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A structure-preserving method for solving the complex $\top$-Hamiltonian eigenvalue problem

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In this work, we present a new structure-preserving method to compute the structured Schur form of a dense complex $\top$-Hamiltonian matrix $\mathscr{H}$ of moderate size. Origination of the complex $\top$-Hamiltonian eigenvalue problem outside the control theory is briefly discussed. Specifically, our method consists of three main stages. At the first stage, we compute eigenvalues of $\mathscr{H}$ using the $\top$-symplectic URV-decomposition of complex $\mathscr{H}$ followed up with the complex periodic QR algorithm to thoroughly respect the $(\lambda, -\lambda)$ pairing of eigenvalues. At the second stage, we construct the $\top$-isotropic invariance subspace of $\mathscr{H}$ from suitable linear combination of columns of U and V matrices from the first stage. At the third stage, we find a $\top$-symplectic-orthogonal basis of this invariance subspace, which immediately provides the structured Schur form of $\mathscr{H}$. Several numerical results are presented to demonstrate the effectiveness and accuracy of our method.

Keywords and phrases: Complex $\top$-Hamiltonian eigenvalue problem, $\top$-symplectic URV-decomposition, complex periodic QR algorithm, complex $\top$-Hamiltonian Schur form.

1. Introduction

In this paper, we consider solving in a structure-preserving manner the following structured eigenvalue problem

$$\mathscr{H}\mathbf{x} \equiv \begin{bmatrix} A & G \\ F & -A^\top \end{bmatrix} \begin{bmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{bmatrix} = \lambda \begin{bmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{bmatrix}, \tag{1}$$

where $A \in \mathbb{C}^{n\times n}, G = G^\top \in \mathbb{C}^{n\times n}$ and $F = F^\top \in \mathbb{C}^{n\times n}$ with a moderate n. Here, $A^\top$ denotes the transpose of A. In addition, $\bar{A}$ and A^* denote the complex conjugate and conjugate transpose of A, respectively. The matrix $\mathscr{H}$ in (1) acquires the $\top$-Hamiltonian structure which will be more clear

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below, hence, the standard eigenvalue problem (1) is called the complex $\top$-Hamiltonian eigenvalue problem ($\top$HEP). Hereafter, we directly call (1) with $\mathscr{H} \in \mathbb{R}^{2n\times 2n}$ the real HEP, and simply call (1) with $\mathscr{H} \in \mathbb{C}^{2n\times 2n}$ the $\top$HEP, if no confusion occurs.

The $\top$HEP does have some important physical originations. For example, as noted in [19], the block structure of $\mathscr{H}$ is common to a variety of quantum chemistry theories with distinct response functions, and provides a united framework to formulate the response theory which describes molecules which are either isolated or embedded in a polarizable environment. In regard to the response of isolated molecules, the recognition of the Hamiltonian structure with additional block structure $A = A^*$ and $F = -\bar{G}$ in some linear response theory has been documented as early as in 1980s [22], and is studied in [1, 8, 9, 16, 24]. On the other hand, in the non-variational coupled cluster theory [19], which describes the response of molecules embedded in the polarizable environment, the set of coupled response equations lead to a $\top$HEP as shown in (1), where $A, -F$ and G in $\mathscr{H}$ have clear physical meaning. The pairing property of eigenvalues of $\mathscr{H}$ discussed below has also been noticed by some quantum chemists.

To facilitate the discussion of the specific structures of (1), we lay out the following definitions:

- $\mathcal{J}_{2n} := \begin{bmatrix} 0 & I_n \\ -I_n & 0 \end{bmatrix}$, where I_n is the identity matrix of size $n \times n$.
- $\mathcal{U} \in \mathbb{C}^{2n\times 2n}$ is called $\top$-symplectic if $\mathcal{U}^\top \mathcal{J}_{2n}\mathcal{U} = \mathcal{J}_{2n}$. We denote the set of unitary $\top$-symplectic matrices in $\mathbb{C}^{2n\times 2n}$ by $\mathbb{U}\top\mathbb{S}_{2n} := \{\mathcal{U} \in \mathbb{C}^{2n\times 2n} | \mathcal{U}^*\mathcal{U} = I_{2n}, \mathcal{U}^\top \mathcal{J}_{2n}\mathcal{U} = \mathcal{J}_{2n}\}$.
- $\mathcal{H} \in \mathbb{C}^{2n\times 2n}$ is called $\top$-Hamiltonian or $\top$-skew-Hamiltonian if $(\mathcal{H}\mathcal{J}_{2n})^\top = \mathcal{H}\mathcal{J}_{2n}$ or $(\mathcal{H}\mathcal{J}_{2n})^\top = -\mathcal{H}\mathcal{J}_{2n}$, respectively.
- A subspace $X \in \mathbb{C}^{2n\times m}$ with $1 \le m \le n$ is called $\top$-isotropic if $X^\top \mathcal{J}_{2n} X = 0$, and it is called a $\top$-Lagrangian subspace if it is $\top$-isotropic and $m = n$.

Moreover, it is rather easy to verify the following results, just by applying the definitions above.

Proposition 1.

- A $\top$-Hamiltonian matrix has the block form $\begin{bmatrix} A & G \\ F & -A^\top \end{bmatrix}$, where $A \in \mathbb{C}^{2n\times 2n}$, $F = F^\top \in \mathbb{C}^{2n\times 2n}$ and $G = G^\top \in \mathbb{C}^{2n\times 2n}$. Eigenvalues of a $\top$-Hamiltonian matrix always occur in pairs $(\lambda, -\lambda)$.

- A ⊤-skew-Hamiltonian matrix has the block form $\begin{bmatrix} A & G \\ F & A^\top \end{bmatrix}$, where $A \in \mathbb{C}^{2n\times 2n}$, $F = -F^\top \in \mathbb{C}^{2n\times 2n}$ and $G = -G^\top \in \mathbb{C}^{2n\times 2n}$. The eigenvalue of a ⊤-skew-Hamiltonian matrix always has even multiplicity.
- Any $U \in \mathbb{U}\top\mathbb{S}_{2n}$ can be partitioned as $\begin{bmatrix} U_1 & U_2 \\ -\overline{U}_2 & \overline{U}_1 \end{bmatrix}$, with $U_1, U_2 \in \mathbb{C}^{n\times n}$.

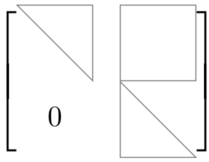
In addition, the ⊤HEP with $A = A^*$ and $F = -\bar{G}$ has more structures, which are exploited in [1, 8, 9, 16, 24]. However, it is unclear to us how the published techniques and computational methods for this special ⊤HEP can be conveniently adopted for solving the ⊤HEP (1) with $A \neq A^*$ and $F \neq -\bar{G}$.

In [2], the ⊤HEP, which is called complex J-symmetric eigenvalue problem there, is considered to some depth, and one of the foremost contributions is that the existence of the structured Jordan form and complex ⊤-Hamiltonian Schur form of $\mathscr{H}$ are proved rigorously for the first time in some sense. Moreover, three structure-preserving methods have been proposed for the ⊤HEP (1)—the QR-like algorithm, SR-like algorithm and embedding complex $\mathscr{H}$ into a real Hamiltonian matrix, with the emphasis put on the second algorithm, *i.e.*, the structure-preserving SR-like algorithm and the resulting complex ⊤-symplectic Lanczos algorithm for the small dense $\mathscr{H}$ and large sparse $\mathscr{H}$, respectively. Besides, the main features of these three algorithms are also summarized there. Specifically, the complexity of the first method is as high as $\mathcal{O}(n^4)$ for $\mathscr{H}$ of size $n \times n$, which is quite expensive, while the complexity of the latter two methods is $\mathcal{O}(n^3)$ or less. However, the second one is not backward stable. The third one is numerically stable but relies on the inverse iteration, which could be relatively expensive, to pick out the correct eigenvalues.

In this work, we will propose an alternative algorithm to solve the ⊤HEP (1) which is of $\mathcal{O}(n^3)$ complexity, structure-preserving, numerically stable, and free of deficiencies as just mentioned. In a nutshell, our method amounts to computing the complex ⊤-Hamiltonian Schur form of $\mathscr{H}$. The complex ⊤-Hamiltonian Schur form (2) is pivotal to the ⊤HEP (1). Once the ⊤-Hamiltonian Schur form is available, all eigenvalues of $\mathscr{H}$ are automatically known, and more importantly, it is routine to retrieve eigenvectors of $\mathscr{H}$. Therefore, it is our main task in this paper to compute the complex ⊤-Hamiltonian Schur form (2). Furthermore, we note that the complex ⊤-Hamiltonian Schur form always exists for any complex ⊤-Hamiltonian $\mathscr{H}$ in (1). This fact is guaranteed by Theorem 1 [2] below.

Theorem 1. [2] For any complex $\top$-Hamiltonian matrix $\mathscr{H}$, there always exists such $Q \in \mathbb{U}\top\mathbb{S}_{2n}$ that

$$(2) \qquad Q^*\mathscr{H}Q = \begin{bmatrix} R & C \\ 0 & -R^\top \end{bmatrix} =$$



$$, \qquad C = C^\top, R \in \mathbb{C}^{n\times n}.$$

In contrast to Theorem 1, the real Hamiltonian Schur form does NOT always exist for a real Hamiltonian matrix [7]. In some cases, only the *partial* real Hamiltonian Schur form can be computed by some sophisticated method [21].

Hereafter, for convenience, we directly call (2) the $\top$-Hamiltonian Schur form. We make the following contributions in this paper on solving the dense $\top$HEP:

- We establish a stable structure-preserving method to compute all eigenvalues of the $\top$HEP, without embedding the complex $\mathscr{H}$ into a real Hamiltonian matrix of the double size. Hence, we are free from filtering away the spurious eigenvalues.
- We provide a different perspective of how to construct the $\top$-isotropic invariant subspace of $\mathscr{H}$. This perspective in combination of some procedure to determine the orthogonal basis of the $\top$-isotropic invariant subspace leads to an efficient method to compute the $\top$-Hamiltonian Schur form (2), which is of $\mathcal{O}(n^3)$ complexity, and easy to understand and implement, though it is not strongly backwards stable for $\mathscr{H}$. We also show how this perspective helps us to understand the method developed in [11].

The rest of this paper is organized as follows. In Sec. 2, we give a brief overview of the structure-preserving algorithms to solve the *real* HEP. In Sec. 3, we discuss the stable and structure preserving algorithm to calculate all eigenvalues of the $\top$HEP. In Sec. 4, we propose a simple and efficient algorithm to compute the $\top$-Hamiltonian Schur form, and we also address the connection between our method and other related works.

Notations. The set $\mathbb{C}_+ := \{z \in \mathbb{C} | \Re(z) > 0\} \cup \{z \in \imath\mathbb{R} | \Im(z) > 0\}$ with $\imath = \sqrt{-1}$ denotes all complex numbers lying in the right open half plane or on the positive imaginary axis. For $x \in \mathbb{C}$, we define the `sign` function by

$$\mathtt{sign}(x) = \begin{cases} x/|x| & \text{if} \quad x \neq 0, \\ 1 & \text{if} \quad x = 0. \end{cases}$$

ε is the machine precision $2^{-64} \approx 2.22 \times 10^{-16}$. $A \oplus B$ denotes the direct sum of matrices A and B. $\|\cdot\|_F$ denotes the Frobenius norm of a vector or a matrix. $\mathbf{e}_j := I_n(:, j)$ denotes the j-th column of the identity matrix of size n-by-n, where n can be known from the context.

2. Overview of the algorithm for the real HEP

The Hamiltonian structure and its properties are widely known within the control theory [13, 14], particularly because of the intimate relation between the stable invariant subspace of the *real* $\mathscr{H}$ and the stabilizing solution to some quadratic matrix equation of great importance [14]. In passing, in control theory, eigenvalues of $\mathscr{H}$ with negative real part are called stable eigenvalues, and the corresponding invariant subspace is called the stable invariant subspace of $\mathscr{H}$.

For the past several decades, solving the real HEP has been studied extensively from the numerical linear algebra perspective, *e.g.*, [4, 5, 7, 15, 17, 18, 23, 25] amongst other seminal works. In particular, Van Loan [25] has first established the square-reduced method, which simply means that the eigenvalues of $\mathscr{H}$ are obtained by taking the square root of those of $\mathscr{H}^2$, on the basis of the structure-preserving algorithm to compute the skew-Hamiltonian Schur form [23] of $\mathscr{H}^2$. However, this simple idea suffers from a possible loss of accuracy of $\sqrt{\varepsilon}$ for tiny eigenvalues of $\mathscr{H}$. The Van Loan's curse [23], which is an open question related to the derivation of a numerically strongly backward stable method of $\mathcal{O}(n^3)$ scaling to compute the real Hamiltonian Schur form of a real Hamiltonian matrix, has plagued the researchers for a long time. A breakthrough along this direction is made in [4, 5].

Briefly speaking, the breakthrough consists in utilizing the symplectic URV-decomposition of $\mathscr{H}$ and the relationship between the invariant subspaces of a real Hamiltonian matrix $\mathscr{H}$ and the extended matrix $\left[\begin{smallmatrix} 0 & \mathscr{H} \\ \mathscr{H} & 0 \end{smallmatrix}\right]$, which can be seen as the implicit version of the square-reduced method without the loss of accuracy due to explicit squaring of the matrix. The accompanying algorithm, which we call the BMX algorithm, can compute eigenvalues of $\mathscr{H}$ in a structure-preserving manner, and compute the stable invariant subspace of $\mathscr{H}$ satisfactorily if $\mathscr{H}$ has no eigenvalues near the imaginary axis.

Furthermore, the long-standing Van Loan's curse has finally been resolved in a more recent work [7]. With the assumption that the real Hamiltonian matrix has no purely imaginary eigenvalues, authors of [7] have shown step by step that the real Hamiltonian Schur form of the real Hamiltonian matrix can indeed be computed in a numerically strongly backward stable way in $\mathcal{O}(n^3)$ flops. To have a completely different insight into why the new method in [7] works even if the real Hamiltonian matrix has eigenvalues near the imaginary axis, we refer the reader to [26]. The block version of this method has also been developed in [21], which shares the same insight with [26] and allows $\mathscr{H}$ to have tightly clustered groups of eigenvalues and purely imaginary eigenvalues. This block algorithm arguably represents the state-of-the-art method to solve the real HEP.

3. A stable algorithm to solve the eigenvalues of the ⊤HEP

In this section, closely following the BMX algorithm, we present the structure-preserving method to compute all eigenvalues of the complex ⊤-Hamiltonian matrix $\mathscr{H}$, before the ⊤-Hamiltonian Schur form (2) of $\mathscr{H}$ is actually computed.

3.1. The ⊤-symplectic URV decomposition

First of all, our method rests essentially on the following basic fact.

Theorem 2. For any $W \in \mathbb{C}^{2n\times 2n}$, there exist matrices $U, V \in \mathbb{U}\top\mathbb{S}_{2n}$ such that

$$U^*WV = \begin{bmatrix} R_1 & R_3 \\ 0 & R_2 \end{bmatrix}, \tag{3}$$

where $R_1 \in \mathbb{C}^{n\times n}$ is upper triangular and $R_2 \in \mathbb{C}^{n\times n}$ is lower Hessenberg and $R_3 \in \mathbb{C}^{n\times n}$ is a general matrix.

The proof of this theorem is constructive. That is, we will propose an algorithm to reduce a general complex matrix of even dimension into a form on the right hand side of (3). To this end, extensive use will be made of two types of elementary unitary complex ⊤-symplectic matrices [23]: the complex ⊤-symplectic Givens matrices and complex ⊤-symplectic Householder matrices.

Specifically, given $\mathbf{v} \in \mathbb{C}^{2n}$ and $j \in \mathbb{N}$ with $1 \le j \le n$, the complex ⊤-symplectic Givens matrix has a special form

$$G_j(c,s) = \begin{bmatrix} C_j(c) & S_j(s) \\ -\overline{S_j(s)} & \overline{C_j(c)} \end{bmatrix} \in \mathbb{C}^{2n\times 2n} \tag{4}$$

with

$$C_j(c) = I_n + (c-1)\mathbf{e}_j\mathbf{e}_j^\top, \quad S_j(s) = s\mathbf{e}_j\mathbf{e}_j^\top, \tag{5a}$$

and $\left[\begin{smallmatrix} c & s \\ -\bar{s} & c \end{smallmatrix}\right]$ being a Givens rotation such that

$$\begin{bmatrix} c & s \\ -\bar{s} & c \end{bmatrix} \begin{bmatrix} v_j \\ v_{n+j} \end{bmatrix} = \begin{bmatrix} \mathtt{sign}(v_j)\sqrt{|v_j|^2 + |v_{n+j}|^2} \\ 0 \end{bmatrix}. \tag{5b}$$

That is to say,

$$(c,s) = \begin{cases} (1,0) & \text{if} \quad v_j = 0 = v_{n+j}, \\ \left(\frac{|v_j|}{\sqrt{|v_j|^2+|v_{n+j}|^2}}, \frac{\mathtt{sign}(v_j)\overline{v_{n+j}}}{\sqrt{|v_j|^2+|v_{n+j}|^2}}\right) & \text{otherwise.} \end{cases} \tag{5c}$$

The complex ⊤-symplectic Householder matrices is a direct sum of two n-by-n Householder matrices,

$$H_j(\mathbf{u}) \oplus \overline{H_j(\mathbf{u})} := \left(I_n - \frac{2}{\|\mathbf{u}\|^2}\mathbf{u}\mathbf{u}^*\right) \oplus \left(I_n - \frac{2}{\|\mathbf{u}\|^2}\bar{\mathbf{u}}\mathbf{u}^\top\right), \tag{6}$$

where $\mathbf{u}$ is a complex vector of length n with its first $j-1$ entries vanishing. As is known, the Householder matrix is widely used to zero out last several entries of a vector. Here, given $\mathbf{x} \in \mathbb{C}^n$ and $j \in \mathbb{N}$ with $1 \leq j \leq n$, if the vector $\mathbf{u}$ in (6) is specified by its entries as follows

$$u_k = \begin{cases} 0 & \text{if} \quad 1 \leq k \leq j-1, \\ x_k + \|x(j\!:\!n)\|\mathtt{sign}(x_k) & \text{if} \quad k = j, \\ x_k & \text{if} \quad j < k \leq n, \end{cases} \tag{7}$$

then the Householder matrix $H_j(\mathbf{u})$ defined in (6) can zero out last $n-j$ entries of $\mathbf{x}$, as one can verify that

$$H_j(\mathbf{u})^*\mathbf{x} = [x_1, \cdots, x_{j-1}, -\|x(j\!:\!n)\|\mathtt{sign}(x_k), 0, \cdots, 0]^\top. \tag{8}$$

In addition, please note that the Hermiticity of the complex Householder matrix is not essential. Other variants of the complex Householder matrix can achieve the similar goal as (8) does.

Moreover, to simplify the notation, for a given $\mathbf{x} \in \mathbb{C}^{2n}$ and $j \in \mathbb{N}$, we define

$$E_j(\mathbf{x}) \equiv (H_j(\mathbf{w})^* \oplus H_j(\mathbf{w})^\top)G_j(c,s)(H_j(\mathbf{u})^* \oplus H_j(\mathbf{u})^\top), \tag{9}$$

Algorithm 1 Elementary eliminators

Input: $\mathbf{x} \in \mathbb{C}^{2n}$ and $j \in \mathbb{N}$ with $j \leq n$.
Output: $\mathbf{u}, \mathbf{w} \in \mathbb{C}^n$ and $c, s \in \mathbb{C}$ and the updated $\mathbf{x} \in \mathbb{C}^{2n}$.

Determine $\mathbf{u} \in \mathbb{C}^n$ and $H_j(\mathbf{u})$ such that the last $n-j$ entries of $\mathbf{x} \leftarrow (H_j(\mathbf{u})^* \oplus H_j(\mathbf{u})^\top)\mathbf{x}$ are zero, according to (7) and (8).
Determine c and s from the j-th and $(n+j)$-th entries of $\mathbf{x}$ according to (5b) and (5c). Update $\mathbf{x} \leftarrow G_j(c,s)\mathbf{x}$.
Determine $\mathbf{w} \in \mathbb{C}^n$ and $H_j(\mathbf{w})$ such that the $(j+1)$-th to the n-th entries of $\mathbf{x} \leftarrow (H_j(\mathbf{w})^* \oplus H_j(\mathbf{w})^\top)\mathbf{x}$ are zero, according to (7) and (8).

where $H_j(\mathbf{u}), H_j(\mathbf{w})$ and $G_j(c,s)$ are computed via Algorithm 1, and

$$E_{n+j}(\mathbf{x}) \equiv \begin{bmatrix} 0 & I_n \\ I_n & 0 \end{bmatrix} E_j\left(\mathbf{x}([n+1:2n, 1:n])\right) \begin{bmatrix} 0 & I_n \\ I_n & 0 \end{bmatrix}. \tag{10}$$

On the basis of Algorithm 1, we propose Algorithm 2 to construct the complex $\top$-symplectic URV-decomposition (3) of a general complex matrix. In particular, if W in (3) is complex $\top$-Hamiltonian, then a simple calculation yields

$$U^* W^2 U = \begin{bmatrix} -R_1 R_2^\top & R_1 R_3^\top - R_3 R_1^\top \\ 0 & -R_2 R_1^\top \end{bmatrix}, \tag{11}$$

which means that eigenvalues of W are square roots of those of the Hessenberg matrix $-R_1 R_2^\top$ or $-R_2 R_1^\top$.

Algorithm 2 Complex $\top$-symplectic URV decomposition

Input: A general matrix $W \in \mathbb{C}^{n \times n}$.
Output: Unitary $\top$-symplectic matrices $U, V \in \mathbb{U}\top\mathbb{S}_{2n}$ and $U^* W V$ of the form (3).

```
U ← I_{2n} and V ← I_{2n}.
for j = 1 : n do
    Set v = W e_j.
    Compute E_j(v) using (9) and Algorithm 1.
    Update W ← E_j(v) W and U ← U E_j(v)^*.
    if j < n then
        Set u ← W^⊤ e_{n+j}.
        Compute E_{n+j+1}(u) using (10) and Algorithm 1.
        Update W ← W E_{n+j+1}(u)^⊤ and V ← V E_{n+j+1}(u)^⊤.
    end if
end for
```

3.2. The complex periodic QR algorithm

Recall that, although the singular values of A are square root of eigenvalues of AA^* or A^*A by definition, it is inadvisable to carry out the explicit matrix multiplication in practical calculations, due to the loss of accuracy of $\sqrt{\varepsilon}$ for small singular values. More generally, the same rule holds for the product eigenvalue problem, in which the matrix is given as the product of several matrices, *e.g.*, $-R_2^\top R_1$ in (11). In this case, the periodic QR algorithm [6, 12] is the first choice. In a word, the complex periodic QR algorithm computes two unitary matrices Z_1 and Z_2 such that $Z_1^* A Z_2$ and $Z_2^* B Z_1$ are both upper triangular matrices.

Specifically, since the matrix factors R_1 and $R_2^\top$ are already in the upper triangular and upper Hessenberg form, respectively, we can directly perform implicit QR steps by 'bulge-chasing' [6, 12], which is the key of the periodic QR algorithm. Here, we only briefly describe one iteration of the 'bulge-chasing' for $AB \in \mathbb{C}^{n\times n}$ in Algorithm 3, which bears a strong resemblance with the single-shift complex QZ algorithm for a complex generalized eigenvalue problem.

After running several iterations of Algorithm 3, some subdiagonal entry $A(k+1,k)$ of the Hessenberg matrix A will be regarded as zero if it satisfies

$$|A(k+1,k)| \le \varepsilon(|A(k,k)| + |A(k+1,k+1)|). \tag{12}$$

Then eigenvalues of the original product AB become the union of those of two or more uncoupled matrix products of smaller sizes, as illustrated in the following

$$AB = \begin{bmatrix} A_1 & * \\ 0 & A_2 \end{bmatrix} \begin{bmatrix} B_1 & * \\ 0 & B_2 \end{bmatrix} = \begin{bmatrix} A_1B_1 & * \\ 0 & A_2B_2 \end{bmatrix}. \tag{13}$$

Hence Algorithm 3 will be applied to A_1B_1 and A_2B_2 separately. This procedure is repeated until A is reduced to the upper triangular form while B remains upper triangular.

It could happen that one or more diagonal entries of the upper triangular matrix B become negligibly small after running Algorithm 3 several times. With regard to this, authors of [3] suggest that a diagonal entry $B(k,k)$ of B can be set to zero if it satisfies

$$|B(k,k)| \le \varepsilon(|B(k-1,k)| + |B(k,k+1)|). \tag{14}$$

Once $B(k,k) = 0$, one eigenvalue of AB directly becomes zero, and by virtue of the deflation method discussed in [6], the rest eigenvalues of AB

Algorithm 3 One iteration of the complex periodic QR algorithm [3]

Input: An upper Hessenberg matrix $A \in \mathbb{C}^{n\times n}$ and an upper triangular matrix $B \in \mathbb{C}^{n\times n}$ with $n \geq 2$.

Output: Unitary matrices Z_1, Z_2; the upper Hessenberg matrix $Z_1^* A Z_2 \in \mathbb{C}^{n\times n}$ and the upper triangular matrix $Z_2^* B Z_1 \in \mathbb{C}^{n\times n}$.

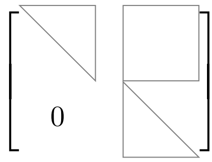
Set $Z_1 \leftarrow I_n$ and $Z_2 \leftarrow I_n$.
Compute shifts σ_1 as the eigenvalue of the 2-by-2 bottom right submatrix of AB which is more close to the last entry of AB.
Set $\mathbf{v} \leftarrow (AB - \sigma I_n)\mathbf{e}_1$.
Determine the Givens rotation $K = \left[\begin{smallmatrix} c & s \\ -\bar{s} & c \end{smallmatrix}\right]$ from $v(1)$ and $v(2)$ according to (5b) and (5c).
Update $A(1{:}2,:) \leftarrow KA(1{:}2,:)$, $B(:,1{:}2) \leftarrow B(:,1{:}2)K^*$ and $Z_1(:,1{:}2) \leftarrow Z_1(:,1{:}2)K^*$.
Set $\mathbf{u} \leftarrow B(1{:}2,1)$.
Determine the Givens rotation $K = \left[\begin{smallmatrix} c & s \\ -\bar{s} & c \end{smallmatrix}\right]$ from $u(1)$ and $u(2)$ according to (5b) and (5c).
Update $A(:,1{:}2) \leftarrow A(:,1{:}2)K^*$, $B(1{:}2,:) \leftarrow KB(1{:}2,:)$ and $Z_2(:,1{:}2) \leftarrow Z_2(:,1{:}2)K^*$.
for $j = 2 : n-1$ **do**
    Set $\mathbf{v} \leftarrow A(j{:}j+1, j-1)$.
    Determine the Givens rotation $K = \left[\begin{smallmatrix} c & s \\ -\bar{s} & c \end{smallmatrix}\right]$ from $v(1)$ and $v(2)$ according to (5b) and (5c).
    Update $A(j{:}j+1,:) \leftarrow KA(j{:}j+1,:)$, $B(:,j{:}j+1) \leftarrow B(:,j{:}j+1)K^*$ and $Z_1(:,j{:}j+1) \leftarrow Z_1(:,j{:}j+1)K^*$.
    Set $\mathbf{u} \leftarrow B(j{:}j+1, j)$.
    Determine the Givens rotation $K = \left[\begin{smallmatrix} c & s \\ -\bar{s} & c \end{smallmatrix}\right]$ from $u(1)$ and $u(2)$ according to (5b) and (5c).
    Update $A(:,j{:}j+1) \leftarrow A(:,j{:}j+1)K^*$, $B(j{:}j+1,:) \leftarrow KB(j{:}j+1,:)$ and $Z_2(:,j{:}j+1) \leftarrow Z_2(:,j{:}j+1)K^*$.
end for

are the union of those of two independent matrix products of smaller sizes, which is similar to (13). However, so far, we are not quite convinced by the error analysis in regard to (14). Especially, when (14) is fulfilled but is intentionally neglected, the square root of the resulting eigenvalues of AB could be comparable to $\sqrt{\varepsilon}$. We are not quite sure that such an eigenvalue of AB should be treated as zero. Therefore, at the moment we decide to disregard the deflation induced by the criterion (14) in our computation.

To conclude this section, we summarize the main results in this and previous subsections into the following theorem and corollary.

Theorem 3. For any complex $\top$-Hamiltonian matrix $\mathscr{H}$, there always exist matrices $U, V \in \mathbb{U}\top\mathbb{S}_{2n}$ such that

$$U^* \mathscr{H} V = \mathcal{R} = \begin{bmatrix} R_1 & R_3 \\ 0 & R_2 \end{bmatrix} = \tag{15}$$



,

where $R_1 \in \mathbb{C}^{n\times n}$ is upper triangular and $R_2 \in \mathbb{C}^{n\times n}$ is lower triangular.

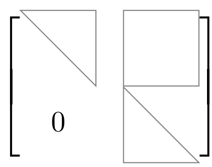
Remark 1. To distinguish with ⊤-symplectic URV-decompositions in (3) and (15), we call (3) and (15) the *unreduced* and *reduced* ⊤-symplectic URV-decomposition, respectively. However, we intentionally use the same notations U, V, R_1, R_2 and R_3 in (3) and (15), since in programming they just go through the following in-place update from (3) to (15),

$$\begin{aligned} &R_1 \leftarrow Z_2^* R_1 Z_1, \quad U \leftarrow U(Z_2 \oplus \overline{Z_2}), \\ &R_2 \leftarrow Z_2^\top R_2 \overline{Z_1}, \quad V \leftarrow V(Z_1 \oplus \overline{Z_1}), \quad R_3 \leftarrow Z_2^* R_3 \overline{Z_1}, \end{aligned}$$

where Z_1 and Z_2 are two unitary matrices computed by the complex periodic QR algorithm.

Corollary 1. Given a complex ⊤-Hamiltonian matrix $\mathscr{H}$ and (15), $\mathscr{H}^2$ is transformed into the following ⊤-skew-Hamiltonian Schur form [23]

$$U^* \mathscr{H}^2 U = \begin{bmatrix} T_1 & * \\ 0 & T_1^\top \end{bmatrix} = \begin{bmatrix} -R_1 R_2^\top & * \\ 0 & -R_2 R_1^\top \end{bmatrix} = \tag{16}$$



.

Similarly, it holds that

$$V^* \mathscr{H}^2 V = \mathcal{J}_{2n} \mathcal{R}^\top \mathcal{J}_{2n} \mathcal{R} = \begin{bmatrix} T_2 & * \\ 0 & T_2^\top \end{bmatrix} = \begin{bmatrix} -R_2^\top R_1 & * \\ 0 & -R_1^\top R_2 \end{bmatrix}, \tag{17}$$

where $T_2 \in \mathbb{C}^{n\times n}$ is upper triangular. Moreover, $(\lambda_j, -\lambda_j)$ is one pair of eigenvalues of $\mathscr{H}$ with $\lambda_j = \sqrt{-R_1(j,j)R_2(j,j)}$, $j = 1, 2, \cdots, n$.

Remark 2. Throughout this paper, unless otherwise specified, we adopt the convention of the square root function that $\sqrt{z} \in \mathbb{C}_+$ for any $z \in \mathbb{C}\backslash\{0\}$, *i.e.*,

$$\sqrt{(b + \imath c)^2} = \mathtt{sign}(b)(b + \imath c), \quad b \in \mathbb{R}\backslash\{0\},\ c \in \mathbb{R}, \tag{18a}$$

$$\sqrt{-a^2} = \imath |a|, \quad a \in \mathbb{R}\backslash\{0\}. \tag{18b}$$

4. A stable algorithm to compute the $\top$-Hamiltonian Schur form

4.1. $\top$-Lagrangian invariant subspace of $\mathscr{H}$

Similar to the real Hamiltonian Schur form, we can also require that all eigenvalues of R in the $\top$-Hamiltonian Schur form (2) belong to $\mathbb{C}_+$.

Below, we will explicate how the $\top$-Hamiltonian Schur form is related to the reduced $\top$-symplectic URV-decomposition of $\mathscr{H}$.

Lemma 1. [21] Given a non-singular complex $\top$-Hamiltonian $\mathscr{H} \in \mathbb{C}^{2n\times 2n}$ and its invariant subspace $X_k \in \mathbb{C}^{2n\times k}$ for some $k \leq n$

$$\mathscr{H} X_k = X_k B_k, \tag{19}$$

where the eigenvalues of $B_k \in \mathbb{C}^{k\times k}$ belong to $\mathbb{C}_+$, it holds that

$$X_k^\top \mathcal{J}_{2n} X_k = 0, \tag{20}$$

i.e., X_k is $\top$-isotropic.

Proof. It follows from (19) that

$$\mathcal{J}_{2n} X_k B_k = \mathcal{J}_{2n}\mathscr{H} X_k = -\mathscr{H}^\top \mathcal{J}_{2n} X_k,$$

hence,

$$X_k^\top \mathcal{J}_{2n} X_k B_k = -(\mathscr{H} X_k)^\top J_{2n} X_k = -B_k^\top X_k^\top \mathcal{J}_{2n} X_k.$$

That is, $Y_k := X_k^\top \mathcal{J}_{2n} X_k$ satisfies the following Lyapunov equation

$$B_k^\top Y_k + Y_k B_k = 0.$$

Since the pairwise sums of eigenvalues of B_k are nonzero, then this Lyapunov equation only admits a trivial solution $Y_k = X_k^\top \mathcal{J}_{2n} X_k = 0$. □

It is highlighted that the machinery used above to guarantee the $\top$-isotropy of some invariant subspaces of $\mathscr{H}$ is quite general in the sense that it works for any non-singular complex $\top$-Hamiltonian matrix and real Hamiltonian matrix without purely imaginary eigenvalues. Moreover, in Lemma 1 no orthogality between columns of X_k is required.

In particular, to solve the $\top$HEP (1) with non-singular $\mathscr{H}$, the invariant subspace X_k in Lemma 1 with $k = n$ is most useful. As soon as the invariant subspace X_n of a complex ⊤-Hamiltonian matrix $\mathscr{H}$ is found with the associated eigenvalues all in $\mathbb{C}_+$ or none in $\mathbb{C}_+ \cup \{0\}$, half of our task to compute the ⊤-Hamiltonian Schur form is done, since $\operatorname{span}(X_n)$ is essentially the same as $\operatorname{span}(Q(:,1\!:\!n))$, where Q is the main object to be known in (2).

Suppose that the invariant subspace X_n in Lemma 1 is found, then the next step is to find a ⊤-isotropic orthonormal basis of $\operatorname{span}(X_n)$. To this purpose, the economy-sized QR decomposition of X_n can be utilized, however, it could happen that the produced $Q(:,1\!:\!n)$ fails to be ⊤-isotropic to working precision. Therefore, we resort to the complex ⊤-symplectic QR decomposition [3, 12] whenever X_n is given as nonorthogonal columns. With the ⊤-isotropic orthonormal basis of $\operatorname{span}(X_n)$ at hand, the ⊤-Hamiltonian Schur form of $\mathscr{H}$ can be constructed.

In what follows, we make use of the reduced ⊤-symplectic URV decomposition (15) of $\mathscr{H}$ to construct the invariant subspace X_n of $\mathscr{H}$.

If X_n satisfies (19) for $k = n$, then it holds that

$$\mathscr{H}^2 X_n = X_n B_n^2. \tag{21}$$

That is, X_n is a ⊤-Lagrangian invariant subspace of $\mathscr{H}^2$. On the other hand, by (16) and (17), $U(:,1\!:\!n)$ and $V(:,1\!:\!n)$ are both ⊤-Lagrangian invariant subspaces of $\mathscr{H}^2$, too. It is natural to ask how this unknown X_n is related to $[U(:,1\!:\!n), V(:,1\!:\!n)]$, since there can be at most $2n$ linearly independent columns among $X_n, U(:,1\!:\!n)$ and $V(:,1\!:\!n)$.

In essence, the reduced ⊤-symplectic URV-decomposition (15) of $\mathscr{H}$ can be reformulated as

$$\mathscr{H} Y_{UV} = Y_{UV} M, \tag{22}$$

where

$$Y_{UV} = [U(:,1\!:\!n), V(:,1\!:\!n)] \in \mathbb{C}^{2n\times 2n}, \tag{23}$$

$$M = \begin{bmatrix} 0 & R_1 \\ -R_2^\top & 0 \end{bmatrix} \in \mathbb{C}^{2n\times 2n}. \tag{24}$$

Eigenvalues of M are just those $\pm\lambda_j$'s of $\mathscr{H}$ stated in Corollary 1. Furthermore, by some routine procedures specified in Sec. 4.2 to construct a desired unitary matrix P, this M can be transformed into an upper triangular matrix $\widetilde{M} = P^* M P \in \mathbb{C}^{2n\times 2n}$ such that its first n diagonal entries all belong to $\mathbb{C}_+$. Immediately, we arrive at the main result of this section.

Theorem 4. Given a non-singular $\top$-Hamiltonian $\mathscr{H}$ with Y_{UV} and M satisfying (22) and

$$\widetilde{M} = P^* M P \in \mathbb{C}^{2n\times 2n} \tag{25}$$

mentioned above, it holds that

$$\mathscr{H}\widetilde{X}_k = \widetilde{X}_k \widetilde{M}(1\!:\!k, 1\!:\!k), \tag{26}$$

where

$$\widetilde{X}_k := Y_{UV} P(:, 1\!:\!k), \quad 1 \le k \le n, \tag{27}$$

satisfies

$$\widetilde{X}_k^\top \mathcal{J}_{2n} \widetilde{X}_k = 0. \tag{28}$$

Moreover, $\operatorname{span}(\widetilde{X}_n)$ is a $\top$-Lagrangian subspace.

Proof. Since by construction $\widetilde{M}$ is upper triangular, the equality (26) follows directly from (22) and (27). Since all eigenvalues of $\widetilde{M}(1\!:\!k, 1\!:\!k)$ belong to $\mathbb{C}_+$, the $\top$-isotropy of $\widetilde{X}_k$ follows immediately from Lemma 1. Moreover, comparing with (2), n columns of $\widetilde{X}_n$ spans the same invariant subspace of $\mathscr{H}$ as $Q(:, 1 : n)$, therefore $\widetilde{X}_n$ has full column rank and $\operatorname{span}(\widetilde{X}_n)$ is a $\top$-Lagrangian subspace. $\square$

Note that the columns of $\widetilde{X}_k$ defined in (27) are usually not orthogonal to each other for $2 \le k \le n$. However, since $\widetilde{X}_n$ satisfies (28), *i.e.*, it contains the first n columns of a $2n$-by-$2n$ $\top$-symplectic matrix, then there exists a $Q \in \mathbb{U}\top\mathbb{S}_{2n}$ such that

$$\widetilde{X}_n = Q \begin{bmatrix} R_{11} \\ 0 \end{bmatrix} = Q \begin{bmatrix} \diagdown \\ 0 \end{bmatrix}, \tag{29}$$

where $R_{11} \in \mathbb{C}^{n\times n}$ is upper triangular. (29) is called the complex $\top$-symplectic QR decomposition [3, 12] of $\widetilde{X}_n$. Moreover, R_{11} in (29) is invertible, since $\operatorname{span}(\widetilde{X}_n)$ is a $\top$-Lagrangian subspace as shown in Theorem 4.

Theorem 5. $Q^*\mathscr{H}Q$ becomes the $\top$-Hamiltonian Schur form with the very Q in (29).

Proof. Substituting (29) to (26) with $k = n$, we have

$$\mathscr{H} Q(:, 1\!:\!n) R_{11} = Q(:, 1\!:\!n) R_{11} \widetilde{M}(1\!:\!n, 1\!:\!n),$$

or rather

$$\mathscr{H} Q(:, 1\!:\!n) = Q(:, 1\!:\!n) \left(R_{11} \widetilde{M}(1\!:\!n, 1\!:\!n) R_{11}^{-1} \right), \tag{30}$$

where the last factor on the right hand side is upper triangular. Further, as soon as we set $R = R_{11} \widetilde{M}(1\!:\!n, 1\!:\!n) R_{11}^{-1}$, (30) becomes $\mathscr{H} Q(:, 1\!:\!n) = Q(:, 1\!:\!n) R$; hence $Q(:, 1\!:\!n)^* \mathscr{H} Q(:, 1\!:\!n) = R$. In addition,

$$\begin{aligned} &Q(:, n+1\!:\!2n)^* \mathscr{H} Q(:, n+1\!:\!2n) = Q(:, 1\!:\!n)^\top \mathcal{J}_{2n} \mathscr{H} \mathcal{J}_{2n}^\top \overline{Q}(:, 1\!:\!n) \\ &= -(Q(:, 1\!:\!n)^* \mathscr{H} Q(:, 1\!:\!n))^\top = -R^\top. \end{aligned}$$

Therefore, $Q^* \mathscr{H} Q$ is the ⊤-Hamiltonian Schur form (2). □

Remark 3. In practice, rather than compute R in this way, we would compute $R = Q(:, 1 : n)^* \mathscr{H} Q(:, 1 : n)$ for the sake of stability. Similarly, the off-diagonal block C of the ⊤-Hamiltonian Schur form is computed by $C = Q(:, 1\!:\!n)^* \mathscr{H} Q(:, n+1\!:\!2n)$.

Remark 4. Although we have not proven that $Y_{UV} \in \mathbb{C}^{2n \times 2n}$ defined in (23) is invertible, we can expediently think that (22) implies $M = Y_{UV}^{-1} \mathscr{H} Y_{UV}$, *i.e.*, $\mathscr{H}$ is similar to M in (24), but not via a unitary ⊤-symplectic matrix. In this sense, our method using the results in Theorem 4 and Theorem 5 to compute the ⊤-Hamiltonian Schur form is some variant of the Laub trick [14], which is NOT truly structure-preserving. However, we believe that our method is stable, straightforward and friendly to the implementation.

4.2. The algorithm to compute the ⊤-Hamiltonian Schur form

Here, we specify how to unitarily transform M defined in (24) into $\widetilde{M}$ defined in (25) with the particular ordering of the eigenvalues. By the perfect shuffle matrix

$$P_1 = [\mathbf{e}_1, \mathbf{e}_{n+1}, \mathbf{e}_2, \mathbf{e}_{n+2}, \cdots, \mathbf{e}_n, \mathbf{e}_{2n}] \in \mathbb{R}^{2n \times 2n}, \tag{31}$$

M is permuted into a quasi-upper triangular matrix $P_1^* M P_1$. Note that the 2-by-2 blocks

$$D_j = \begin{bmatrix} 0 & R_1(j,j) \\ -R_2(j,j) & 0 \end{bmatrix}, \quad 1 \le j \le n,$$

along the diagonal of $P_1^* M P_1$ are special complex $\top$-Hamiltonian matrices, which can be transformed into the Schur form by Givens rotations. Specifically, since $D_j^2 \mathbf{e}_1 = \lambda_j^2 \mathbf{e}_1$ with $\lambda_j = \sqrt{-R_1(j,j)R_2(j,j)}$, then $\lambda_j \mathbf{e}_1 + D_j \mathbf{e}_1$ is the eigenvector of D_j, *i.e.*,

$$D_j \begin{bmatrix} \lambda_j \\ -R_2(j,j) \end{bmatrix} = \lambda_j \begin{bmatrix} \lambda_j \\ -R_2(j,j) \end{bmatrix}.$$

After determining the Givens rotation K_j such that $K_j[\lambda_j, \ -R_2(j,j)]^\top \propto [1, \ 0]^\top$ according to (5b) and (5c), $K_j D_j K_j^*$ becomes a 2-by-2 upper triangular matrix

$$K_j D_j K_j^* = \begin{bmatrix} \lambda_j & * \\ 0 & -\lambda_j \end{bmatrix}, \quad 1 \le j \le n.$$

Letting

$$K = K_1 \oplus K_2 \oplus \cdots \oplus K_n, \tag{32}$$

consequently, $K P_1^* M P_1 K^*$ is upper triangular. Moreover, we would like to swap all diagonal entries of $K P_1^* M P_1 K^*$ which belong to $\mathbb{C}_+$ to the leading block while the rest diagonal entries are moved to the bottom block. This reordering is a routine task in numerical linear algebra. Some highly efficient algorithm has been developed, *e.g.*, in [12], to compute a unitary matrix P_2 and the upper triangular matrix $P_2^* K P_1^* M P_1 K^* P_2$ with the specified ordering of the eigenvalues. Now, denote $P = P_1 K^* P_2$, then this $P_2^* K P_1^* M P_1 K^* P_2$ can be identified with the desired $\widetilde{M}$ in Theorem 4.

Remark 5. When the Schur form $K P_1^* M P_1 K^*$ is reordered, to prevent the numerical instability, we also need to identify the clusters of eigenvalues of $\mathscr{H}$ if they exist. To this end, we can adopt the criterion used in [21].

In [7, 21, 26], in order to preserve the $\top$-skew-Hamiltonian form $U^* \mathscr{H}^2 U$ in (16) at each step of transforming $U^* \mathscr{H} U$ to the $\top$-Hamiltonian Schur form, some sophisticated procedures are proposed to construct the Q matrix.

However, in our problem it is only necessary that $Q^* \mathscr{H}^2 Q$ is in the $\top$-skew-Hamiltonian form at the end, therefore, we decide to resort to the procedure in Algorithm 4 to compute the complex $\top$-symplectic QR decomposition of $\widetilde{X}_n$, where only the elementary eliminators (9) are used, to find an orthonormal basis of $\mathrm{span}(\widetilde{X}_n)$.

Now, we summarize the above derivations and discussions into Algorithm 5 to compute the $\top$-Hamiltonian Schur form (2) of a non-singular complex $\top$-Hamiltonian matrix $\mathscr{H}$.

Algorithm 4 ⊤-symplectic QR decomposition [3, 12]

Input: A general matrix $W \in \mathbb{C}^{2n\times m}$ with $n \geq m > 1$.
Output: $P \in \mathbb{U}\top\mathbb{S}_{2n}$ and $P^*W \in \mathbb{C}^{2n\times m}$.

1: Set $P \leftarrow I_{2n}$.
2: **for** $j = 1\!:\!m$ **do**
3: Set $\mathbf{x} = W(:, j)$.
4: Compute $E_j(\mathbf{x})$ using (9) and Algorithm 1.
5: Update $W \leftarrow E_j(\mathbf{x})^*W$.
6: Update $P \leftarrow PE_j(\mathbf{x})$.
7: **end for**

Algorithm 5 A stable algorithm to compute the ⊤-Hamiltonian Schur form

Input: A non-singular complex ⊤-Hamiltonian matrix $\mathscr{H}$.
Output: The ⊤-Hamiltonian Schur form (2).

1: Compute the reduced ⊤-symplectic URV decomposition of $\mathscr{H}$ (15) using Algorithm 2 followed by Algorithm 3.
2: Form M in (24) and set $P = P_1$ with P_1 in (31).
3: Update $M \leftarrow P^*MP$.
4: **for** $j = 1\!:\!n$ **do**
5: Construct the Givens rotation K_j from $\lambda_j = \sqrt{-R_1(j,j)R_2(j,j)}$ and $-R_2(j,j)$ according to (5b) and (5c).
6: **end for**
7: Construct K in (32).
8: Update $M \leftarrow KMK^*$ and $P \leftarrow PK^*$.
9: Determine a unitary matrix P_2 such that the first n diagonal entries of the reordered Schur form $P_2^*MP_2$ belong to $\mathbb{C}_+$.
10: Update $P \leftarrow PP_2$.
11: Compute $\widetilde{X}_n$ according to (27).
12: Compute $Q \in \mathbb{U}\top\mathbb{S}_{2n}$ via the ⊤-symplectic QR decomposition of $\widetilde{X}_n$ using Algorithm 4.
13: Compute $R = Q(:, 1\!:\!n)^*\mathscr{H}Q(:, 1\!:\!n)$.
14: Compute $C = Q(:, 1\!:\!n)^*\mathscr{H}Q(:, n+1\!:\!2n)$.

With the ⊤-Hamiltonian Schur form (2) ready, it is rather easy to compute eigenvectors of $\mathscr{H}$. To compute eigenvectors of ⊤-Hamiltonian Schur form is almost the same as those of the common Schur form, based on which the eigenvectors of $\mathscr{H}$ are obtained. Hence, we will not discuss the details here.

4.3. Connection with other methods to compute the $\top$-isotropic invariant subspace of $\mathscr{H}$

By Theorem 2.1 of [4], the stable invariant subspace of a real $\mathscr{H}$ is computed using some invariant subspace of the extended matrix $\left[\begin{smallmatrix} 0 & \mathscr{H} \\ \mathscr{H} & 0 \end{smallmatrix}\right]$ in [3, 4]. By simple calculations, one can verify that Theorem 2.1 of [4] leads to the identical invariant subspace $\widetilde{X}_n$ of $\mathscr{H}$ defined in (27) with the associated eigenvalues of $\mathscr{H}$ belong to $\mathbb{C}_+$. However, our main conclusion in Theorem 4 is directly obtained from (22), instead of a more complicated extended matrix.

In section 3 of [11], a method has been proposed to extract the stable invariant subspace of a large sparse real Hamiltonian matrix $\mathscr{H}$ from the invariant subspace of $\mathscr{H}^2$. Here we re-derive that method from (22) with the aid of the `sign` function of M.

For convenience, we denote the `sign` function of M by $\texttt{signm}(M)$. In light of the special form of M in (24), by Chapter 5 of [10], we have

$$\texttt{signm}(M) = M\left(\texttt{sqrtm}(M^2)\right)^{-1} = \begin{bmatrix} & R_1\left(\texttt{sqrtm}(T_2)\right)^{-1} \\ -R_2^\top\left(\texttt{sqrtm}(T_1)\right)^{-1} & \end{bmatrix}, \tag{33}$$

where T_1 and T_2 are defined in Corollary 1 and $\texttt{sqrtm}(T_1)$ denotes the square root function of T_1. In addition, even if T_1 has some *negative* eigenvalues, so long as the convention (18) of the square root function is adopted, $\texttt{sqrtm}(T_1)$ is well-defined via the established Schur-Parlett algorithm [10] and its eigenvalues still belong to $\mathbb{C}_+$. Moreover, by Theorem 5.1 in [10], $(I_{2n} + \texttt{signm}(M))[I_n,\ 0]^\top$ is the invariant subspace of M associated with the eigenvalues in $\mathbb{C}_+$. Indeed, with (33), it is easy to see that

$$\begin{aligned} M(I_{2n} + \texttt{signm}(M))\begin{bmatrix} I_n \\ 0 \end{bmatrix} &= \begin{bmatrix} 0 & R_1 \\ -R_2^\top & 0 \end{bmatrix}\begin{bmatrix} I_n \\ -R_2^\top\left(\texttt{sqrtm}(T_1)\right)^{-1} \end{bmatrix} \\ &= \begin{bmatrix} \texttt{sqrtm}(T_1) \\ -R_2^\top \end{bmatrix} = \begin{bmatrix} I_n \\ -R_2^\top\left(\texttt{sqrtm}(T_1)\right)^{-1} \end{bmatrix}\texttt{sqrtm}(T_1). \end{aligned} \tag{34}$$

Let

$$\widetilde{U}_n := Y_{UV}\begin{bmatrix} I_n \\ -R_2^\top\left(\texttt{sqrtm}(T_1)\right)^{-1} \end{bmatrix} = U(:,1\!:\!n) - V(:,1\!:\!n)R_2^\top\left(\texttt{sqrtm}(T_1)\right)^{-1}, \tag{35}$$

then it follows from (22) that

$$\mathscr{H}\widetilde{U}_n = \widetilde{U}_n\texttt{sqrtm}(T_1). \tag{36}$$

Furthermore, by noting that $V(:,1\!:\!n)(-R_2^\top) = \mathscr{H}U(:,1\!:\!n)$, we can alternatively define

$$\widetilde{U}_n = \mathscr{H}U(:,1\!:\!n) + U(:,1\!:\!n)\texttt{sqrtm}(T_1), \tag{37}$$

instead of (35), which still satisfies (36). One can verify that $\widetilde{U}_n$ defined in (37) is identical to the invariant subspace of $\mathscr{H}$ constructed in section 3 of [11]. In passing, by Lemma 1, $\widetilde{U}_n$ is ⊤-isotropic.

Since both $P(:,1:n)$ in (27) and $(I_{2n} + \texttt{signm}(M))[I_n,\ 0]^\top$ spans the same invariant subspace of M, we must have

$$-R_2^\top (\texttt{sqrtm}(T_1))^{-1} = P(n+1\!:\!2n,1\!:\!n)P(1\!:\!n,1\!:\!n)^{-1}.$$

However, in practice, we should avoid using $P(:,1\!:\!n)$ in (27) to compute $\widetilde{U}_n$ in (34), especially when $P(1\!:\!n,1\!:\!n)$ is ill-conditioned.

5. Numerical results

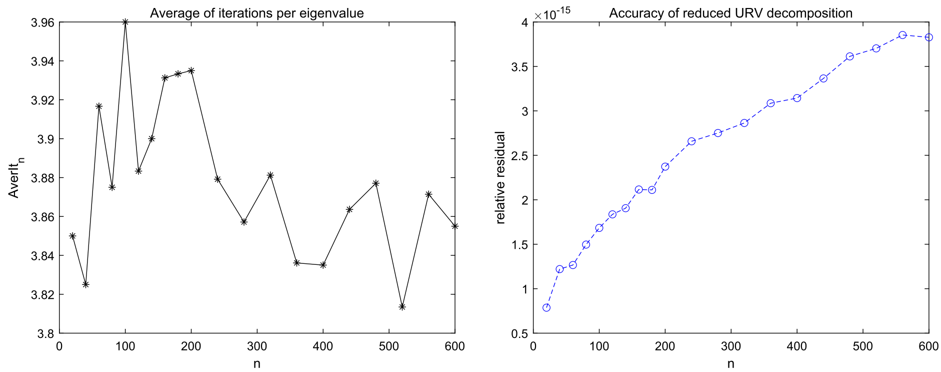
We have implemented the algorithms in previous sections in MATLAB [20] language. All numerical computations in this paper are performed in double precision by running MATLAB [20] of version 2019b on a laptop with an Intel Core i7-8650U 1.90GHz CPU and 16GB RAM.

5.1. Accuracy and efficiency of the reduced ⊤-symplectic URV-decomposition

We test Algorithm 2 followed by the complex periodic QR algorithm on a series of random ⊤-Hamiltonian matrices $\mathscr{H} \in \mathbb{C}^{2n\times 2n}$ with n ranging from 20 to 600. These matrices are generated by the function `rand` of MATLAB. Since the most time-consuming step is the complex periodic QR algorithm, which is implemented without any blocking techniques, we decide to use the average number iterations of Algorithm 3 to characterize its efficiency. Specifically, for $\mathscr{H} \in \mathbb{C}^{2n\times 2n}$, the average number of iterations ($AverIt_n$) is defined by

$$AverIt_n = \frac{\text{the total number of times Algorithm 3 is executed}}{n},$$

In Figure 1a, we plot the results of $AverIt_n$ versus n, from which it is seen that roughly 4 iterations of Algorithm 3 should be executed to obtain one pair of eigenvalues of $\mathscr{H}$.



(a) Average number of iterations of Algorithm 3

(b) Relative residual of (22)

Figure 1: The efficiency and accuracy of the reduced ⊤-symplectic URV-decomposition.

To characterize the accuracy of the reduced ⊤-symplectic URV-decomposition (15) of $\mathscr{H}$, we consider the relative residual

$$r = \|\mathscr{H} Y_{UV} - Y_{UV} M\|_F / \|\mathscr{H}\|_F \tag{38}$$

of (22) with Y_{UV} defined in (23) and M defined in (24). For the same set of ⊤-Hamiltonian matrices $\mathscr{H} \in \mathbb{C}^{2n\times 2n}$, we plot r defined in (38) versus n in Figure 1b. Since these examples are not pathological, we have not encountered numerical difficulties during computing (15), hence the accuracy is quite good, as shown in Figure 1b.

5.2. Accuracy of the ⊤-Hamiltonian Schur form

As mentioned in Sec. 2, the block method to compute the real Hamiltonian Schur form has been developed in [21]. We also implement the complex version of this method in MATLAB language. For comparison, we also implement a variant of Algorithm 5 which is based on $\widetilde{U}_n$ in (35) to construct the ⊤-Lagrangian invariant subspace of $\mathscr{H}$. In brief, to compute the term $-R_2^\top(\mathtt{sqrtm}(T_1))^{-1}$ in (35), we need to first compute $\mathtt{signm}(M)$ using the Parlett algorithm [10] and the relation

$$\mathtt{signm}(M) = P_1 \mathtt{signm}(P_1^* M P_1) P_1^*.$$

To characterize the accuracy of the computed ⊤-Hamiltonian Schur form, we denote the relative residual of (2) by

$$r_s = \|\mathscr{H}Q(:,1:n) - Q(:,1:n)R\|_F / \|\mathscr{H}\|_F,$$

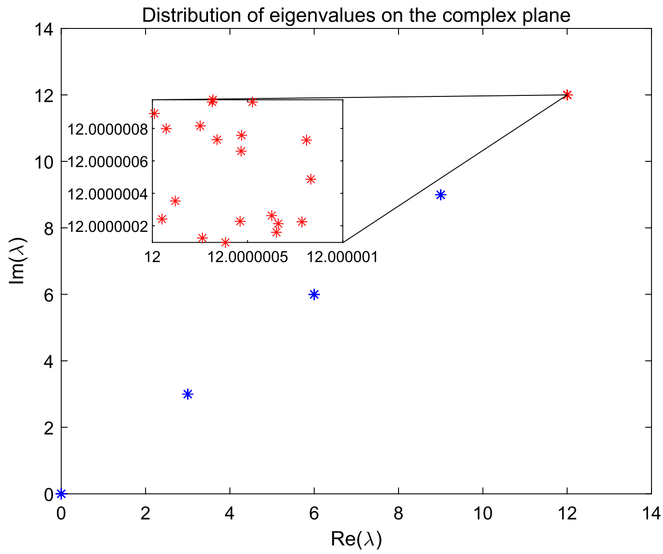
where $s = schur, sign$, and blk corresponding to Algorithm 5, the variant of Algorithm 5 using (35) and the block method in [21]. We test these three methods on some challenging cases, as shown below.

Each ⊤-Hamiltonian matrix below is constructed using (2). Specifically, we prepare a diagonal matrix D containing eigenvalues of $\mathscr{H} \in \mathbb{C}^{2n\times 2n}$ in accordance with a specific requirement, and the upper triangular matrix $R \in \mathbb{C}^{n\times n}$ in (2) is obtained by computing the Schur decomposition of $Z^*DZ \in \mathbb{C}^{n\times n}$ with Z being a random unitary matrix. In addition, the C block in (2) is generated by the function `rand` of MATLAB, and Q is just a random unitary ⊤-symplectic matrix.

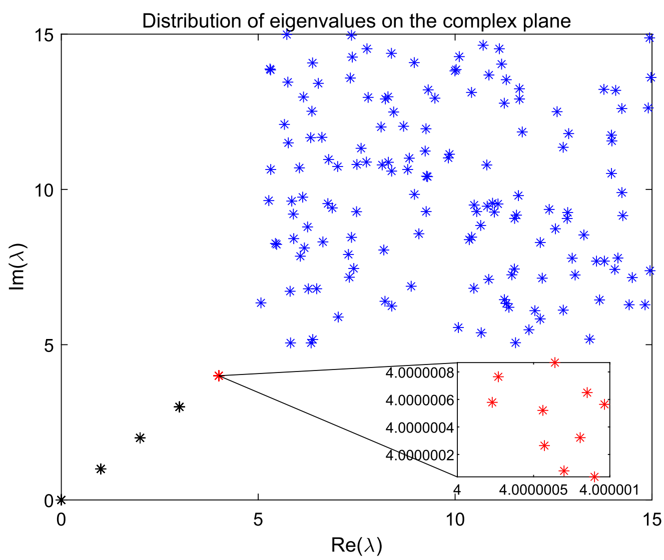
Example 5.1. In this example, a complex ⊤-Hamiltonian matrix $\mathscr{H} \in \mathbb{C}^{100\times 100}$ is built with only one cluster consisting of 50 eigenvalues around -1. These eigenvalues are clustered within a circle centered at -1 with the radius being 10^{-6}. For this $\mathscr{H}$, we obtain the residual $r_{schur} = 2.34\times 10^{-15}$, $r_{sign} = 2.53 \times 10^{-11}$, and $r_{blk} = 1.25 \times 10^{-15}$ for the three methods respectively. In this example, the first method is as accurate as the third method, however, the second method is obviously less accurate, which could be due to the relatively large error of the computed `signm`(M).

Example 5.2. In this example, we generate a complex ⊤-Hamiltonian matrix $\mathscr{H} \in \mathbb{C}^{200\times 200}$ with 10 tight eigenvalue clusters on the left half complex plane, which is illustrated in Figure 2a. The radius of each cluster is at most 10^{-6}. Note that the correct index of clusters should be assigned to each eigenvalue before the function `ordschur` of MATLAB is invoked. For this $\mathscr{H}$, we obtain the relative residual $r_{schur} = 3.41\times 10^{-15}$, $r_{sign} = 3.37\times 10^{-15}$ and $r_{blk} = 3.62 \times 10^{-15}$ for the three methods respectively. In this example, the three methods are equally accurate.

Example 5.3. In this example, we construct a complex ⊤-Hamiltonian matrix $\mathscr{H} \in \mathbb{C}^{400\times 400}$ with 5 tight eigenvalue clusters and some unclustered eigenvalues, which is illustrated in Figure 2b. In the block method, 21 blocks with different sizes are involved. We obtain the relative residual $r_{schur} = 4.69 \times 10^{-15}$, $r_{sign} = 4.79 \times 10^{-15}$ and $r_{blk} = 5.31 \times 10^{-15}$ for the three methods respectively. Again, in this example, the three methods are equally accurate.



(a) Eigenvalue distribution of Example 5.2.



(b) Eigenvalue distribution of Example 5.3.

Figure 2: The distribution of eigenvalues in Examples 5.2 and 5.3.

6. Concluding remarks

In this paper, we present an $\mathcal{O}(n^3)$ structure-preserving and numerically stable algorithm to compute all eigenvalues of a complex ⊤-Hamiltonian matrix $\mathscr{H}$ in (1). Unlike the third algorithm proposed in [2], our method deals with $\mathscr{H}$ directly and consequently computes no redundant eigenvalues.

We also provide a simple perspective to construct the ⊤-Lagrangian invariant subspace of $\mathscr{H}$, based on which the complex ⊤-Hamiltonian Schur form of $\mathscr{H}$ can be readily computed, without considering the extended matrix $\left[\begin{smallmatrix} 0 & \mathscr{H} \\ \mathscr{H} & 0 \end{smallmatrix}\right]$ or $\mathscr{H}^2$. In our numerical experiments, by testing three methods on several challenging examples, we find that Algorithm 5 to compute the ⊤-Hamiltonian Schur form of $\mathscr{H}$ is competitive with the state-of-the-art method in [21], and is simpler to understand and implement.

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