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Some remarks on the complex J-symmetric eigenproblem

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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 [21] 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.

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1. Introduction

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

$H_C \in \mathbb{C}^{2n\times 2n}$	complex 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., [11,18,19]. Here $J = \left[\begin{smallmatrix} 0 & I \\ -I & 0 \end{smallmatrix}\right]$ 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, H is complex 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 [19]: 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 $\left[\begin{smallmatrix} A & C \\ D & -A^T \end{smallmatrix}\right]$ 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 $\left[\begin{smallmatrix} A & C \\ D & -A^H \end{smallmatrix}\right]$ 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 [22,23] for determining electronic excitation energies. Solving the Bethe–Salpeter equations numerically, the eigenvalue problem $H_{BS}x = \lambda x$ for complex matrices

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

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

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

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 $(\lambda, -\lambda, \overline{\lambda}, -\overline{\lambda})$. Moreover, for $\lambda \in \mathbb{C}$, $H_{BS}x = \lambda x$ implies $H_{BS}K\overline{x} = -\overline{\lambda}K\overline{x}$ and $H_{BS}y = -\lambda y$ implies $H_{BS}K\overline{y} = \overline{\lambda}K\overline{y}$ with*