^*$  yields (2.5).  $\square$ 

Analogously, one has

**Proposition 2.2.** The matrix  $\mathcal{D}_{-1}$ , (2.1), shows the property

(2.8) 
$$(E F_{2n} \overline{\Omega}_{2n}) \mathcal{D}_{-1} (E F_{2n} \overline{\Omega}_{2n})^* = \begin{pmatrix} D_0 & & & \\ & D_1 & & \\ & & \ddots & \\ & & & D_{n-1} \end{pmatrix}.$$

Here,  $\Omega_{2n}$  is the  $(2n \times 2n)$ -matrix defined by (2.4). Moreover,  $D_0, \ldots, D_{n-1}$  are

still of the form (2.6), however now with

(2.9) 
$$S_l = \sum_{i=0}^{2n-1} a_i \sigma_{2n}^i (\omega_{2n}^l)^i$$
 and  $T_l = \sum_{i=0}^{2n-1} b_i \sigma_{2n}^{i-1} (\omega_{2n}^l)^i$ ,  $l = 0, \dots, 2n-1$ .

E is the same permutation matrix as in the previous proposition.

Proof. Notice that

$$\overline{\Omega}_{2n} \, \mathcal{D}_{-1} \, \Omega_{2n} = \text{dcirc} \left( \begin{array}{ccc} a_0 & a_1 \sigma_{2n} & \cdots & a_{2n-1} \sigma_{2n}^{2n-1} \\ b_0 \sigma_{2n}^{-1} & b_1 & \cdots & b_{2n-1} \sigma_{2n}^{2n-2} \end{array} \right),$$

and proceed similarly as above.  $\Box$ 

**Corollary 2.1.** The set of eigenvalues of the doubly circulant matrix  $\mathcal{D}_1$ , (respectively of the doubly skew-circulant matrix  $\mathcal{D}_{-1}$ ), is the union of the sets of solutions of the quadratic equations

$$(2.10) det (D_k - \lambda) = 0, k = 0, \dots, n - 1,$$

where the matrices  $D_k$  are of the form (2.6), with  $S_k$  and  $T_k$  given by (2.7), (respectively, by (2.9)).

2.2. Application to finite element matrices. For the consistent mass FE-approximation of (1.2), we consider a quadratic mesh, consisting of n identical subintervals (taking the nodes in each interval to be the endpoints and the midpoint). Number the nodes in [0,1] globally from 1 to 2n+1 and let  $\varphi_i$  be the usual (piecewise quadratic) cardinal basis function, associated to the i-th global node, see e.g.  $[4, \S 2.3.1]$ . Then the set of 2n functions

$$\phi_1 = \varphi_1 + \alpha \varphi_{2n+1}, \ \phi_2 = \varphi_2, \dots, \ \phi_{2n} = \varphi_{2n},$$

is easily seen to form a suitable basis for the FE-spaces  $\subset V^{\alpha}$  ( $\alpha = 1$  or  $\alpha = -1$ ).

Due to this proper choice of the basis, the  $(2n \times 2n)$ -matrices K and M entering (1.3) are found to be of the form

(2.11) 
$$X = \begin{pmatrix} a^{X} & b^{X} & c^{X} & & & \alpha c^{X} & \alpha b^{X} \\ b^{X} & d^{X} & b^{X} & & & & & \\ c^{X} & b^{X} & a^{X} & b^{X} & c^{X} & & & & \\ & & b^{X} & d^{X} & b^{X} & & & & \\ & & & & & & & a^{X} & b^{X} \\ \alpha c^{X} & & & & & & a^{X} & b^{X} \\ \alpha b^{X} & & & & & b^{X} & d^{X} \end{pmatrix},$$

(with the convention that the non-written entries are zero). Here X = K or X = M, and  $\alpha$  is again 1 or -1. The respective non-zero matrix entries are given

by

$$a^K = \frac{14}{3}n, \ b^K = -\frac{8}{3}n, \ c^K = \frac{1}{3}n, \ d^K = \frac{16}{3}n,$$

and

$$a^M = \frac{4}{15n}, \ b^M = \frac{1}{15n}, \ c^M = \frac{1}{30n}, \ d^M = \frac{8}{15n}.$$

Referring to the notations (2.2), we clearly have

$$X = \operatorname{dcirc} \left( \begin{array}{cccc} a^{X} & b^{X} & c^{X} & 0 & \cdots & 0 & c^{X} & b^{X} \\ b^{X} & d^{X} & b^{X} & 0 & & \cdots & 0 \end{array} \right), \quad \text{when } \alpha = 1,$$

and

$$X = \operatorname{dscirc} \left( \begin{array}{cccc} a^X & b^X & c^X & 0 & \cdots & 0 & -c^X & -b^X \\ b^X & d^X & b^X & 0 & \cdots & 0 \end{array} \right), \quad \text{when } \alpha = -1.$$

From Propositions 2.1–2.2 it follows that the matrices M and K can be brought into the block diagonal form (2.5) by the same unitary transformation, viz  $(E F_{2n})$ , when  $\alpha = 1$ , and  $(E F_{2n} \overline{\Omega}_{2n})$ , when  $\alpha = -1$ . The k-th block along the diagonal  $(k = 0, \ldots, n-1)$  is found to be

$$X_{k} = \begin{pmatrix} \frac{a^{X} + d^{X}}{2} + 2b^{X} \cos \frac{\eta(k)\pi}{2n} + c^{X} \cos \frac{\eta(k)\pi}{n} & \frac{a^{X} - d^{X}}{2} + c^{X} \cos \frac{\eta(k)\pi}{n} \\ \frac{a^{X} - d^{X}}{2} + c^{X} \cos \frac{\eta(k)\pi}{n} & \frac{a^{X} + d^{X}}{2} - 2b^{X} \cos \frac{\eta(k)\pi}{2n} + c^{X} \cos \frac{\eta(k)\pi}{n} \end{pmatrix},$$

where, again, X = K or X = M, and where

(2.12) 
$$\eta(k) = \begin{cases} 2k, & \text{when } \alpha = 1, \\ 2k+1, & \text{when } \alpha = -1. \end{cases}$$

This leads us to the main result of this section.

**Theorem 2.1.** The eigenvalues of the present EVP (1.3) are given by

$$(2.13) \quad \lambda^{(1)}(k) \\ \lambda^{(2)}(k) = \frac{2N^2 \left( 11 + 4\cos^2\frac{\eta(k)\pi}{2n} \mp \sqrt{1 + 268\cos^2\frac{\eta(k)\pi}{2n} - 44\cos^4\frac{\eta(k)\pi}{2n}} \right)}{2 - \cos^2\frac{\eta(k)\pi}{2n}},$$

where k = 0, ..., n-1 and where  $\eta(k)$  is given by (2.12).

Proof. Leaning upon well-known properties of block matrices, see e.g. [1, §2.1],  $M^{-1}K$  can be transformed into a block diagonal form by the same unitary transformation as the matrices M and K, the blocks along the diagonal being  $M_k^{-1}K_k$ ,  $k=0,\ldots,n-1$ . Thus, on account of Corollary 2.1, the eigenvalues of the present EVP (1.3) are given by the union of the sets of solutions of the

quadratic equations

(2.14) 
$$\det(M_k^{-1}K_k - \lambda) = 0, \quad k = 0, \dots, n - 1.$$

These last equations can be written explicitly as

$$\lambda^{2} - N^{2} \frac{44 + 16\cos^{2} \frac{\eta(k)\pi}{2n}}{2 - 2\cos^{2} \frac{\eta(k)\pi}{2n}} \lambda + 240N^{4} \frac{1 - \cos^{2} \frac{\eta(k)\pi}{2n}}{2 - \cos^{2} \frac{\eta(k)\pi}{2n}} = 0, \quad k = 0, \dots, n-1. \ \Box$$

# 3. Some computational aspects.

(a) Case of periodic BCs ( $\alpha = 1$ ). The exact eigenvalues of the differential EVP (1.1) are directly found to be

(3.1) 
$$\lambda_1 = 0$$
, and  $\lambda_m = \lambda_{m+1} = m^2 \pi^2$ ,  $m = 2, 4, 6, \dots$ 

We aim at establishing an explicit form of the approximation error, by comparing (3.1) with the closed expression (2.13), derived for the approximate eigenvalues. To this end, note that

$$\lambda^{(1)}(k) = \lambda^{(1)}(n-k)$$
 and  $\lambda^{(2)}(k) = \lambda^{(2)}(n-k)$ ,  $k = 1, \dots, n-1$ .

Hence, all approximate eigenvalues are double, except  $\lambda^{(1)}(0)$ , and, when n is even, also except the eigenvalues  $\lambda^{(1)}(\frac{n}{2})$  and  $\lambda^{(2)}(\frac{n}{2})$ , which are simple.

To fix the ideas, we take n to be odd. A straightforward calculation reveals that, for  $k = 0, \ldots, \frac{n-1}{2}, \lambda^{(1)}(k)$  is an increasing function of k, while  $\lambda^{(2)}(k)$  is a decreasing function of k. Thus, the approximate eigenvalues, numbered in increasing order of magnitude, read

(3.2) 
$$\begin{cases} \lambda_1^h = \lambda^{(1)}(0), \\ \lambda_m^h = \lambda_{m+1}^h = \begin{cases} \lambda^{(1)}(\frac{m}{2}), & m = 2, 4, \dots, n-1, \\ \lambda^{(2)}(n - \frac{m}{2}), & m = n+1, n+3, \dots, 2n-2, \end{cases} \\ \lambda_{2n}^h = \lambda^{(2)}(0). \end{cases}$$

Note that  $\lambda_1 = 0$  is recovered exactly. For the other eigenvalues, combination of (3.2) and (3.1) leads to

(3.3) 
$$\lambda_m^h - \lambda_m = \lambda_{m+1}^h - \lambda_{m+1} = \frac{1}{720} \pi^6 m^6 h^4 + \mathcal{O}(h^6), \quad m = 2, 4, 6, \dots,$$
  
when  $n > m + 1$ .

(b) Case of semi-periodic BCs ( $\alpha = -1$ )

Here, the exact eigenvalues of (1.1) are given by

(3.4) 
$$\lambda_m = \lambda_{m+1} = m^2 \pi^2, \quad m = 1, 3, 5, \dots$$

Again we notice some symmetries in the set of approximate eigenvalues (2.13), viz

$$\lambda^{(1)}(k) = \lambda^{(1)}(n-k-1)$$
 and  $\lambda^{(2)}(k) = \lambda^{(2)}(n-k-1)$ ,  $k = 0, \dots, n-1$ .

Here, all eigenvalues are double, except, when n is odd, the eigenvalues  $\lambda^{(1)}(\frac{n-1}{2})$  and  $\lambda^{(2)}(\frac{n-1}{2})$ , which are simple.

Hence, in this case we take n to be even. By similar arguments as above, the approximate eigenvalues, numbered in increasing order of magnitude, are found to be

(3.5) 
$$\lambda_m^h = \lambda_{m+1}^h = \begin{cases} \lambda^{(1)}(\frac{m-1}{2}), & m = 1, 3, \dots, n-1, \\ \lambda^{(2)}(n-1-\frac{m-1}{2}), & m = n+1, n+3, \dots, 2n-1. \end{cases}$$

Thus, by combination of (3.4) and (3.5), we infer (3.3) to hold again, however now for  $m = 1, 3, 5, \ldots$ , when  $n \ge m + 1$ .

Consequently, in both cases, the theoretical order  $h^4$ -convergence for a quadratic FE-mesh is recovered.

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