



MAX-PLANCK-GESELLSCHAFT

Max Planck Institute Magdeburg Preprints

Peter Benner

Heike Faßbender

Chao Yang

Some Remarks on the Complex J -Symmetric Eigenproblem



Author's addresses:

Peter Benner

Computational Methods in Systems and Control Theory
Max Planck Institute for Dynamics of Complex Technical Systems
Sandtorstraße 1, 39106 Magdeburg, Germany

benner@mpi-magdeburg.mpg.de

Heike Faßbender

Institut Computational Mathematics/AG Numerik
TU Braunschweig
Pockelsstr. 14, 38106 Braunschweig, Germany

h.fassbender@tu-bs.de

Chao Yang

Computational Research Division
Lawrence Berkeley National Laboratory
Berkeley, CA 94720, USA

CYang@lbl.gov

Imprint:

Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg

Publisher:

Max Planck Institute for
Dynamics of Complex Technical Systems

Address:

Max Planck Institute for
Dynamics of Complex Technical Systems
Sandtorstr. 1
39106 Magdeburg

<http://www.mpi-magdeburg.mpg.de/preprints/>

Abstract

The eigenproblem for complex J -symmetric matrices $H_C = \begin{bmatrix} A & C \\ D & -A^T \end{bmatrix}$, $A, C = C^T, D = D^T \in \mathbb{C}^{n \times n}$ is considered. A proof of the existence of a transformation to the complex J -symmetric Schur form proposed in [16] is given. The complex symplectic unitary QR decomposition and the complex symplectic SR decomposition are discussed. It is shown that a QR-like method based on the complex symplectic unitary QR decomposition is not feasible here. A complex symplectic SR algorithm is presented which can be implemented such that one step of the SR algorithm can be carried out in $\mathcal{O}(n)$ arithmetic operations. Based on this, a complex symplectic Lanczos method can be derived. Moreover, it is discussed how the $2n \times 2n$ complex J -symmetric matrix H_C can be embedded in a $4n \times 4n$ real Hamiltonian matrix.

Keywords. Complex J -symmetric eigenproblem, real Hamiltonian matrix, complex Hamiltonian matrix, structure-preserving, SR algorithm.

1 Introduction

The basic algebraic structures and properties of the following classes of matrices

$H_C \in \mathbb{C}^{2n \times 2n}$	J -symmetric	$JH_C = (JH_C)^T$
$H_H \in \mathbb{C}^{2n \times 2n}$	J -Hermitian (complex Hamiltonian)	$JH_H = (JH_H)^H$
$H \in \mathbb{R}^{2n \times 2n}$	real Hamiltonian	$JH = (JH)^H = (JH)^T$

are well-known, see, e.g., [7, 13, 14]. Here $J = \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix}$ and I is the $n \times n$ identity matrix. X^T denotes transposition, $Y = X^T, y_{ij} = x_{ji}$, no matter whether X is real or complex, while X^H denotes conjugate transposition, $Y = X^H, y_{ij} = \overline{x_{ji}}$. In case $H \in \mathbb{R}^{2n \times 2n}$, the structures coalesce, A is J -symmetric and J -Hermitian. Each of the three classes of matrices forms a Lie algebra. The eigenvalues of real Hamiltonian matrices H and of complex J -symmetric matrices H_C display a symmetry [14]: they appear in pairs $(\lambda, -\lambda)$. If x is the right eigenvector corresponding to λ , $Bx = \lambda x$, then Jx is the left eigenvector corresponding to the eigenvalue $-\lambda$ of $B = H$ or $B = H_C$, $(Jx)^T B = -\lambda(Jx)^T$. Moreover, the matrices in these two classes can always be written in block form $\begin{bmatrix} A & C \\ D & -A^T \end{bmatrix}$ with $C = C^T, D = D^T$, where either $A, C, D \in \mathbb{R}^{n \times n}$ or $A, C, D \in \mathbb{C}^{n \times n}$. In contrast, complex Hamiltonian matrices have a block form $\begin{bmatrix} A & C \\ D & -A^H \end{bmatrix}$ with $A, C = C^H, D = D^H \in \mathbb{C}^{n \times n}$; the eigenvalues display the symmetry $(\lambda, -\overline{\lambda})$.

A particular instance of the J -symmetric eigenproblem arises in the context of estimating the absorption spectra in molecules and solids using the Bethe-Salpeter equations [17, 18] for determining electronic excitation energies. Solving the Bethe-Salpeter equations numerically, the eigenvalue problem $H_{BS}x = \lambda x$ for complex matrices

$$H_{BS} = \begin{bmatrix} A & -D^H \\ D & -A^T \end{bmatrix} \in \mathbb{C}^{2n \times 2n}, \quad A = A^H, D = D^T \in \mathbb{C}^{n \times n} \quad (1)$$

arises. The matrices H_{BS} belong to the slightly more general class of matrices of complex J -symmetric matrices

$$H_C = \begin{bmatrix} A & C \\ D & -A^T \end{bmatrix} \in \mathbb{C}^{2n \times 2n}, \quad A, C = C^T, D = D^T \in \mathbb{C}^{n \times n}. \quad (2)$$

As already discussed, the eigenvalues of H_C display the symmetry $(\lambda, -\lambda)$. Clearly, H_{BS} inherits these properties. There is even more structure in the eigenvalues and eigenvectors of H_{BS} .

Theorem 1. *Eigenvalues of H_{BS} that are real or purely imaginary appear in pairs $(\lambda, -\lambda)$, other eigenvalues appear in quadruples $(\lambda, -\lambda, \bar{\lambda}, -\bar{\lambda})$. Moreover, for $\lambda \in \mathbb{C}$, $H_{BS}x = \lambda x$ implies $H_{BS}K\bar{x} = -\bar{\lambda}K\bar{x}$ and $H_{BS}y = -\lambda y$ implies $H_{BS}K\bar{y} = \bar{\lambda}K\bar{y}$ with*

$$K = \begin{bmatrix} 0 & I \\ I & 0 \end{bmatrix}.$$

For $\lambda \in \mathbb{R}$, it follows that $H_{BS}x = \lambda x$ implies $H_{BS}K\bar{x} = -\lambda K\bar{x}$ (as $-\lambda = -\bar{\lambda}$).

Proof. The equation $H_{BS}x = \lambda x$ reads

$$\begin{aligned} Ax_1 - D^H x_2 &= \lambda x_1 \\ Dx_1 - A^T x_2 &= \lambda x_2 \end{aligned}$$

for $x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$, $x_1, x_2 \in \mathbb{C}^n$. Reversing the order of the two equations, multiplying by -1 and taking the conjugate of each equation yields

$$\begin{aligned} -D^H \bar{x}_1 + A \bar{x}_2 &= -\bar{\lambda} \bar{x}_2 \\ -A^T \bar{x}_1 + D \bar{x}_2 &= -\bar{\lambda} \bar{x}_1 \end{aligned}$$

(recall that $D = D^T$, hence $\bar{D} = D^H$ and, as $A = A^H$, we have $\bar{A} = A^T$). This is the same as $H_{BS}K\bar{x} = -\bar{\lambda}K\bar{x}$.

An analogous argument shows that $H_{BS}y = -\lambda y$ implies $H_{BS}K\bar{y} = \bar{\lambda}K\bar{y}$. \square

In this paper, we analyze structure-preserving methods for solving the eigenproblem for H_C , and thus also for H_{BS} .

Numerical algorithms for the real Hamiltonian eigenproblem are a well-studied field of research, see, e.g., [8] for an overview. It is of particular interest to use structure-preserving methods which guarantee that the computed eigenvalues come in pairs. This is, due to rounding errors, not necessarily the case when using standard eigensolvers like the QR method [12]. A backward stable structure-preserving algorithm for the real Hamiltonian eigenproblem has been proposed in [3, 4]. The complex Hamiltonian eigenproblem is dealt with, e.g., in [5]. In [19] it is noted, that the eigenproblem for (1) is equivalent to a real Hamiltonian eigenproblem with $H = \begin{bmatrix} \operatorname{Im}(A+D) & \operatorname{Re}(A+D) \\ \operatorname{Re}(D-A) & -\operatorname{Im}(A+D)^T \end{bmatrix}$. [19] discusses structure-preserving parallel algorithms for solving this special eigenproblem.

The only algorithm for solving the eigenproblem for complex J -symmetric matrices H_C which we could find in the literature is a Jacobi algorithm [16]. It transforms H_C to

its complex J -symmetric Schur form from which the eigenvalues can be read off. Much to our surprise, the existence of the transformation to complex J -symmetric Schur form has not been proved in the literature. In Section 3 we fill this gap using a result on the structured Jordan canonical form of complex J -symmetric matrices from [15].

The Jacobi algorithm [16] is inherently structure-preserving (that is, each iterate is complex J -symmetric). Section 4 briefly summarizes our findings on other structure-preserving algorithms. The structure-preserving algorithms are based on similarity transformations with complex symplectic matrices $S_C \in \mathbb{C}^{2n \times 2n}$ defined by the property $S_C^T J S_C = J$. These matrices form the automorphism group associated with the Lie algebra of complex J -symmetric matrices. The similarity transformation $S_C^{-1} H_C S_C$ yields a complex J -symmetric matrix.

Most structure-preserving algorithms are based on suitable matrix decompositions which can replace the standard QR decomposition in the QR algorithm. Hence, in Section 2 the decomposition of general $2n \times 2n$ matrices into the product of a complex symplectic and another suitable matrix is considered. In particular, the complex symplectic unitary QR decomposition and the complex symplectic SR decomposition are discussed which are the basis for the algorithms considered in Section 4. In Section 4.1 it is discussed why a QR-like method based on the complex symplectic unitary QR decomposition is not feasible here. Section 4.2 presents the complex symplectic SR algorithm which is analogous to the SR algorithm for real Hamiltonian matrices [9]. Based on this, a complex symplectic Lanczos method can be derived which projects the large, sparse $2n \times 2n$ complex J -symmetric matrix H_C onto a small, dense $2k \times 2k$ complex J -symmetric J -Hessenberg matrix. This $2k \times 2k$ complex J -symmetric matrix is uniquely determined by $4k - 1$ parameters. Using these $4k - 1$ parameters, one step of the SR algorithm can be carried out in $\mathcal{O}(k)$ arithmetic operations (compared to $\mathcal{O}(k^3)$ arithmetic operations when working on the actual matrix). Moreover, the complex J -symmetric structure, which will be destroyed in the numerical process due to roundoff errors when working with a complex J -symmetric matrix, will be forced by working just with the parameters. Finally, in Section 4.3 it is discussed how the $2n \times 2n$ complex J -symmetric matrix H_C can be embedded in a $4n \times 4n$ real Hamiltonian matrix. Hence, any method for solving the Hamiltonian eigenproblem can be used to solve the complex J -symmetric one. Conclusions are given in Section 5.

2 Complex symplectic decompositions

It is well-known that each complex matrix $A \in \mathbb{C}^{n \times n}$ can be decomposed into the product of a unitary matrix Q and an upper triangular matrix R . Based on this decomposition, the standard QR algorithm can be used to transform A into Schur form using similarity transformations with unitary matrices.

In order to derive a QR-like structure-preserving algorithm for complex J -symmetric matrices, a suitable matrix decomposition which can replace the standard QR decomposition in the QR iteration is needed. As a similarity transformation with a complex symplectic matrix preserves the complex J -symmetric structure, complex symplectic

decompositions of square matrices of even dimension are considered in this section.

Hence we will consider decompositions of a complex matrix $A \in \mathbb{C}^{2n \times 2n}$ into the product of a complex symplectic matrix S and a suitable matrix R . First, the numerically desirable case of a decomposition into the product of a unitary and complex symplectic matrix S and a suitable matrix R is discussed. Next, the requirement of S being unitary is dropped, and a decomposition into the product of a complex symplectic matrix S and a suitable matrix R is presented. Our discussion closely resembles the discussion in [6] where matrix decompositions of the type $A = SR$ into the product of a symplectic matrix S (that is, $S^H JS = J, S \in \mathbb{C}^{2n \times 2n}$) or a unitary and symplectic matrix S (that is, $S^H S = I, S^H JS = J, S \in \mathbb{C}^{2n \times 2n}$) and an upper triangular-like matrix R for complex matrices $A \in \mathbb{C}^{2n \times 2n}$ have been considered.

Theorem 2 (Complex symplectic unitary QR decomposition).

For any $A \in \mathbb{C}^{2n \times 2n}$, there always exists a decomposition of the form

$$A = QR, \quad Q^T J Q = J, Q^H Q = I$$

for a complex symplectic and unitary matrix $Q \in \mathbb{C}^{2n \times 2n}$ and

$$R = \begin{bmatrix} R_{11} & R_{12} \\ R_{21} & R_{22} \end{bmatrix} = \begin{bmatrix} \nabla & \square \\ \circ \nabla & \square \\ \vdots & \vdots \\ \circ \nabla & \square \end{bmatrix}, \quad (3)$$

where R_{11} is upper triangular and R_{21} is strictly upper triangular. If A is nonsingular, then R_{11} is nonsingular.

If A is real, Q and R can be chosen to be real.

Proof. Partition the matrix A into $n \times n$ blocks

$$A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}.$$

The complex symplectic and unitary matrix Q can be constructed by using a suitable sequence of complex symplectic and unitary Householder and Givens transformations to turn A columnwise to the desired form (3). Essentially for every column, first a Householder transformation is used to eliminate the corresponding entries under the diagonal in the $(2, 1)$ block, then a Givens transformation is used to eliminate the diagonal element in the $(2, 1)$ block. Finally, a Householder transformation is used to eliminate the corresponding entries under the diagonal in the $(1, 1)$ block. \square

The proof makes use of complex symplectic Householder and Givens transformations which are defined as follows:

- A complex symplectic Givens transformation $G_C^{(j)}$ differs from the identity I_{2n} in four elements $(j, j), (j, n+j), (n+j, j)$ and $(n+j, n+j)$. Let G denote a unitary 2×2 Givens rotation. Then $(G_C^{(j)})_{jj} = g_{11}, (G_C^{(j)})_{j, n+j} = g_{12}, (G_C^{(j)})_{n+j, j} = g_{21}, (G_C^{(j)})_{n+j, n+j} = g_{22}$. G is chosen to zero out either the j th or the $(n+j)$ th component of $x \in \mathbb{C}^{2n}$ (see [13, Section 4.6.1]).

- A complex symplectic Householder transformation is set up in a similar way by embedding a $k \times k$ Householder matrix $H(u)$ and $\overline{H(u)}$ into I_{2n} , $k \leq n$. The vector $u \neq 0$ is chosen to map k coordinates from among the first n (alternatively, from among the last n) coordinates of $x \in \mathbb{C}^{2n}$ to a specific vector in \mathbb{C}^k (see [13, Section 4.6.2]).

Corollary 1. *If A is complex symplectic, then R in (3) has additional structure: $R_{21} = 0$ and $R_{22} = R_{11}^{-T}$,*

$$R = \begin{bmatrix} \square & \square \\ 0 & \square \end{bmatrix}.$$

Proof. As A is complex symplectic and has a complex symplectic QR decomposition, $A = QR$, the matrix R needs to be complex symplectic as well:

$$J = A^T J A = R^T Q^T J Q R = R^T J R.$$

This gives

$$I = R_{11}^T R_{22} - R_{21}^T R_{12}, \quad (4)$$

$$0 = R_{11}^T R_{21} - R_{21}^T R_{11}. \quad (5)$$

Hence, $R_{11}^T R_{21}$ is symmetric due to (5), $R_{11}^T R_{21} = R_{21}^T R_{11} = (R_{11}^T R_{21})^T$.

In the matrix R from (3) R_{11} is upper triangular and R_{21} is strictly upper triangular. As A is nonsingular, R_{11} is nonsingular. That is, $r_{jj}^{11} \neq 0$, $j = 1, \dots, n$. Here the elements of $R_{k\ell}$ are denoted by $r_{ij}^{k\ell}$, $k, \ell = 1, 2$, $i, j = 1, \dots, n$. Now it follows from the (strict) upper triangular structure of R_{11} and R_{21} that $R_{21} = 0$. Consider the product $Z = R_{11}^T R_{21}$. Its first column is equal to zero. As Z is symmetric, this implies that its first row has to be equal to zero as well. As $z_{1j} = r_{11}^{11} r_{1j}^{21}$ for $j = 2, \dots, n$, and $r_{11}^{11} \neq 0$, this implies that the first row of R_{21} is zero, $r_{1j}^{21} = 0$. From this it follows that the second column of Z is zero as well. Hence the second row of Z is zero, that is $z_{2j} = r_{22}^{11} r_{2j}^{21} = 0$ for $j = 3, \dots, n$. As $r_{22}^{11} \neq 0$, we have $r_{2j}^{21} = 0$, $j = 3, \dots, n$. From this it follows that the third column of Z is zero. Z is symmetric, so that its third row has to be equal to zero as well. Continuing in this fashion, one can argue that $R_{21} = 0$.

Now (4) implies that $R_{11}^T R_{22} = I$, which gives $R_{22} = R_{11}^{-T}$. \square

Theorem 2 and Corollary 1 are analogues of Corollary 4.5 in [6]. Note that the unitary symplectic SR decomposition in [6] yields a matrix R almost of the form (3), just the diagonal entries of R_{21} are purely imaginary numbers, not zeros. However, not surprisingly, in the real case, Q and R can be chosen real and the matrix R is as in (3).

Unfortunately, a QR-like method based on the complex symplectic unitary QR decomposition is not viable due to the lack of an appropriate reduced form which can replace the Hessenberg form in the standard QR iteration (see Section 4.1 for a discussion). Therefore, a decomposition into a complex symplectic matrix S and a suitable matrix R is considered next.

The following theorem is the analogue of Theorem 3.8 in [6]. Please note that in [6] the decomposition of $2n \times 2n$ matrices A into the product of a symplectic matrix S ($S^H JS = J$) and a matrix R which is a permuted version of an upper triangular matrix is considered. It is proven that the set of matrices which have such a decomposition is dense in $\mathbb{R}^{2n \times 2n}$, but not dense in $\mathbb{C}^{2n \times 2n}$. Making use of complex symplectic matrices in the decomposition of a complex $2n \times 2n$ matrix, we obtain a result analogously to the real case in [6] (in the real case, the theorem below is just the result from [6]).

Theorem 3 (Complex symplectic SR decomposition). *Let $A \in \mathbb{C}^{2n \times 2n}$ be nonsingular. There exists a decomposition of the form*

$$A = SR, \quad S^T JS = J$$

for a complex symplectic matrix $S \in \mathbb{C}^{2n \times 2n}$ and an (upper) J -triangular matrix

$$R = \begin{bmatrix} R_{11} & R_{12} \\ R_{21} & R_{22} \end{bmatrix} = \begin{bmatrix} \diagdown & \diagdown \\ \circ \cdots \circ & \diagdown \end{bmatrix}$$

if and only if $\det((\widehat{P}A^T J A \widehat{P}^T)[2k, 2k]) \neq 0$ for all $k = 1, \dots, n$. Here \widehat{P} is the permutation matrix $\widehat{P} = [e_1, e_3, \dots, e_{2n-1}, e_2, e_4, \dots, e_{2n}]$ which permutes R into upper triangular form and $A[k, k]$ denotes the leading $k \times k$ principal submatrix of A of dimension $k \times k$.

Proof. Theorem 3.8 and Remark 3.9 in [6] states the above result for real matrices A , the proof also holds for complex A . \square

The complex symplectic SR decomposition is unique up to a trivial factor.

Corollary 2. *Let $A \in \mathbb{C}^{2n \times 2n}$. Let $A = SR$ and $A = \widetilde{S}\widetilde{R}$ be complex symplectic SR factorizations of A . Then there exists a trivial matrix D , that is, D is complex symplectic and J -triangular, such that $\widetilde{S} = SD^{-1}$ and $\widetilde{R} = DR$. D is trivial if and only if it has the form*

$$D = \begin{bmatrix} C & F \\ 0 & C^{-1} \end{bmatrix} = \begin{bmatrix} \diagdown & \diagdown \\ 0 & \diagdown \end{bmatrix}, \quad (6)$$

where C and $F \in \mathbb{C}^{n \times n}$ are diagonal matrices.

Proof. Proposition 3.3 in [9] states the above result for real matrices A , the proof also holds for complex A and the complex symplectic SR decomposition. \square

A straightforward adaption of the algorithm for computing the real SR decomposition as given in [9] gives an algorithm for computing the complex symplectic SR decomposition of an arbitrary matrix $A \in \mathbb{C}^{2n \times 2n}$. Besides the complex symplectic Householder and Givens transformations already introduced in Section 3, complex symplectic shears for Gauss-like eliminations are needed, see [13, Section 4.6.3] for a definition.

3 (Structured) normal forms for complex J -symmetric matrices

The standard QR algorithm transforms a complex matrix A into its Schur form. A structure-preserving analogue for complex J -symmetric matrices A will attempt to transform A into an appropriate complex J -symmetric Schur form.

Any complex J -symmetric matrix X is said to be in complex J -symmetric Schur form if

$$X = \begin{bmatrix} R & B \\ 0 & -R^T \end{bmatrix} = \begin{bmatrix} \nabla & \square \\ 0 & \nabla \end{bmatrix}, \quad R, B = B^T \in \mathbb{C}^{n \times n}, \quad (7)$$

where the nonzero eigenvalues of R either have positive real part or zero real part and positive imaginary part, see, e.g. [16]. Much to our surprise, we could not find a proof of the following fact in the literature.

Theorem 4. *For any complex J -symmetric matrix H_C there exists a complex symplectic and unitary matrix $W \in \mathbb{C}^{2n \times 2n}$ satisfying*

$$W^T J W = J, \quad W^H W = I,$$

such that $W^H H_C W$ is in complex J -symmetric Schur form (7).

We will present a proof for Theorem 4 which makes use of the structured Jordan form for complex J -symmetric matrices [15]. For the ease of the reader, this structured Jordan form is presented here. Before we do so, some notation needs to be introduced.

A matrix $X = X_1 \oplus \cdots \oplus X_p$ denotes a block diagonal matrix X with diagonal blocks X_1, \dots, X_p (in that order). The symbol Σ_p denotes the $p \times p$ reverse identity with alternating signs

$$\Sigma_p = \begin{bmatrix} 0 & & (-1)^0 \\ & \ddots & \\ (-1)^{p-1} & & 0 \end{bmatrix}.$$

Moreover, $\mathcal{J}_p(\lambda)$ denotes the upper bidiagonal Jordan block of size p associated with the eigenvalue λ . Finally, a matrix $X \in \mathbb{C}^{p \times p}$ is called \mathfrak{J} -decomposable if there exists a nonsingular matrix $P \in \mathbb{C}^{p \times p}$ such that

$$P^{-1} X P = X_1 \oplus X_2, \quad P^T \mathfrak{J} P = \mathfrak{J}_1 \oplus \mathfrak{J}_2,$$

where $X_1, \mathfrak{J}_1 \in \mathbb{C}^{m \times m}$ and $X_2, \mathfrak{J}_2 \in \mathbb{C}^{p-m \times p-m}$ for some $0 < m < p$. Otherwise, X is called \mathfrak{J} -indecomposable. Clearly, any matrix X can always be decomposed as

$$P^{-1} X P = X_1 \oplus \cdots \oplus X_k, \quad P^T J P = \mathfrak{J}_1 \oplus \cdots \oplus \mathfrak{J}_k,$$

where X_j is \mathfrak{J}_j -indecomposable, $j = 1, \dots, k$. A classification of indecomposable matrices is given in [15].

Now we can state the structured Jordan form for complex J -symmetric matrices. As already observed, all nonzero eigenvalues come in pairs $(\lambda, -\lambda)$. The Jordan block associated with $-\lambda$ is just minus the transpose of the Jordan block associated with λ . Moreover, Jordan blocks associated with the eigenvalue zero either are of even size or appear in pairs. In particular, it holds

Theorem 5 ([15, Theorem 8.3]). *(Canonical form for complex J -symmetric matrices)*
There exists a nonsingular matrix Q such that

$$Q^{-1}H_C Q = \mathfrak{H}_1 \oplus \cdots \oplus \mathfrak{H}_p, \quad Q^T J Q = \mathfrak{J}_1 \oplus \cdots \oplus \mathfrak{J}_p, \quad (8)$$

where \mathfrak{H}_j is \mathfrak{J}_j -indecomposable and where \mathfrak{H}_j and \mathfrak{J}_j have one of the following forms:

i) blocks associated with $\lambda_j = 0$, where $n_j \in \mathbb{N}$ is even:

$$\mathfrak{H}_j = \mathcal{J}_{n_j}(0), \quad \mathfrak{J}_j = \Sigma_{n_j};$$

ii) paired blocks associated with $\lambda_j = 0$, where $m_j \in \mathbb{N}$ is odd:

$$\mathfrak{H}_j = \begin{bmatrix} \mathcal{J}_{m_j}(0) & 0 \\ 0 & -(\mathcal{J}_{m_j}(0))^T \end{bmatrix}, \quad \mathfrak{J}_j = J_{m_j};$$

iii) blocks associated with a pair $(\lambda_j, -\lambda_j) \in \mathbb{C} \times \mathbb{C}$, where $\operatorname{Re}(\lambda_j) > 0$ or $\operatorname{Im}(\lambda_j) > 0$ if $\operatorname{Re}(\lambda_j) = 0$ and $m_j \in \mathbb{N}$:

$$\mathfrak{H}_j = \begin{bmatrix} \mathcal{J}_{m_j}(\lambda_j) & 0 \\ 0 & -(\mathcal{J}_{m_j}(\lambda_j))^T \end{bmatrix}, \quad \mathfrak{J}_j = J_{m_j}.$$

Moreover, the form (8) is unique up to the permutation of blocks.

With this theorem we are ready to present a proof of Theorem 4 using Theorem 5.

Proof of Theorem 4. Consider equation (8). The first step in proving Theorem 4 will be to construct a matrix Y to transform $Q^{-1}H_C Q$ such that $Y^{-1}Q^{-1}H_C Q Y = T$ is in complex J -symmetric Schur form (7) and such that $Y^T Q^T J Q Y = J$. For this, only permutations and diagonal scaling have to be used. Let Y be this transformation matrix and set $Z = QY$. In a second step, decompose the complex symplectic matrix Z into the product of a complex symplectic and unitary matrix S and a matrix R as in (3). As Z is complex symplectic, R is of the form given in Corollary 1. Then

$$S^T J S = J$$

and

$$R^{-1}S^{-1}H_C S R = T \Leftrightarrow S^{-1}H_C S = R T R^{-1} = \tilde{T},$$

where \tilde{T} is in complex J -symmetric Schur form (7) as

$$R T R^{-1} = R T J R^T J = \begin{bmatrix} \tilde{T}_{11} & \tilde{T}_{12} \\ 0 & \tilde{T}_{22} \end{bmatrix}$$

with

$$\begin{aligned} \tilde{T}_{11} &= -R_{11} T_{11} R_{11}^{-1}, \\ \tilde{T}_{12} &= -R_{11} T_{12} R_{11}^T + R_{11} T_{11} R_{11}^T + R_{12} T_{11}^T R_{11}^T = \tilde{T}_{12}^T, \\ \tilde{T}_{22} &= R_{11}^{-T} T_{11}^T R_{11}^T = -\tilde{T}_{11}^T, \end{aligned}$$

and \tilde{T}_{11} is an upper triangular matrix as products and inverses of upper triangular matrices are upper triangular again [12, Chapter 3.1.7].

This leaves to discuss the first step of constructing Y . The blocks \mathfrak{H}_j in cases ii) and iii) are of even dimension having the block form

$$\begin{bmatrix} \mathcal{J}_j(\lambda) & 0 \\ 0 & -\mathcal{J}_j^T(\lambda) \end{bmatrix}.$$

The corresponding blocks \mathfrak{J}_j are just small copies of J , $\mathfrak{J}_j = J_j$. Our first goal is to transform the blocks corresponding to case i) to be of the same form as those for the cases ii) and iii), even so the Jordan structure will be lost. Then it will be possible to reorder the blocks in the different \mathfrak{H}_j such that all upper bidiagonal blocks are moved to the upper block and all lower bidiagonal blocks will be moved to the lower block of the resulting 2×2 block matrix with $n \times n$ blocks.

The blocks $\mathfrak{H}_j = \mathcal{J}_j(0)$ in case i) corresponding to zero eigenvalues have even dimension as well. Hence they can be partitioned into blocks of size $j/2 \times j/2$

$$\mathfrak{H}_j = \begin{bmatrix} \mathcal{J}_{j/2}(0) & \widehat{B} \\ 0 & \mathcal{J}_{j/2}(0) \end{bmatrix}, \quad \mathcal{J}_{j/2}, \widehat{B} \in \mathbb{R}^{j/2 \times j/2},$$

where \widehat{B} is zero up to the only nonzero entry 1 in the position $(j/2, 1)$. Unlike the \mathfrak{H}_j block in the cases ii) and iii), here the second diagonal block is upper bidiagonal, not lower bidiagonal. Applying the permutation \mathcal{P}_j

$$\mathcal{P}_j = \begin{bmatrix} I_{j/2} & 0 \\ 0 & P_{j/2} \end{bmatrix}, P_{j/2} = \begin{bmatrix} 0 & 1 \\ & \ddots \\ 1 & 0 \end{bmatrix} \in \mathbb{R}^{j/2 \times j/2} \quad (9)$$

to \mathfrak{H}_j yields

$$\mathcal{P}_j \begin{bmatrix} \mathcal{J}_{j/2}(0) & \widehat{B} \\ 0 & \mathcal{J}_{j/2}(0) \end{bmatrix} \mathcal{P}_j = \begin{bmatrix} \mathcal{J}_{j/2}(0) & \widehat{B}P_{j/2} \\ 0 & \mathcal{J}_{j/2}(0)^T \end{bmatrix},$$

so that the second diagonal block is of lower bidiagonal form. The only nonzero entry in \widehat{B} ends up in the (n, n) -position in $\widehat{B}P_{j/2}$. Applying \mathcal{P}_j to the corresponding \mathfrak{J}_j block gives

$$\mathcal{P}_j^T \Sigma_j \mathcal{P}_j = \mathcal{P}_j \begin{bmatrix} 0 & \Sigma_{j/2} \\ -\Sigma_{j/2} & 0 \end{bmatrix} \mathcal{P}_j = \begin{bmatrix} 0 & \Sigma_{j/2}P_{j/2} \\ -P_{j/2}\Sigma_{j/2} & 0 \end{bmatrix}$$

with

$$\Sigma_{j/2}P_{j/2} = \text{diag}(-(-1)^0, (-1)^1, \dots, (-1)^{j/2}) = D_{j/2}.$$

Using diagonal scaling with the matrix

$$\mathcal{D}_j = \begin{bmatrix} D_{j/2} & 0 \\ 0 & I_{j/2} \end{bmatrix},$$

the matrix $\mathcal{P}_j \Sigma_j \mathcal{P}_j$ can easily be transformed to the matrix J_j :

$$\mathcal{D}_j^T \mathcal{P}_j \Sigma_j \mathcal{P}_j \mathcal{D}_j = J_j.$$

In order to conclude the transformation, \mathcal{D}_j needs to be applied to $\mathcal{P}_j \mathfrak{H}_j \mathcal{P}_j$

$$\mathcal{D}_j^{-1} \begin{bmatrix} \mathcal{J}_{j/2}(0) & \widehat{B}P_{j/2} \\ 0 & \mathcal{J}_{j/2}(0)^T \end{bmatrix} \mathcal{D}_j = \begin{bmatrix} -\mathcal{J}_{j/2}(0) & D_{j/2} \widehat{B}P_{j/2} \\ 0 & \mathcal{J}_{j/2}(0)^T \end{bmatrix}.$$

Let $G = \widetilde{G}_1 \oplus \cdots \oplus \widetilde{G}_p$ be partitioned as the matrices in (8), where

$$\widetilde{G}_j = \begin{cases} I_j & \text{if the block corresponds to case ii) or iii),} \\ \mathcal{P}_j \mathcal{D}_j & \text{if the block corresponds to case i).} \end{cases}$$

Then

$$G^{-1} Q^{-1} H_C Q G = \widetilde{\mathfrak{H}}_1 \oplus \cdots \oplus \widetilde{\mathfrak{H}}_p, \quad G^T Q^T J Q G = \widetilde{\mathfrak{J}}_1 \oplus \cdots \oplus \widetilde{\mathfrak{J}}_p,$$

where

$$\begin{aligned} \widetilde{\mathfrak{H}}_j &= \begin{bmatrix} \mathcal{E}_j & \mathcal{B}_j \\ 0 & -\mathcal{E}_j^T \end{bmatrix}, \\ \widetilde{\mathfrak{J}}_j &= J_j. \end{aligned}$$

Here \mathcal{E}_j is upper bidiagonal and \mathcal{B}_j is zero for the cases ii) and iii), and has one nonzero entry in the $(j/2 \times j/2)$ position for the case i).

Next permute $G^{-1} Q^{-1} H_C G$ such that

$$\widehat{P} G^{-1} H_C G \widehat{P} = \begin{bmatrix} \widetilde{R} & \widetilde{B} \\ 0 & -\widetilde{R}^T \end{bmatrix}, \quad \widehat{P} G^T J G \widehat{P} = J \quad (10)$$

for an upper bidiagonal \widetilde{R} and a symmetric \widetilde{B} . Such a permutation \widehat{P} always exists. Each of the blocks $\widetilde{\mathfrak{H}}_j$ has diagonal blocks of the form $\text{diag}(\mathcal{J}_j, -\mathcal{J}_j^T)$. Hence, the permutation has to take the leading diagonal block of \mathfrak{H}_j as the j th diagonal block of \widetilde{R} (which implies that the trailing diagonal block will be the j th diagonal block of $-\widetilde{R}^T$). In case there is a nonzero off-diagonal block \mathcal{B}_j in \mathfrak{H}_j , it will be moved to \widetilde{B} such that the nonzero entry ends up on the diagonal of the upper right block \widetilde{B} .

In order to illustrate this, consider the following small example

$$\begin{bmatrix} \mathcal{E}_{j_1}(0) & \mathcal{B}_{j_1} & & \\ & -\mathcal{E}_{j_1}^T(0) & & \\ & & \mathcal{E}_{j_2}(\lambda) & \\ & & & -\mathcal{E}_{j_2}^T(\lambda) \end{bmatrix}.$$

Using

$$\widehat{P} = \begin{bmatrix} I & 0 & 0 & 0 \\ 0 & 0 & I & 0 \\ 0 & I & 0 & 0 \\ 0 & 0 & 0 & I \end{bmatrix}$$

yields

$$\begin{aligned}
& \widehat{\mathcal{P}} \begin{bmatrix} \mathcal{E}_{j_1}(0) & \mathcal{B}_{j_1} & & \\ & -\mathcal{E}_{j_1}^T(0) & & \\ & & \mathcal{E}_{j_2}(\lambda) & \\ & & & -\mathcal{E}_{j_2}^T(\lambda) \end{bmatrix} \begin{bmatrix} I & 0 & 0 & 0 \\ 0 & 0 & I & 0 \\ 0 & I & 0 & 0 \\ 0 & 0 & 0 & I \end{bmatrix} \\
&= \begin{bmatrix} I & 0 & 0 & 0 \\ 0 & 0 & I & 0 \\ 0 & I & 0 & 0 \\ 0 & 0 & 0 & I \end{bmatrix} \begin{bmatrix} \mathcal{E}_{j_1}(0) & 0 & \mathcal{B}_{j_1} & 0 \\ 0 & 0 & -\mathcal{E}_{j_1}^T(0) & 0 \\ 0 & \mathcal{E}_{j_2}(\lambda) & 0 & 0 \\ 0 & 0 & 0 & -\mathcal{E}_{j_2}^T(\lambda) \end{bmatrix} \\
&= \left[\begin{array}{cc|cc} \mathcal{E}_{j_1}(0) & 0 & \mathcal{B}_{j_1} & 0 \\ 0 & \mathcal{E}_{j_2}(\lambda) & 0 & 0 \\ \hline 0 & 0 & -\mathcal{E}_{j_1}^T(0) & 0 \\ 0 & 0 & 0 & -\mathcal{E}_{j_2}^T(\lambda) \end{array} \right].
\end{aligned}$$

Applying this permutation to $G^T Q^T J Q G$ yields

$$\begin{aligned}
& \begin{bmatrix} I & 0 & 0 & 0 \\ 0 & 0 & I & 0 \\ 0 & I & 0 & 0 \\ 0 & 0 & 0 & I \end{bmatrix} \begin{bmatrix} 0 & I_{j_1} & 0 & 0 \\ -I_{j_1} & 0 & 0 & 0 \\ 0 & 0 & 0 & I_{j_2} \\ 0 & 0 & -I_{j_2} & 0 \end{bmatrix} \begin{bmatrix} I & 0 & 0 & 0 \\ 0 & 0 & I & 0 \\ 0 & I & 0 & 0 \\ 0 & 0 & 0 & I \end{bmatrix} \\
&= \begin{bmatrix} I & 0 & 0 & 0 \\ 0 & 0 & I & 0 \\ 0 & I & 0 & 0 \\ 0 & 0 & 0 & I \end{bmatrix} \begin{bmatrix} 0 & 0 & I_{j_1} & 0 \\ -I_{j_1} & 0 & 0 & 0 \\ 0 & 0 & 0 & I_{j_2} \\ 0 & -I_{j_2} & 0 & 0 \end{bmatrix} \\
&= \left[\begin{array}{cc|cc} 0 & 0 & I_{j_1} & 0 \\ 0 & 0 & 0 & I_{j_2} \\ \hline -I_{j_1} & 0 & 0 & 0 \\ 0 & -I_{j_2} & 0 & 0 \end{array} \right] = J.
\end{aligned}$$

Hence, there is always a permutation $\widehat{\mathcal{P}}$ in order to achieve (10). \square

Note that H_C is in complex J -symmetric Schur form if and only if the matrix $\mathcal{P}H_C\mathcal{P}$ with \mathcal{P} as in (9) is in standard Schur form.

In [16], a Jacobi algorithm for computing the complex J -symmetric Schur form of a complex J -symmetric matrix is given.

4 Algorithms

The only algorithm for computing the complex J -symmetric Schur form of H_C which we could find in the literature is a Jacobi algorithm [16]. The algorithms proposed there are based either on solving a suitable 2×2 or a 4×4 complex J -symmetric subproblem. Asymptotic quadratic convergence is proven under a specific scheme on

the choice of the sweeps (that is, a sequence of Jacobi steps in which each element in the strict lower triangular part of $\mathcal{P}H_C\mathcal{P}$ is annihilated at least once). Even so, a proof of global convergence is still missing. The Jacobi algorithm is structure-preserving and backward stable. The Jacobi algorithm is inherently parallel, since the solutions of the 2×2 or a 4×4 subproblems rely only on local information. But if one is not interested in high accuracy computation, then for large-scale computations, Jacobi's method is not regarded as competitive, not even for modern parallel computers [11].

Hence, in this section other structure-preserving algorithms for computing the eigenvalues of complex J -symmetric matrices are derived.

4.1 QR-like algorithm

The most popular way to compute the standard Schur form of a general matrix is the QR algorithm. It first transforms the given matrix into upper Hessenberg form and then iterates on that to converge towards the Schur form. It is tempting to derive a structured QR algorithm for transforming H_C iteratively into complex J -symmetric Schur form. In order to do so, we need a structured Hessenberg form. The most natural way to define this is the following: a complex J -symmetric matrix is in structured Hessenberg form if it is of the form

$$H_{hess} = \begin{bmatrix} F & G \\ E & -F^T \end{bmatrix} = \begin{bmatrix} \diagdown & \square \\ * & \diagdown \end{bmatrix}, \quad F, E, G = G^T \in \mathbb{C}^{n \times n},$$

where F is upper Hessenberg and $E = \alpha e_n e_n^T$. A matrix H_C is in structured Hessenberg form if and only if $\mathcal{P}H_C\mathcal{P}$ is in standard Hessenberg form for \mathcal{P} as in (9).

Assume that a complex symplectic and unitary matrix Q exists which transforms H_C into unreduced structured Hessenberg form $Q^H H_C Q$. Let $Q = [q_1 \dots q_n \ q_{n+1} \dots q_{2n}]$ with $q_{n+j} = J\bar{q}_j$. Given q_1 , it is straightforward to see from $H_C Q = Q H_{hess}$ that $H_C q_j = \sum_{k=1}^{j+1} f_{kj} q_k$, while from $Q^H H_C Q = H_{hess}$ we have for $i, j = 1, \dots, n$

$$(H_{hess})_{n+i,j} = e_{ij} = q_i^H J^T H_C q_j = q_i^H J^T \left(\sum_{k=1}^{j+1} h_{kj} q_k \right) = - \sum_{k=1}^{j+1} h_{kj} q_i^H J q_k.$$

For the structured Hessenberg form e_{ij} needs to be zero. As the complex symplecticity of Q only gives information about $q_i^T J q_j$, not about $q_i^H J q_j$, we can not argue that $e_{ij} = 0$ in general (only in the real case, we have $e_{ij} = 0$). Therefore, in general we can not construct a complex symplectic and unitary matrix Q which transforms H_C into a structured Hessenberg matrix. This cannot be used as a basis for a structured QR algorithm.

However, for any complex matrix $X \in \mathbb{C}^{2n \times 2n}$ there exists a unitary and complex symplectic transformation to a condensed form with more nonzero entries.

Theorem 6. *There exists a complex symplectic and unitary matrix Q which transforms*

any $X \in \mathbb{C}^{2n \times 2n}$ into the form

$$Q^H X Q = M = \begin{bmatrix} \diagdown & \square \\ M_{21} & \square \end{bmatrix},$$

where M_{21} is such that $m_{ji}^{21} = 0$ for $j = i + 3, \dots, n, i = 1, \dots, n - 1$. If $X = H_C$ is complex J -symmetric, then this reduces to

$$Q^H H_C Q = M = \begin{bmatrix} \diagdown & \square \\ M_{21} & \diagdown \end{bmatrix}, \quad (11)$$

where $M_{22} = -M_{11}^T$, $M_{12} = M_{12}^T$ and $M_{21} = M_{21}^T$. M_{21} is pentadiagonal, that is, $m_{ji}^{21} = m_{ij}^{21} = 0$ for $j = i + 3, \dots, n, i = 1, \dots, n - 1$.

Proof. Q can be constructed from a sequence of complex symplectic Householder transformations. First construct a complex symplectic Householder transformation H_1 such that it eliminates the entries $(3, 1), \dots, (n, 1)$ in X . The similarity transformation $X_1 = H_1 X H_1^H$ gives zero entries in X_1 in the positions $(3, 1), \dots, (n, 1)$. Next construct a complex symplectic Householder transformation H_2 such that it eliminates the entries $(n + 4, 1), \dots, (2n, 1)$ in X_1 . Perform the similarity transformation $X_2 = H_2 X_1 H_2^H$. This gives zero entries in X_2 in the positions $(n + 4, 1), \dots, (2n, 1)$. The already created zeros in the upper part of the first column are not destroyed. Now construct a complex symplectic Householder transformation H_3 such that it eliminates the entries $(4, 2), \dots, (n, 2)$ in X_2 , perform the similarity transformation $X_3 = H_3 X_2 H_3^H$, construct a complex symplectic Householder transformation H_4 such that it eliminates the entries $(n + 5, 2), \dots, (2n, 2)$ in X_3 . Perform the similarity transformation $X_4 = H_4 X_3 H_4^H$. This gives zero entries in X_4 in the positions $(4, 2), \dots, (n, 2)$ and $(n + 5, 2), \dots, (2n, 2)$. The already created zeros in the first column are not destroyed. Continue in this fashion. \square

The reduced form (11) may serve as the basis of a unitary complex symplectic QR-like algorithm for complex J -symmetric matrices. But the reduced form (11) will not be preserved in the iteration as products of the form

$$\begin{bmatrix} \diagdown & \square \\ 0 & \diagdown \end{bmatrix} \begin{bmatrix} \diagdown & \square \\ M_{12} & \diagdown \end{bmatrix} \begin{bmatrix} \diagdown & \square \\ 0 & \diagdown \end{bmatrix}$$

are in general not of the form (11). In each iteration step, the reduced form (11) is lost and would have to be restored. Even so all necessary computations are numerically stable, this seems to be no promising way to solve the eigenproblem for H_C due to a computational complexity of $\mathcal{O}((2n)^4)$.

A similar observation has been made for the symplectic case ($S^H J S = J$), see, e.g. [6, Theorem 4.7] and the discussion given there. Please note that the derivations presented there have no direct analogue here as they heavily depend on the relations $S^H J S = J$ and $S^H S = I$.

errors when working on a complex J -symmetric matrix will be forced by working just with the parameters. The complex symplectic SR iteration proceeds until the problem has completely decoupled into complex J -symmetric subproblems of size 2×2 or 4×4 . In a final step each of these subproblems has to be transformed into a form from which the eigenvalues can be read off.

Please note, that as S is complex symplectic, but not unitary, the complex symplectic SR algorithm is structure-preserving for complex J -symmetric eigenproblems, but not backward stable. The algorithm uses a sequence of unitary complex symplectic Givens- and Householder-like transformations matrices as well as some complex symplectic shears which are not unitary. But whenever a complex symplectic shear transformation has to be used, the complex symplectic shear among all possible ones with optimal (smallest possible) condition number is chosen.

In case a large and sparse complex J -symmetric eigenproblem is to be solved, the complex symplectic SR algorithm might not be the appropriate tool. Based on the complex symplectic SR algorithm and the complex J -symmetric J -Hessenberg form, a Lanczos-like algorithm can be derived which reduces a complex J -symmetric matrix H_C to complex symmetric J -Hessenberg form just like the symplectic Lanczos algorithm for (real) Hamiltonian matrices in, e.g., [1]. The algorithm projects the large, sparse $2n \times 2n$ complex J -symmetric matrix onto a small $2k \times 2k$ one from which approximations to a few extremal (or interior) eigenvalues can be obtained. Basically all comments given for the symplectic Lanczos algorithm for real Hamiltonian matrices hold here as well. Like any unsymmetric Lanczos algorithm, the complex symplectic Lanczos algorithm for complex J -symmetric matrices may break down; serious breakdown may occur. There is freedom in the choice of the parameters $\alpha_j, \beta_j, \gamma_j, \delta_j$ which may be used in order to construct a numerically safe algorithm.

A Krylov-Schur-type restart might be possible, analogous to the Hamiltonian case [2].

4.3 Embedding H_C into a real Hamiltonian matrix

A different approach is to embed H_C into a matrix of double size to make everything real and permute everything in order to collect the real and imaginary parts of A, C, D parts into joint blocks. Let

$$\begin{aligned} A &= A_R + \iota A_I, \\ C &= C_R + \iota C_I, \\ D &= D_R + \iota D_I \end{aligned}$$

with $A_R, A_I, C_R, C_I, D_R, D_I \in \mathbb{R}^{n \times n}$. As $C = C^T$ and $D = D^T$, it follows that

$$C_R = C_R^T, \quad C_I = C_I^T, \quad D_R = D_R^T, \quad D_I = D_I^T. \quad (13)$$

Then

$$H_C = \begin{bmatrix} A & C \\ D & -A^T \end{bmatrix} = \begin{bmatrix} A_R & C_R \\ D_R & -A_R^T \end{bmatrix} + \iota \begin{bmatrix} A_I & C_I \\ D_I & -A_I^T \end{bmatrix} = H_R + \iota H_I,$$

with Hamiltonian real and imaginary part $H_R \in \mathbb{R}^{2n \times 2n}$ and $H_I \in \mathbb{R}^{2n \times 2n}$,

$$(H_R J)^T = H_R J \quad \text{and} \quad (H_I J)^T = H_I J.$$

Let

$$Y = \frac{\sqrt{2}}{2} \begin{bmatrix} I & \imath I \\ I & -\imath I \end{bmatrix} \in \mathbb{C}^{4n \times 4n}$$

and

$$P = \begin{bmatrix} I & 0 & 0 & 0 \\ 0 & 0 & I & 0 \\ 0 & I & 0 & 0 \\ 0 & 0 & 0 & -I \end{bmatrix}.$$

Then $P^T P = P P^T = I$ and Y is unitary, that is, $Y^H Y = I = Y Y^H$.

It is straightforward that

$$\begin{aligned} P^T Y^H \begin{bmatrix} H_C & 0 \\ 0 & \overline{H_C} \end{bmatrix} Y P &= P^T \begin{bmatrix} H_R & -H_I \\ H_I & H_R \end{bmatrix} P \in \mathbb{R}^{4n \times 4n} \\ &= \left[\begin{array}{cc|cc} A_R & -A_I & C_R & C_I \\ A_I & A_R & C_I & -C_R \\ \hline D_R & -D_I & -A_R^T & -A_I^T \\ -D_I & -D_R & A_I^T & -A_R^T \end{array} \right] \\ &= \left[\begin{array}{c|c} \mathcal{A} & \mathcal{C} \\ \hline \mathcal{D} & -\mathcal{A}^T \end{array} \right] = \mathcal{H} \in \mathbb{R}^{4n \times 4n}. \end{aligned} \quad (14)$$

As $\mathcal{C} = \mathcal{C}^T$ and $\mathcal{D} = \mathcal{D}^T$, \mathcal{H} is Hamiltonian.

Clearly, the spectrum $\sigma(\mathcal{H})$ of \mathcal{H} is the union of the spectrum of H_C and the one of $\overline{H_C}$,

$$\sigma(\mathcal{H}) = \sigma(H_C) \cup \sigma(\overline{H_C}).$$

The structured Jordan form of \mathcal{H} can be inferred from that of H_C (8). Hence, the nonzero eigenvalues of \mathcal{H} come in quadruples $(\lambda, -\lambda, \bar{\lambda}, -\bar{\lambda})$. In particular, the real and purely imaginary eigenvalues of \mathcal{H} have even multiplicity.

When solving the eigenproblem for H_C by solving the eigenproblem for \mathcal{H} , eigenvalues of H_C can be deduced from those of \mathcal{H} , but eigenvectors can not. They have to be determined using inverse iteration. Moreover, one has to decide which of the computed eigenvalues are eigenvalues of H_C . For real and purely imaginary eigenvalues of \mathcal{H} , this is straightforward. They appear in quadruples $(\lambda, -\lambda, \bar{\lambda}, -\bar{\lambda})$, that is we have for real λ

$$(\lambda, -\lambda, \bar{\lambda}, -\bar{\lambda}) = (\text{Re}(\lambda), -\text{Re}(\lambda), \text{Re}(\lambda), -\text{Re}(\lambda))$$

and similar for purely imaginary λ

$$(\lambda, -\lambda, \bar{\lambda}, -\bar{\lambda}) = (\text{Im}(\lambda), -\text{Im}(\lambda), \text{Im}(\lambda), -\text{Im}(\lambda)).$$

As the eigenvalues of H_C appear in pairs, each real and purely eigenvalue quadruple of \mathcal{H} gives an eigenvalue pair $(\lambda, -\lambda)$ of H_C . For complex eigenvalues of \mathcal{H} there is no obvious

way to determine whether $(\lambda, -\lambda)$ or whether $(\bar{\lambda}, -\bar{\lambda})$ is the corresponding eigenpair of H_C . This needs to be tested, e.g., using inverse iteration.

The eigenproblem for \mathcal{H} can be solved by the numerically stable, structure preserving method for computing the eigenvalues of real Hamiltonian matrices proposed in [4] (or any other method proposed for the Hamiltonian eigenproblem).

The additional explicit structure in H_{BS} (1) can not be made use of in any of the ideas discussed above. E.g., the Hamiltonian matrix (14) has additional structure

$$\mathcal{H} = \left[\begin{array}{c|c} \mathcal{A} & -\mathcal{D} \\ \hline \mathcal{D} & -\mathcal{A}^T \end{array} \right], \quad \mathcal{D} = \mathcal{D}^T, \mathcal{A} = \mathcal{A}^T$$

which is so far of no use.

5 Conclusions

Structure-preserving algorithms for the complex J -symmetric eigenproblem have been discussed. When choosing an algorithm for a specific problem at hand one should take the following into account.

- The Jacobi-like algorithm [16] is backward stable and inherently parallelizable. Asymptotic quadratic convergence has been proven, but a global convergence proof is missing. In case of convergence, the iterates converge towards the complex J -symmetric Schur form (7).
- A backward stable QR-like algorithm based on the complex symplectic unitary QR decomposition as given in Theorem 2 can be derived, but there seems to be no suitable Hessenberg-like form to decrease the computational complexity $\mathcal{O}((2n)^4)$.
- The complex symplectic SR algorithm based on the complex symplectic SR decomposition as given in Theorem 3 is structure-preserving, but not backward stable. When using the reduction to complex J -symmetric J -Hessenberg form (12) as a first step of the algorithm, the complex-symplectic SR algorithm can be implemented such that only $\mathcal{O}(n)$ flops per iteration steps are required. The iteration proceeds until the problem has completely decoupled into complex J -symmetric subproblems of size 2×2 or 4×4 .
- A complex symplectic Lanczos algorithm suitable for large sparse complex J -symmetric eigenproblems can be devised based on the complex symplectic SR algorithm. (Serious) breakdown may occur.
- Any complex J -symmetric matrix H_C can be embedded into a real Hamiltonian matrix \mathcal{H} of double size. The real Hamiltonian eigenproblem can be solved by the numerically stable, structure-preserving method [4]. Eigenvalues of H_C can be deduced from those of \mathcal{H} , eigenvectors have to be determined via inverse iteration.

References

- [1] P. Benner and H. Faßbender. An implicitly restarted symplectic Lanczos method for the Hamiltonian eigenvalue problem. *Linear Algebra Appl.*, 263:75–111, 1997.
- [2] P. Benner, H. Faßbender, and M. Stoll. Hamiltonian Krylov-Schur-type method based on the symplectic Lanczos method. *Linear Algebra Appl.*, 435:578–600, 2011.
- [3] P. Benner, V. Mehrmann, and H. Xu. A new method for computing the stable invariant subspace of a real Hamiltonian matrix. *J. Comput. Appl. Math.*, 86(1):17–43, 1997.
- [4] P. Benner, V. Mehrmann, and H. Xu. A numerically stable, structure preserving method for computing the eigenvalues of real Hamiltonian or symplectic pencils. *Numer. Math.*, 78(3):329–358, 1998.
- [5] P. Benner, V. Mehrmann, and H. Xu. A note on the numerical solution of complex Hamiltonian and skew-Hamiltonian eigenvalue problems. *Electron. Trans. Numer. Anal. (ETNA)*, 8:115–126, 1999.
- [6] A. Bunse-Gerstner. Matrix factorizations for symplectic QR-like methods. *Linear Algebra Appl.*, 83:49–77, 1986.
- [7] A. Bunse-Gerstner, R. Byers, and V. Mehrmann. A chart of numerical methods for structured eigenvalue problems. *SIAM J. Matrix Anal. Appl.*, 13(2):419–453, 1992.
- [8] A. Bunse-Gerstner and H. Faßbender. Breaking Van Loan’s curse: A quest for structure-preserving algorithms for dense structured eigenvalue problems. In Peter Benner, Matthias Bollhöfer, Daniel Kressner, Christian Mehl, and Tatjana Stykel, editors, *Numerical Algebra, Matrix Theory, Differential-Algebraic Equations and Control Theory*, pages 3–23. Springer International Publishing, 2015.
- [9] A. Bunse-Gerstner and V. Mehrmann. A symplectic QR-like algorithm for the solution of the real algebraic Riccati equation. *IEEE Trans. Automat. Control*, AC-31:1104–1113, 1986.
- [10] H. Faßbender. The parameterized SR algorithm for Hamiltonian matrices. *Electron. Trans. Numer. Anal. (ETNA)*, 26:121–145, 2007.
- [11] Gene H. Golub and Henk A. van der Vorst. Eigenvalue computation in the 20th century. *J. Comput. Appl. Math.*, 123:35–65, 2000.
- [12] G.H. Golub and C.F. Van Loan. *Matrix Computations*. Johns Hopkins University Press, Baltimore, MD, USA, fourth edition, 2013.
- [13] D.S. Mackey, N. Mackey, and F. Tisseur. Structured tools for structured matrices. *Electronic Journal of Linear Algebra (ELA)*, 10:106–145, 2003.

- [14] D.S. Mackey, N. Mackey, and F. Tisseur. Structured factorizations on scalar product spaces. *SIAM J. Matrix Anal. Appl.*, 27(3):821–850, 2006.
- [15] C. Mehl. On classification of normal matrices in indefinite inner product spaces. *Electronic Journal of Linear Algebra (ELA)*, 15:84–106, 2006.
- [16] C. Mehl. On asymptotic convergence of nonsymmetric Jacobi algorithms. *SIAM J. Matrix Anal. Appl.*, 30:291–311, 2008.
- [17] E. Ribolini, J. Toulouse, and A. Savin. Electronic excitation energies of molecular systems from the Bethe-Salpeter equation: Example of H_2 molecule. In S. Ghosh and P. Chattaraj, editors, *Concepts and Methods in Modern Theoretical Chemistry*, volume 1: Electronic Structure and Reactivity, page 367. 2013.
- [18] E. Ribolini, J. Toulouse, and A. Savin. Electronic excitations from a linear-response range-separated hybrid scheme. *Molecular Physics*, 111:1219, 2013.
- [19] M Shao, F. H. da Jornada, C. Yang, J. Deslippe, and S. G. Louie. Structure preserving parallel algorithms for solving the Bethe-Salpeter eigenvalue problem. *submitted to Linear Algebra Appl.*, 2015.

