Electronic Transactions on Numerical Analysis.
Volume 8, pp. 115-126, 1999.

ISSN 1068-9613.

ETNA
Kent State University
etna@mcs.kent.edu

A NOTE ON THE NUMERICAL SOLUTION OF COMPLEX HAMILTONIAN AND SKEW-HAMILTONIAN EIGENVALUE PROBLEMS*

PETER BENNER†, VOLKER MEHRMANN‡, AND HONGGUO XU§

Abstract. In this paper we describe a simple observation that can be used to extend two recently proposed structure preserving methods for the eigenvalue problem for real Hamiltonian matrices to the case of complex Hamiltonian and skew-Hamiltonian matrices.

Key words. eigenvalue problem, Hamiltonian matrix, skew-Hamiltonian matrix, algebraic Riccati equation, invariant subspace.

AMS subject classifications. 65F15, 93B40, 93B36, 93C60.

1. Introduction. In two recent papers [4, 5], the authors developed new structure preserving numerical methods for the computation of eigenvalues and invariant subspaces of real Hamiltonian matrices. The new methods are a large step in the direction of solving an open problem posed by Paige/Van Loan [17], i.e., to develop a method for the computation of the Hamiltonian Schur form having a complexity of $O(n^3)$ and being strongly backward stable. Such a method would compute the exact Hamiltonian Schur form of a nearby Hamiltonian matrix. For real *skew-Hamiltonian* matrices a method satisfying the above requirements can immediately be derived from the method proposed by Van Loan in [18] for determining the eigenvalues for real Hamiltonian matrices. But this method is not applicable in the complex case and also is not able to yield certain Lagrangian invariant subspaces of *Hamiltonian* matrices that are needed in the context of computing the solution to algebraic Riccati equations or optimal control problems; see, e.g., [11, 15]. The new structure preserving methods of [5, 4] also cannot deal with the case of complex Hamiltonian matrices, but there are several important applications where the eigenvalue problem for complex Hamiltonian matrices has to be solved; see, e.g., [6, 16]. In this paper we therefore discuss structured methods for complex Hamiltonian and skew-Hamiltonian matrices.

Let us first introduce some notation. We will denote by $\Lambda(A)$ the spectrum of a matrix A, by $\Lambda_+(A)$, $\Lambda_-(A)$ the subsets of $\Lambda(A)$ of eigenvalues with positive and negative real parts, respectively and we will denote by $\mathrm{Inv}_+(A)$, $\mathrm{Inv}_-(A)$ the invariant subspaces of A corresponding to $\Lambda_+(A)$, $\Lambda_-(A)$, respectively. Superscripts T and H denote the transpose and the conjugate transpose, respectively.

DEFINITION 1.1. *Let* $J := \begin{bmatrix} 0 & I_n \\ -I_n & 0 \end{bmatrix}$, *where I_n is the $n \times n$ identity matrix.*

*i) A matrix $H \in \mathbb{C}^{2n\times 2n}$ is called **Hamiltonian** if $(HJ)^H = HJ$. The Lie algebra of Hamiltonian matrices in $\mathbb{C}^{2n\times 2n}$ is denoted by $\mathbf{H}_{2n}$. A Hamiltonian matrix has the block form* $\begin{bmatrix} F & D \\ G & -F^H \end{bmatrix}$, *where $F, D, G \in \mathbb{C}^{n\times n}$, $D = D^H$, and $G = G^H$.*

*ii) A matrix $N \in \mathbb{C}^{2n\times 2n}$ is called **skew-Hamiltonian** if $(NJ)^H = -NJ$. The Jordan algebra of skew-Hamiltonian matrices in $\mathbb{C}^{2n\times 2n}$ is denoted by $\mathbf{SH}_{2n}$. A skew-*

* Received August 25, 1998. Accepted for publication February 26, 1999. Recommended by D. Calvetti. This work was supported by *Deutsche Forschungsgemeinschaft*, Research Grant Me 790/7-2.

† Zentrum für Technomathematik, Fachbereich 3/Mathematik und Informatik, Universität Bremen, D-28334 Bremen, Germany.

‡ Fakultät für Mathematik, TU Chemnitz, D-09107 Chemnitz, Germany.

§ Fakultät für Mathematik, TU Chemnitz, D-09107 Chemnitz, Germany. Supported partially by the Chinese National Natural Science Foundation.

ETNA
Kent State University
etna@mcs.kent.edu

Hamiltonian matrix has the block form $\begin{bmatrix} F & D \\ G & F^H \end{bmatrix}$*, where* $F, D, G \in \mathbb{C}^{\mathrm{n}\times\mathrm{n}}$*,* $D = -D^H$*, and* $G = -G^H$*.*

iii) *A matrix* $S \in \mathbb{C}^{2\mathrm{n}\times 2\mathrm{n}}$ *is called* ***symplectic*** *if* $SJS^H = J$*. The Lie group of symplectic matrices in* $\mathbb{C}^{2\mathrm{n}\times 2\mathrm{n}}$ *is denoted by* $\mathbf{S}_{2n}$*.*

iv) *The Lie group of unitary matrices in* $\mathbb{C}^{\mathrm{n}\times\mathrm{n}}$ *is denoted by* $\mathbf{U}_n$ *and the Lie group of unitary symplectic matrices in* $\mathbb{C}^{2\mathrm{n}\times 2\mathrm{n}}$ *is denoted by* $\mathbf{US}_{2n}$*.*

Hamiltonian and skew-Hamiltonian matrices have certain obvious properties, which follow directly from the definition.

PROPOSITION 1.2.

i) *Multiplication with* $i := \sqrt{-1}$ *represents an isomorphism between the classes of complex Hamiltonian and skew-Hamiltonian matrices, i.e.,* $H \in \mathbf{H}_{2n}$ *if and only if* $iH \in \mathbf{SH}_{2n}$*.*

ii) *For* $H \in \mathbf{H}_{2n}$*, if* $\lambda \in \Lambda(H)$*, then also* $-\bar{\lambda} \in \Lambda(H)$*. Furthermore, if* H *is real, then also* $-\lambda, \bar{\lambda} \in \Lambda(H)$*.*

iii) *For* $N \in \mathbf{SH}_{2n}$*, if* $\lambda \in \Lambda(N)$*, then* $\bar{\lambda} \in \Lambda(N)$*. Furthermore, if* N *is real, then each eigenvalue of* N *has even algebraic multiplicity.*

iv) *Similarity transformations with symplectic matrices leave the classes of Hamiltonian and skew-Hamiltonian matrices invariant, i.e., if* $U \in \mathbf{S}_{2n}$*,* $H \in \mathbf{H}_{2n}$*, and* $N \in \mathbf{SH}_{2n}$*, then* $U^{-1}HU \in \mathbf{H}_{2n}$ *and* $U^{-1}NU \in \mathbf{SH}_{2n}$*.*

v) *If* $U \in \mathbf{US}_{2n}$*, then* U *can be partitioned as*

$$U = \begin{bmatrix} U_1 & U_2 \\ -U_2 & U_1 \end{bmatrix}, \qquad U_1, U_2 \in \mathbb{C}^{\mathrm{n}\times\mathrm{n}}.$$

For a Hamiltonian matrix $H \in \mathbf{H}_{2n}$ that has no purely imaginary eigenvalues, Paige and Van Loan [17] showed that there exists a matrix $U \in \mathbf{US}_{2n}$ so that

$$Q^H H Q = \begin{bmatrix} R & T \\ 0 & -R^H \end{bmatrix}, \qquad T = T^H, \quad R \text{ is upper triangular,} \tag{1.1}$$

which is called the *Hamiltonian Schur form*. The same proof also works for the skew-Hamiltonian case. For a real skew-Hamiltonian matrix, however, such a form always exists without any restriction on the eigenvalues [18]. Necessary and sufficient conditions for the existence of the Hamiltonian Schur form if the matrix has purely imaginary eigenvalues are given in [11, 13, 14].

Unfortunately, the construction of a method for the computation of this Schur form that has complexity $O(n^3)$ and is strongly stable, i.e., computes the Hamiltonian Schur form of a nearby Hamiltonian matrix, is still an open problem, although a lot of progress has been made in recent years [1, 4, 5, 8].

For real skew-Hamiltonian matrices N, Van Loan's method presented in [18] can be used to develop a structural QR algorithm as follows. First, a real matrix $Q_1 \in \mathbf{US}_{2n}$ is computed such that

$$Q_1^T N Q_1 =: \begin{bmatrix} F_1 & D_1 \\ 0 & F_1^T \end{bmatrix}, \tag{1.2}$$

where F_1 is upper Hessenberg and D_1 is skew symmetric. Then an orthogonal matrix $\tilde{Q}_2 \in \mathbf{U}_n$ is computed by the standard QR algorithm (see, e.g., [9]) such that $F_2 := \tilde{Q}_2^T F_1 \tilde{Q}_2$ is in real Schur form. Hence, with $Q_2 := \mathrm{diag}(\tilde{Q}_2, \tilde{Q}_2) \in \mathbf{US}_{2n}$ we obtain that

$$Q_2^T Q_1^T N Q_1 Q_2 =: \begin{bmatrix} F_2 & D_2 \\ 0 & F_2^T \end{bmatrix} \tag{1.3}$$

ETNA
Kent State University
etna@mcs.kent.edu

is in skew-Hamiltonian Schur form. But this method is not applicable in the case that N has a nontrivial complex part, since then the initial transformation to the Hessenberg-like form (1.2) is in general not possible as can be seen from the following example.

EXAMPLE 1. Let $N = \begin{bmatrix} -1 & -i \\ i & -1 \end{bmatrix} \in \mathbf{SH}_2$, then $\Lambda(N) = \{-2, 0\}$. Obviously, N cannot have a Hessenberg form as in (1.2). The methods derived in [4, 5] for the Hamiltonian eigenvalue problem can also not be used in the complex case. These methods compute in an initial step the *symplectic URV decomposition* of a Hamiltonian matrix H, that is, two real matrices $U, V \in \mathbf{US}_{2n}$ are computed such that

$$U^T H V = \begin{bmatrix} H_1 & H_2 \\ 0 & H_3^T \end{bmatrix}, \tag{1.4}$$

where H_1 is upper triangular and H_3 is upper Hessenberg. It follows (see [5]) that

$$V^T H^2 V = \begin{bmatrix} -H_3 H_1 & (H_3 H_2)^T - H_3 H_2 \\ 0 & (-H_3 H_1)^T \end{bmatrix}$$

has exactly the form (1.2). But for complex matrices, this initial reduction does not always exist as the next example demonstrates.

EXAMPLE 2. Consider the Hamiltonian matrix

$$H = \frac{\sqrt{2}}{2} \begin{bmatrix} i & -1 \\ 1 & i \end{bmatrix}.$$

Since $H^2 = N$, where N is as in Example 1, H^2 cannot have the form (1.2), and hence H cannot have the form (1.4).

In this paper we will study the case of general complex Hamiltonian and skew-Hamiltonian matrices and show how the method of Van Loan and the new methods of [4, 5] can be extended to this case. In Section 2 we will first show how to compute eigenvalues of complex Hamiltonian and skew-Hamiltonian matrices. The obtained algorithm will be the basis for a method to compute invariant subspaces as presented in Section 3. We will briefly discuss the complexity of the algorithms and their numerical properties in Section 4. Numerical examples in Section 5 demonstrate the reliability and performance of the proposed algorithms. Some concluding remarks are given in Section 6.

2. Eigenvalue Computation. In order to develop a method for the complex case we will first transform the structured complex eigenvalue problem into a structured real problem of double size. After solving the eigenvalue problem for this extended matrix, we will recover the eigenvalues of the original matrix. The method can be viewed as a generalization of the real algorithm proposed in [5], and we will discuss the relationship to this algorithm in Section 4. The basis for our new approach is the following simple observation. If we partition $N \in \mathbf{SH}_{2n}$ as $N = N_1 + iN_2$ with N_1, N_2 real, then $N_1 \in \mathbf{SH}_{2n}, N_2 \in \mathbf{H}_{2n}$. Moreover, by Definition 1.1, N_1 and N_2 can be written as

$$\begin{aligned} N_1 &= \begin{bmatrix} F_1 & D_1 \\ G_1 & F_1^T \end{bmatrix}, \qquad D_1 = -D_1^T, \quad G_1 = -G_1^T, \\ N_2 &= \begin{bmatrix} F_2 & D_2 \\ G_2 & -F_2^T \end{bmatrix}, \qquad D_2 = D_2^T, \quad G_2 = G_2^T. \end{aligned}$$

Thus, if we introduce the unitary matrix

$$Y_{2n} := \frac{\sqrt{2}}{2} \begin{bmatrix} I_{2n} & iI_{2n} \\ I_{2n} & -iI_{2n} \end{bmatrix}, \tag{2.1}$$

ETNA
Kent State University
etna@mcs.kent.edu

and the permutation matrix

$$P := \begin{bmatrix} I_n & 0 & 0 & 0 \\ 0 & 0 & I_n & 0 \\ 0 & I_n & 0 & 0 \\ 0 & 0 & 0 & I_n \end{bmatrix}, \tag{2.2}$$

then we obtain the real matrix

$$\mathcal{N} := P^H Y_{2n}^H \begin{bmatrix} N & 0 \\ 0 & \overline{N} \end{bmatrix} Y_{2n} P = \left[\begin{array}{cc|cc} F_1 & -F_2 & D_1 & -D_2 \\ F_2 & F_1 & D_2 & D_1 \\ \hline G_1 & -G_2 & F_1^T & F_2^T \\ G_2 & G_1 & -F_2^T & F_1^T \end{array}\right] =: \left[\begin{array}{c|c} \mathcal{F} & \mathcal{D} \\ \hline \mathcal{G} & \mathcal{F}^T \end{array}\right]. \tag{2.3}$$

It is easy to verify that $\mathcal{D} = -\mathcal{D}^T$, $\mathcal{G} = -\mathcal{G}^T$, so $\mathcal{N} \in \mathbf{SH}_{4n} \cap \mathbb{R}^{4n\times 4n}$ and thus we can apply Van Loan's algorithm to determine the eigenvalues of $\mathcal{N}$ and also to get the real skew-Hamiltonian Schur form

$$W_1^T \mathcal{N} W_1 = \begin{bmatrix} R & T \\ 0 & R^T \end{bmatrix} =: \mathcal{R}, \tag{2.4}$$

where $R \in \mathbb{R}^{2n\times 2n}$ is quasi upper triangular, $T = -T^T$, and $W_1 \in \mathbf{US}_{4n}$ is real.

By Proposition 1.2 iii), $\Lambda(N) = \Lambda(\overline{N})$ and it is not difficult to see that

$$\Lambda(N) = \Lambda(R). \tag{2.5}$$

Hence the eigenvalues of the complex skew-Hamiltonian matrix N can be computed by applying Van Loan's method to the double size real skew-Hamiltonian matrix $\mathcal{N}$ in (2.3).

Since Van Loan's method is strongly backward stable it is clear that the computed eigenvalues of N are the exact eigenvalues of a real skew-Hamiltonian matrix near to $\mathcal{N}$ and $\mathcal{N}$ is similar to $\operatorname{diag}(N, \overline{N})$. Because R is real, $\Lambda(R)$ is symmetric with respect to the real axis, thus also the symmetry of $\Lambda(N)$ is preserved.

Unfortunately, in general this method does not determine the skew-Hamiltonian Schur form of N. Set

$$V := Y_{2n} P W_1 = \begin{bmatrix} V_{11} & V_{12} \\ V_{21} & V_{22} \end{bmatrix}.$$

Then combining (2.3) and (2.4), we obtain

$$\begin{bmatrix} N & 0 \\ 0 & \overline{N} \end{bmatrix} V = V \begin{bmatrix} R & T \\ 0 & R^T \end{bmatrix}. \tag{2.6}$$

Comparing the (1,1) blocks on both sides of (2.6) yields

$$N V_{11} = V_{11} R.$$

If V_{11} is nonsingular, then we get the Schur decomposition of N via the QR decomposition of V_{11}, but if V_{11} is singular then we only get a certain non-Lagrangian invariant subspace of N from the basis of $\operatorname{range} V_{11}$.

By the isomorphism in Proposition 1.2 i) we also immediately obtain a method for the computation of the eigenvalues of a complex Hamiltonian matrix $H \in \mathbf{H}_{2n}$. Substituting $N = iH$ into (2.3) and using $\overline{iH} = -i\overline{H}$, by (2.4) we obtain with $V = Y_{2n} P W_1$ that

$$V^H \operatorname{diag}(H, -\overline{H}) V = -i\mathcal{R}, \tag{2.7}$$

and by (2.5), we the get the spectrum of H as

$$\Lambda(H) \;=\; -\,i\Lambda(R). \tag{2.8}$$

In this section we have shown how we can use a simple observation on the extension of complex skew-Hamiltonian matrices to a real problem of the same structure to compute the eigenvalues via the structure preserving method of Van Loan. In the next section we discuss the computation of invariant subspaces.

3. Computation of Invariant Subspaces. In this section we show how to compute $\mathrm{Inv}_+(H)$ and $\mathrm{Inv}_-(H)$, the invariant subspaces of a complex matrix $H \in \mathbf{H}_{2n}$, corresponding to the eigenvalues with negative and positive real parts, respectively. These are the important subspaces needed in applications from control theory, see, e.g., [11, 15]. We will assume for simplicity that the Hamiltonian matrices that we discuss have no purely imaginary eigenvalues such that $\dim \mathrm{Inv}_+(H) = n = \dim \mathrm{Inv}_-(H)$. In case there exist purely imaginary eigenvalues, there are several ways to distribute these eigenvalues in the Schur form, and it is still an open question what is the best way to do this. See [4, 14] for detailed comments.

Under these assumptions, $\mathcal{R}$ defined in (2.4) is in $\mathbf{SH}_{4n}$, has no real eigenvalues, and is in real skew-Hamiltonian Schur form. Hence, $-i\mathcal{R} \in \mathbf{H}_{4n}$ is in Hamiltonian Schur form. For matrices in Hamiltonian Schur form, the eigenvalue reordering procedure of Byers [7, 8] can be employed to determine a matrix $W_2 \in \mathbf{US}_{4n}$ such that

$$W_2^H(-i\mathcal{R})W_2 \;=\; \begin{bmatrix} \hat{R} & \hat{T} \\ 0 & -\hat{R}^H \end{bmatrix} \;=:\; \hat{\mathcal{R}} \in \mathbf{H}_{4n}, \tag{3.1}$$

and all eigenvalues of $\hat{R}$ have negative real parts, i.e., $\Lambda(\hat{R}) = \Lambda_-(\hat{\mathcal{R}})$. Let $U := VW_2$, then by (2.7) and (3.1) we have

$$U^H \begin{bmatrix} H & 0 \\ 0 & -\overline{H} \end{bmatrix} U \;=\; \hat{\mathcal{R}}. \tag{3.2}$$

THEOREM 3.1. *Suppose that $H \in \mathbf{H}_{2n}$ has no purely imaginary eigenvalues and suppose that*

$$U^H \begin{bmatrix} H & 0 \\ 0 & -\overline{H} \end{bmatrix} U \;=\; \hat{\mathcal{R}} \;=\; \begin{bmatrix} \hat{R} & \hat{T} \\ 0 & -\hat{R}^H \end{bmatrix} \tag{3.3}$$

is in Hamiltonian Schur form with $\Lambda(\hat{R}) = \Lambda_-(\hat{\mathcal{R}})$. Partition $U = \begin{bmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{bmatrix}$ accordingly. Then there exist matrices $\Phi, \Psi, \Theta \in \mathbf{U}_{2n}$ such that

$$\begin{aligned} U_{11} \;&=\; \Phi \begin{bmatrix} I_n & 0 \\ 0 & 0 \end{bmatrix} \Theta \;=:\; \begin{bmatrix} \Phi_1 & 0 \end{bmatrix} \Theta, \\ U_{21} \;&=\; \Psi \begin{bmatrix} 0 & 0 \\ 0 & I_n \end{bmatrix} \Theta \;=:\; \begin{bmatrix} 0 & \Psi_2 \end{bmatrix} \Theta, \end{aligned} \tag{3.4}$$

and the columns of Φ_1, $\overline{\Psi_2}$ form orthogonal bases of $\mathrm{Inv}_-(H)$ and $\mathrm{Inv}_+(H)$, respectively.

Proof. ¿From (3.3) we obtain

$$HU_{11} \;=\; U_{11}\hat{R}, \qquad H\overline{U_{21}} \;=\; -\,\overline{U_{21}}\overline{\hat{R}}. \tag{3.5}$$

Since $\Lambda(\hat{R}) = \Lambda_-(\hat{\mathcal{R}})$, we have

$$\operatorname{range} U_{11} \subseteq \operatorname{Inv}_-(H), \qquad \operatorname{range} \overline{U_{21}} \subseteq \operatorname{Inv}_+(H). \tag{3.6}$$

By assumption H has no purely imaginary eigenvalues, and thus Proposition 1.2 ii) implies that there are exactly n eigenvalues in $\Lambda_+(H)$ and n eigenvalues in $\Lambda_-(H)$. Hence,

$$\dim \operatorname{Inv}_-(H) \;=\; \dim \operatorname{Inv}_+(H) \;=\; n, \tag{3.7}$$

and thus

$$\operatorname{rank} U_{11} \leq n, \qquad \operatorname{rank} U_{21} \leq n. \tag{3.8}$$

On the other hand, U is unitary. Using the CS decompositions [9] of U_{11} and U_{21} there exist $\Phi, \Psi, \Theta \in \mathbf{U}_{2n}$ so that

$$U_{11} \;=\; \Phi \begin{bmatrix} \Sigma & 0 \\ 0 & 0 \end{bmatrix} \Theta, \quad U_{21} \;=\; \Psi \begin{bmatrix} \Delta & 0 \\ 0 & I_{2n-r} \end{bmatrix} \Theta,$$

where $\Sigma, \Delta \in \mathbb{R}^{r\times r}$ are diagonal with nonnegative diagonal elements, $\Sigma \neq 0$, and $\Sigma^2 + \Delta^2 = I_r$. The first inequality of (3.8) implies $\operatorname{rank}\Sigma \leq n$. If $\operatorname{rank}\Sigma \neq n$, then $\operatorname{rank} U_{21} > n$, which contradicts the second inequality of (3.8). Hence $\operatorname{rank}\Sigma = n$. Moreover $\Sigma = I_n$, since otherwise, $\Delta \neq 0$, and thus $\operatorname{rank} U_{21} > n$ which again contradicts (3.8). This shows (3.4). The remaining assertions follow from (3.6), (3.7) and the fact that $\Phi_1^H\Phi_1 = \Psi_2^H\Psi_2 = I_n$. □

In summary we obtain the following algorithm for the computation of $\operatorname{Inv}_-(H)$.

ALGORITHM 1. *This algorithm computes the (Lagrangian) invariant subspace corresponding to the eigenvalues in the open left half plane of a complex matrix $H \in \mathbf{H}_{2n}$ having no purely imaginary eigenvalues.*

Input: A complex Hamiltonian matrix $H \in \mathbf{H}_{2n}$ having no purely imaginary eigenvalues.

Output: $\Phi_1 \in \mathbb{C}^{2n\times n}$, with $\Phi_1^H\Phi_1 = I_n$, $\operatorname{range}\Phi_1 = \operatorname{Inv}_-(H)$.

Step 1 Set $N = iH$ and determine the matrix $\mathcal{N}$ as in (2.3). Apply Van Loan's algorithm [18] to $\mathcal{N}$ to compute the real skew-Hamiltonian Schur form,

$$W_1^T \mathcal{N} W_1 \;:=\; \begin{bmatrix} R & T \\ 0 & R^T \end{bmatrix} \;=:\; \mathcal{R},$$

where $W_1 \in \mathbf{US}_{4n}$ and R is quasi upper triangular.

Step 2 Determine a matrix $W_2 \in \mathbf{US}_{4n}$ by using Byers' unitary symplectic reordering method [8] applied to $i\mathcal{R}$, so that

$$W_2^H(-i\mathcal{R})W_2 \;=\; \begin{bmatrix} \hat{R} & \hat{T} \\ 0 & -\hat{R}^H \end{bmatrix} =: \hat{\mathcal{R}}$$

with $\Lambda(\hat{R}) \;=\; \Lambda_-(\hat{\mathcal{R}})$.

Set $U_{11} := \begin{bmatrix} I_{2n} & 0 \end{bmatrix} U \begin{bmatrix} I_{2n} \\ 0 \end{bmatrix}$, where $U = Y_{2n}PW_1W_2$.

Step 3 Compute Φ_1, an orthogonal basis of $\operatorname{range} U_{11}$, using any numerically stable orthogonalization scheme, for example a rank-revealing QR-decomposition; see, e.g., [9].

End

The same algorithm can also be used to compute $\mathrm{Inv}_+(H)$. In this case we need to form U_{21}, the $(2,1)$ block of U and then compute an orthogonal basis of $\mathrm{range}\, U_{21}$.

REMARK 1. *There are still some improvements possible in the described algorithm. First it would be nice if it could be performed completely in real arithmetic and second, it would be ideal if the additional structure in the blocks $\mathcal{F}, \mathcal{D}, \mathcal{G}$ could be exploited. At this writing, we are not aware how to achieve this.*

REMARK 2. *In [4] a method similar to Algorithm 1 was proposed for the eigenproblem of real Hamiltonian matrices. The method uses a new matrix factorization, called the symplectic URV decomposition. This factorization in general only exists for real matrices. Using the symplectic URV decomposition, it is possible to compute the Hamiltonian Schur form of the extended matrix*

$$\mathcal{B} := \begin{bmatrix} 0 & H \\ H & 0 \end{bmatrix}, \qquad H \in \mathbf{H}_{2n} \text{ real}$$

or equivalently, the extended Hamiltonian matrix $\hat{\mathcal{B}} := P^T \mathcal{B} P$. The invariant subspace of H is then obtained from the Lagrangian invariant subspace of $\mathcal{B}$ or $\hat{\mathcal{B}}$.

On the other hand with the complex unitary symplectic matrix $X = \mathrm{diag}(I_n, -iI_n, I_n, -iI_n)$, we get

$$-i\mathcal{N} = X^H \hat{\mathcal{B}} X,$$

i.e., the Hamiltonian matrices $\hat{\mathcal{B}}$ and $-i\mathcal{N}$ are symplectically similar. Therefore, both methods can be used for computing the Hamiltonian Schur form of the same matrix $-i\mathcal{N}$. Hence Algorithm 1 shares the same methodology with the method proposed in [4]. Because the symplectic URV decomposition can be used to exploit the given matrix structures more efficiently, this method is more efficient than Algorithm 1 for real Hamiltonian matrices. Thus, the complexity of Algorithm 1 is much higher than that of the algorithm presented in [4]. Hence we recommend to use the method in [4] for real problems; Algorithm 1 should only be used for complex problems as it offers no advantage over the method in [4] with respect to numerical stability and accuracy.

4. Complexity and Error Analysis.

The computational complexities for the three steps of Algorithm 1 are given in Table 4.1. Following [9], any floating point operation ($+$, $-$, $*$, $/$, $\sqrt{\ }$) is counted as a *flop*. Note that in Step 1, only real operations are involved. The flop counts are based on the estimated computational cost of the standard numerical linear algebra algorithms as given in [9] and the estimated flops for Van Loan's algorithm as given in [3, 18]. We assume that the structure of (skew-)Hamiltonian and orthogonal symplectic matrices as given in Definition 1.1 *i), ii)* and Proposition 1.2 *v)* is fully exploited and that in Step 3, a QR factorization with column pivoting is used. The total flop count is based on the assumption that one complex flop is roughly as expensive as four real flops.

Step	1	2	3	total
flops	$397\frac{1}{3}n^3$ (real)	$40n^3$ (complex)	$18\frac{2}{3}n^3$ (complex)	$\approx 158n^3$ (complex)

TABLE 4.1
Flop counts for Algorithm 1

These numbers compare with $205n^3$ complex flops for the computation of the same invariant subspace via the Schur method as suggested in [12]. If only eigenvalues are required, then only Step 1 of Algorithm 1 is performed without accumulating the similarity transformations. This requires about $\frac{320}{3}n^3$ real flops for the computation of the skew-Hamiltonian

ETNA
Kent State University
etna@mcs.kent.edu

Hessenberg form and $\frac{160}{3}n^3$ for the Hessenberg QR algorithm [9], altogether $160n^3$ real flops. The computation of the eigenvalues of a complex $2n \times 2n$ matrix using the nonsymmetric QR algorithm needs about $80n^3$ complex flops.

In [4] we have given the error analysis for the proposed structure preserving method for the Hamiltonian Schur form of the extended Hamiltonian matrix $\hat{\mathcal{B}} = P^T \begin{bmatrix} 0 & H \\ H & 0 \end{bmatrix} P$, and the invariant subspaces of the real Hamiltonian matrix H. By Remark 2 the same error analysis can be carried out for the complex case. Let $W = W_1W_2 \in \mathbf{US}_{4n}$, where $W_1, W_2 \in \mathbf{US}_{4n}$ are updated in Algorithm 1. Let $\hat{\mathcal{R}}$ be the finite precision analogue to the Hamiltonian triangular matrix $\mathcal{R}$ computed by Algorithm 1. We have

$$W^H(-i\mathcal{N})W \;=\; \hat{\mathcal{R}} + \mathcal{E}, \qquad \mathcal{E} \in \mathbf{H}_{4n}, \qquad \|\mathcal{E}\| < c\epsilon\|H\|, \tag{4.1}$$

where $\|\,.\,\|$ is the spectral norm, ϵ is the machine precision, and c is a constant.

By (1.1) there exists a unitary symplectic matrix Q such that

$$Q^HHQ \;=\; \begin{bmatrix} S & L \\ 0 & -S^H \end{bmatrix}, \qquad \Lambda(S) \;=\; \Lambda_-(H). \tag{4.2}$$

Let $K \in \mathbf{US}_{2n}$ be such that

$$K^H \begin{bmatrix} -S^H & 0 \\ L & S \end{bmatrix} K \;=\; \begin{bmatrix} -\hat{S}^H & \hat{L} \\ 0 & \hat{S} \end{bmatrix}, \qquad \Lambda(\hat{S}) \;=\; \Lambda_-(H). \tag{4.3}$$

Then using the *separation* between two matrices as defined by (see, e.g., [9])

$$\operatorname{sep}(A,B) \;:=\; \min_{X\neq 0} \frac{\|AX - XB\|}{\|X\|},$$

and employing

$$\delta \;:=\; \min\{\operatorname{sep}(S^H,-S), \operatorname{sep}(\hat{S},-\hat{S}^H)\}, \tag{4.4}$$

we obtain as in [4] the following result.

THEOREM 4.1. *Let S, L, $\hat{S}$, $\hat{L}$ be defined in (4.2) and (4.3) and δ be as in (4.4). Let $\mathcal{E}$ be the error matrix as in (4.1). Furthermore, let Φ_1 be the output of Algorithm 1 in exact arithmetic and let Φ_ϵ be the computed output in finite arithmetic. Denote by $\xi \in \mathbb{R}^{n\times n}$ the diagonal matrix of canonical angles between* $\operatorname{range}\Phi_1$ *and* $\operatorname{range}\Phi_\epsilon$. *If*

$$8\|\mathcal{E}\|(\delta + \max\{\|L\|, \|\hat{L}\|\}) < \delta^2,$$

then

$$\|\sin\xi\| < c_s\frac{\|\mathcal{E}\|}{\delta} < c_s c\epsilon\frac{\|\mathcal{H}\|}{\delta}, \tag{4.5}$$

with $c_s = 8\,\dfrac{\sqrt{10}+4}{\sqrt{10}+2} \approx 11.1.$

REMARK 3. *The above theorem essentially shows that the invariant subspace computed by Algorithm 1 is as accurate as to be expected from a numerical backward stable method as long as the condition numbers of the stable and unstable H-invariant subspaces given by* $\operatorname{sep}(S^H,-S)$ *and* $\operatorname{sep}(\hat{S},-\hat{S}^H)$*, respectively, are approximately equal. The fact that the* *accuracy of the computed invariant subspace is affected by the conditioning of the complimentary subspace can be expected as Algorithm 1 basically computes both subspaces at the same time.*

By applying the perturbation theory for the Hamiltonian Schur form developed recently in [10] we can get more precise error bounds. But note that this does not affect the qualitative behavior of the error bound as explained above. Therefore and due to its relatively complicated structure, we refrain here from presenting details of the theory in [10].

5. Numerical Examples. We have implemented the computation of the real skew-Hamiltonian Schur form of the matrix $\mathcal{N}$ as in (2.3) and the computation of the eigenvalues of complex Hamiltonian matrices in Fortran 77. We present two examples demonstrating the numerical accuracy and performance of the algorithm.

The test results reported here were obtained on a Sun Ultra10 with 512 MByte main memory and a 299 MHz UltraSPARC-IIi CPU using IEEE double precision arithmetic. All subroutines were compiled using standard optimization and double-word alignment (compiler flags `-O -dalign`). The standard public domain versions of LAPACK and BLAS [2], compiled with the same compiler flags, were used. It should be noted that on the machine used, the cost of complex arithmetic compared to real arithmetic using Fortran 77 code does not follow the model used to estimate flops earlier in this paper. For matrix multiplication of $n \times n$ matrices as implemented in the BLAS Level 3 subroutines DGEMM and ZGEMM for real and complex arithmetic, respectively, the complex version required less than twice the time of the real version for $n = 100$. The ratio even becomes smaller as n is increased. The tests were confirmed by results obtained on a PC with a 200 MHz AMD K6 CPU.

We will compare the subroutine ZHAEV for computing eigenvalues of complex Hamiltonian matrices using the method presented in Section 2 to the LAPACK driver routine ZGEEV for computing eigenvalues of general non-Hermitian matrices based on the QR algorithm.

EXAMPLE 3. [18, Example 2] This example was used in [18] to demonstrate the possible loss of accuracy in the method for computing the eigenvalues of real Hamiltonian matrices. We have turned the example into a complex problem, still having the same real eigenvalues.

Let $A = \mathrm{diag}(1,\, 10^{-2},\, 10^{-4},\, 10^{-6},\, 10^{-8}\,)$. Then a Hamiltonian matrix H is obtained by

$$H = U^H \begin{bmatrix} A & 0 \\ 0 & -A^H \end{bmatrix} U,$$

where $U \in \mathbf{US}_{10}$ is randomly generated by five real symplectic rotations and five complex reflectors. Thus, $\Lambda(H) = \{\pm 1, \pm 10^{-2}, \pm 10^{-4}, \pm 10^{-6}, \pm 10^{-8}\}$.

In Table 5.1 we present the absolute errors of the eigenvalues $\tilde{\lambda}$ computed by ZHAEV and ZGEEV. For demonstration purposes, we also give the results obtained by the implementation of Van Loan's method described in [3] applied to the above example where the transformations accumulated in U are all chosen real.

Here, the loss of accuracy of order $\|H\|_2/|\lambda|$ in Van Loan's method is obvious while both ZHAEV and ZGEEV compute all eigenvalues to full accuracy.

EXAMPLE 4. We tested our subroutines for randomly generated Hamiltonian matrices with entries distributed uniformly in the interval $[-1,\, 1\,]$. The eigenvalues computed by ZHAEV are as accurate as for ZGEEV. In Figure 5.1 we present the minimum singular value of $H - \tilde{\lambda} I_{2n}$, denoted by $\sigma_{\min}(H - \tilde{\lambda} I_{2n})$, for an $n = 50$ example and all eigenvalues in the closed right half plane (in this case, these are 52, i.e., 4 eigenvalues are located on the imaginary axis). The given error measure is the backward error of the computed eigenvalues $\tilde{\lambda}$ in the sense that it equals the 2-norm of the perturbation matrix $E \in \mathbb{C}^{2n \times 2n}$ of smallest 2-norm for which $\tilde{\lambda}$ is an exact eigenvalue of $H + E$. It can be seen from Figure 5.1 that both

ETNA
Kent State University
etna@mcs.kent.edu

λ	ZHAEV	ZGEEV	[3]
1	1.7×10^{-17}	1.6×10^{-15}	1.2×10^{-15}
10^{-2}	1.1×10^{-17}	2.5×10^{-17}	1.0×10^{-17}
10^{-4}	2.6×10^{-17}	3.3×10^{-17}	1.3×10^{-14}
10^{-6}	3.9×10^{-17}	3.2×10^{-17}	1.7×10^{-14}
10^{-8}	1.8×10^{-17}	3.0×10^{-17}	4.3×10^{-11}

TABLE 5.1
Example 3, absolute errors $|\lambda - \tilde{\lambda}|$.

methods compute the eigenvalues accurately with no significant preference of one algorithm over the other.

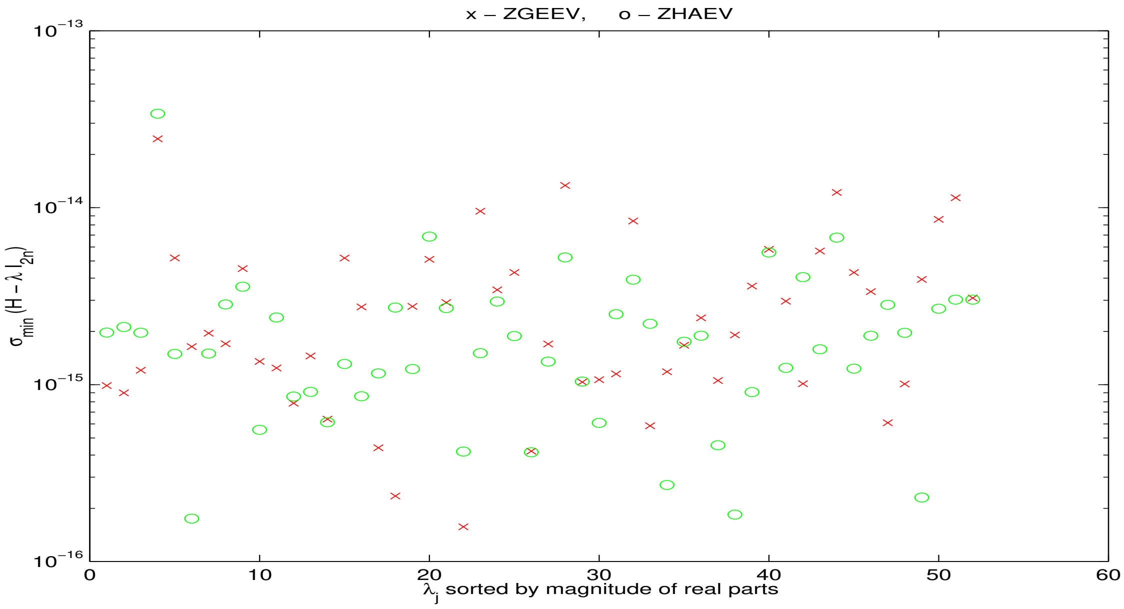

FIG. 5.1. *Example 4, backward error of computed eigenvalues ($n = 50$).*

We also measured the CPU times required by ZHAEV and ZGEEV for $H \in \mathbb{C}^{2n \times 2n}$ with n varying from 50 to 500. For each value of n, we recorded the CPU seconds of execution time required to solve 10 randomly generated Hamiltonian eigenvalue problems. Table 5.2 shows the mean CPU seconds of execution time measured on the Sun Ultra10.

n	50	100	150	200	250	300	350	400	450	500
ZGEEV	0.41	3.1	11.7	28.8	56.8	99.5	157.9	238.1	339.7	470.6
ZHAEV	0.22	1.7	7.1	20.6	47.8	77.9	126.5	193.5	276.8	386.5

TABLE 5.2
Example 4, average CPU seconds of execution times for ZHAEV and ZGEEV across 10 trials.

The table shows that for these Hamiltonian matrices, ZHAEV requires about half of the execution time of ZGEEV for small n and tends to 80% of the execution time of ZGEEV for larger n. This varying ratio of execution times can be explained by the varying ratio of CPU times required for complex operations compared to real operations. Moreover, ZHAEV is implemented using non-blocked algorithms while ZGEEV benefits from its block-oriented (BLAS Level 3 based) implementation in particular for larger n.

Besides the faster computation of the eigenvalues, ZHAEV returns the right pairing of the eigenvalues as $\pm\lambda_i$, $i = 1, \ldots, n$. Since ZGEEV treats a Hamiltonian matrix like an arbitrary nonsymmetric matrix, small perturbations can and do cause computed eigenvalues with small real parts to cross the imaginary axis. Moreover, it is difficult to decide whether eigenvalues are on the imaginary axis or not. In contrast to this, all simple purely imaginary eigenvalues computed by ZHAEV come out having exact real part zero as these are simple real eigenvalues of $\mathcal{R}$ in (2.4).

6. Conclusion. We have demonstrated a simple trick that allows to use Van Loan's method for the computation of Hamiltonian Schur forms of real skew-Hamiltonian matrices to be extended to the case of complex Hamiltonian and skew-Hamiltonian matrices. For this modification we have given an error analysis and also shown its connection to other recent structure preserving methods. Numerical experiments demonstrate that the accuracy of the proposed algorithm for computing eigenvalues is as good as to be expected from the error analysis. The performance of the method in comparison to unstructured methods shows that some benefit is gained from exploiting the structure.

REFERENCES

[1] G. S. Ammar, P. Benner, and V. Mehrmann, *A multishift algorithm for the numerical solution of algebraic Riccati equations*, Electron. Trans. Numer. Anal., 1 (1993), pp. 33–48.

[2] E. Anderson, Z. Bai, C. Bischof, J. Demmel, J. Dongarra, J. Du Croz, A. Greenbaum, S. Hammarling, A. McKenney, S. Ostrouchov, and D. Sorensen, *LAPACK Users' Guide*, 2nd Ed., SIAM, Philadelphia, PA, 1995.

[3] P. Benner, R. Byers, and E. Barth, *HAMEV and SQRED: Fortran 77 subroutines for computing the eigenvalues of Hamiltonian matrices using Van Loan's square reduced method*, Technical Report SFB393/96-06, Fak. f. Mathematik, TU Chemnitz–Zwickau, 09107 Chemnitz, FRG, 1996. Available from `http://www.tu-chemnitz.de/sfb393/sfb96pr.html`.

[4] 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 (1997), pp. 17–43.

[5] ———, *A numerically stable, structure preserving method for computing the eigenvalues of real Hamiltonian or symplectic pencils*, Numer. Math., 78(3) (1998), pp. 329–358.

[6] A. Bunse-Gerstner and V. Mehrmann, *The HHDR-algorithm and its application to optimal control problems*, RAIRO Automat. Prod. Inform. Ind., 23 (1989), pp. 305–329.

[7] R. Byers, *Hamiltonian and Symplectic Algorithms for the Algebraic Riccati Equation*, PhD thesis, Cornell University, Dept. Comp. Sci., Ithaca, NY, 1983.

[8] ———, *A Hamiltonian QR-algorithm*, SIAM J. Sci. Statist. Comput., 7 (1986), pp. 212–229.

[9] G. H. Golub and C. F. Van Loan, *Matrix Computations*, 3rd Ed., Johns Hopkins University Press, Baltimore, 1996.

[10] M. M. Konstantinov, V. Mehrmann, and P. Hr. Petkov, *Perturbation analysis for the Hamiltonian Schur form*, Technical Report SFB393/98-17, Fak. f. Mathematik, TU Chemnitz, 09107 Chemnitz, FRG, 1998.

[11] P. Lancaster and L. Rodman, *The Algebraic Riccati Equation*, Oxford University Press, Oxford, 1995.

[12] A. J. Laub, *A Schur method for solving algebraic Riccati equations*, IEEE Trans. Automat. Control, AC-24 (1979), pp. 913–921.

[13] W.-W. Lin and T.-C. Ho, *On Schur type decompositions for Hamiltonian and symplectic pencils*, Technical report, Institute of Applied Mathematics, National Tsing Hua University, Taiwan, 1990.

[14] W.-W. Lin, V. Mehrmann and H. Xu, *Canonical forms for Hamiltonian and symplectic matrices and pencils*, to appear in Linear Algebra Appl.

[15] V. MEHRMANN, *The Autonomous Linear Quadratic Control Problem, Theory and Numerical Solution*. Number 163 in Lecture Notes in Control and Information Sciences. Springer-Verlag, Heidelberg, July 1991.
[16] *P. C. Müller*, *Allgemeine lineare Theorie für Rotorsysteme ohne oder mit kleinen Unsymmetrien*, Ingenieur Archiv, 51 (1981), pp. 61–74.
[17] C. C. PAIGE AND C. F. VAN LOAN, *A Schur decomposition for Hamiltonian matrices*, Linear Algebra Appl., 14 (1981), pp. 11–32.
[18] C. F. VAN LOAN, *A symplectic method for approximating all the eigenvalues of a Hamiltonian matrix*, Linear Algebra Appl., 61 (1984), pp. 233–251.