

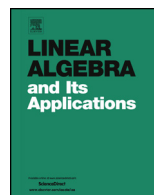


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A symmetric structure-preserving Γ QR algorithm for linear response eigenvalue problems



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ABSTRACT

In this paper, we present an efficient Γ QR algorithm for solving the linear response eigenvalue problem $\mathcal{H}\mathbf{x} = \lambda\mathbf{x}$, where \mathcal{H} is Π^- -symmetric with respect to $\Gamma_0 = \text{diag}(I_n, -I_n)$. Based on newly introduced Γ -orthogonal transformations, the Γ QR algorithm preserves the Π^- -symmetric structure of \mathcal{H} throughout the whole process, and thus guarantees the computed eigenvalues to appear pairwise $(\lambda, -\lambda)$ as they should. With the help of a newly established implicit Γ -orthogonality theorem, we incorporate the implicit multi-shift technique to accelerate the convergence of the Γ QR algorithm. Numerical experiments are given to show the effectiveness of the algorithm.

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1. Introduction

In this paper, we consider the standard eigenvalue problem of the form

$$\mathcal{H} \mathbf{x} \equiv \begin{bmatrix} A & B \\ -B & -A \end{bmatrix} \begin{bmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{bmatrix} = \lambda \mathbf{x}, \tag{1.1}$$

where A and B are $n \times n$ real symmetric matrices. We refer to it a *linear response eigenvalue problem* (LREP). Any complex scalar λ and nonzero $2n$ -dimensional column vector \mathbf{x} that satisfy (1.1) are called an *eigenvalue* and its associated *eigenvector*, respectively, and correspondingly, (λ, \mathbf{x}) is called an *eigenpair*.

Our consideration of this problem is motivated by Casida’s eigenvalue equations in [1–4]. In computational quantum chemistry and physics, the excitation states and response properties of molecules and clusters are predicted by the linear-response time-dependent density functional theory. The excitation energies and transition vectors (oscillator strengths) of molecular systems can be calculated by solving Casida’s eigenvalue equations [1–3]. There has been a great deal of recent work on and interest in developing efficient numerical algorithms and simulation techniques for computing excitation responses of molecules and for material designs in energy science [5–12].

Let

$$\Gamma_0 = \begin{bmatrix} I_n & 0 \\ 0 & -I_n \end{bmatrix}, \Pi \equiv \Pi_{2n} = \begin{bmatrix} 0 & I_n \\ I_n & 0 \end{bmatrix}. \tag{1.2}$$

The matrix \mathcal{H} in (1.1) satisfies

$$\Gamma_0 \mathcal{H} = \begin{bmatrix} A & B \\ B & A \end{bmatrix} \text{ and } \mathcal{H} \Pi = -\Pi \mathcal{H}. \tag{1.3}$$

As a result of the second equation in (1.3), if (λ, \mathbf{x}) is an eigenpair of \mathcal{H} , i.e., $\mathcal{H} \mathbf{x} = \lambda \mathbf{x}$, then $(-\lambda, \Pi \mathbf{x})$ is also an eigenpair of \mathcal{H} , and if also $\lambda \notin \mathbb{R}$, then $(\bar{\lambda}, \bar{\mathbf{x}})$ and $(-\bar{\lambda}, \Pi \bar{\mathbf{x}})$ are eigenpairs of \mathcal{H} as well, where $\bar{\lambda}$ is the complex conjugate of λ and $\bar{\mathbf{x}}$ takes entrywise complex conjugation.

Previously in [5,6,13], LREP (1.1) was well-studied under the condition that $\Gamma_0 \mathcal{H}$ is positive definite. For the case, all eigenvalues of \mathcal{H} are real. Without the positive definite condition, the methods developed in [5,6,13] are not applicable.

Let \mathbb{J}_n be the set of all $n \times n$ diagonal matrices with ± 1 on the diagonal and set

$$\Gamma_{2n} = \{\text{diag}(J, -J) : J \in \mathbb{J}_n\}.$$

Note that $\Gamma_0 = \text{diag}(I_n, -I_n) \in \Gamma_{2n}$. In this paper, we will study an eigenvalue problem for which the condition that $\Gamma_0 \mathcal{H}$ is positive definite is no longer assumed and it in fact includes LREP (1.1) as a special case. Specifically, we will consider the following eigenvalue problem

$$\mathcal{H} \mathbf{x} \equiv \begin{bmatrix} A & B \\ -B & -A \end{bmatrix} \mathbf{x} = \lambda \mathbf{x} \tag{1.4a}$$

with the structure property:

there is a $\Gamma = \text{diag}(J, -J) \in \mathbf{\Gamma}_{2n}$ with $J = \text{diag}(\pm 1) \in \mathbb{J}_n$ such that $\Gamma \mathcal{H} = \begin{bmatrix} JA & JB \\ JB & JA \end{bmatrix}$ with $JA, JB \in \mathbb{R}^{n \times n}$ being symmetric.

(1.4b)

There are two reasons for considering this more general eigenvalue problem (1.4). The first reason is that this includes (1.1), with/without $\Gamma_0 \mathcal{H}$ being positive definite, as a special case, and the second one is that the intermediate eigenvalue problems in our later iterative Γ QR algorithm for solving (1.1) are of this kind, i.e., with $\Gamma \neq \Gamma_0$.

It can be verified that the second equation in (1.3), $\mathcal{H} \Pi = -\Pi \mathcal{H}$, still holds in the case of (1.4b). Therefore the same results about the eigenvalue pattern we mentioned for (1.1) remain valid. Namely, if (λ, \mathbf{x}) is an eigenpair, then $(-\lambda, \Pi \mathbf{x})$ is also an eigenpair, and if also $\lambda \notin \mathbb{R}$, then $(\bar{\lambda}, \bar{\mathbf{x}})$ and $(-\bar{\lambda}, \Pi \bar{\mathbf{x}})$ are eigenpairs as well. Another interesting result is about the Γ -orthogonality among the eigenvectors of \mathcal{H} . Specifically, for two eigenpairs (λ, \mathbf{x}) and (μ, \mathbf{y}) of \mathcal{H} if $\lambda \neq \bar{\mu}$, then it holds that $\mathbf{y}^H \Gamma \mathbf{x} = 0$, where \mathbf{y}^H is the conjugate transpose of \mathbf{y} . This is because using (1.4b), we have

$$\lambda \mathbf{y}^H \Gamma \mathbf{x} = \mathbf{y}^H \Gamma \mathcal{H} \mathbf{x} = \mathbf{y}^H \mathcal{H}^H \Gamma \mathbf{x} = \bar{\mu} \mathbf{y}^H \Gamma \mathbf{x}$$

and thus $(\lambda - \bar{\mu}) \mathbf{y}^H \Gamma \mathbf{x} = 0$ which yields $\mathbf{y}^H \Gamma \mathbf{x} = 0$ when $\lambda \neq \bar{\mu}$.

The matrix \mathcal{H} in (1.4) has some nice block structures. In fact, the eigenvalue problem (1.4) can be transformed into a special Hamiltonian eigenvalue problem

$$\begin{bmatrix} 0 & JM \\ JK & 0 \end{bmatrix} \begin{bmatrix} \mathbf{y}_1 \\ \mathbf{y}_2 \end{bmatrix} = \lambda \begin{bmatrix} \mathbf{y}_1 \\ \mathbf{y}_2 \end{bmatrix} \text{ with } K = A - B, \quad M = A + B, \tag{1.5}$$

$\mathbf{y}_1 = \mathbf{x}_1 - \mathbf{x}_2$, and $\mathbf{y}_2 = \mathbf{x}_1 + \mathbf{x}_2$. There are several existing structure-preserving approaches [14,15,8,16] that can be applied to solve the eigenvalue problem (1.1), (1.4), or (1.5).

(a) A periodic QR (PQR) algorithm [16] can be used to solve the product eigenvalue problem $(JK)(JM)\mathbf{y}_2 = \lambda^2 \mathbf{y}_2$ for (1.5). Note that only \mathbf{y}_2 is computed directly this way, but \mathbf{y}_1 can be recovered through $\lambda \mathbf{y}_1 = JM \mathbf{y}_2$ for nonzero eigenvalues λ . For $\lambda \neq 0$, we may take any \mathbf{y}_1 such that $K \mathbf{y}_1 = 0$. Once \mathbf{y}_1 and \mathbf{y}_2 are known, $\mathbf{x}_1 = (\mathbf{y}_1 + \mathbf{y}_2)/2$ and $\mathbf{x}_2 = (\mathbf{y}_2 - \mathbf{y}_1)/2$ become available. Conceivably, there is a stability concern in recovering \mathbf{y}_1 for eigenvalues λ tiny in magnitude. PQR uses orthogonal transformations. Here, the $n \times n$ block structure in (1.4) is exploited and the symmetry of the spectrum can be preserved. However, the symmetric structures of JA and JB are destroyed during the iterations.

(b) The KQZ algorithm [8] can be applied to solve \mathcal{H} in (1.1). It uses orthogonal and Π -orthogonal transformations. The block structure $\mathcal{H} \Pi = -\Pi \mathcal{H}$ is preserved

during the KQZ iteration. The reduced matrices JA and JB in (1.4b) are no longer symmetric (tridiagonal), but only Hessenberg. It is mathematically different from the PQR algorithm, but they have the similar amount of computational costs. Later at the end of Section 5 and in Section 6, we will show that they are more expensive than the Γ QR algorithm to be presented.

(c) An HR process proposed by Brebner and Grad (BG) [14] is used to reduce the product eigenvalue problem $(JK)(JM)\mathbf{y}_2 = \lambda^2\mathbf{y}_2$ to a pseudosymmetric form $C\mathbf{z} = \lambda^2J'\mathbf{z}$, where C is symmetric tridiagonal and J' is the inertia sign-matrix of JK or JM . The tridiagonal pseudosymmetry in the BG algorithm is preserved during the HR iterations. The BG algorithm has the similar amount of computational costs as our Γ QR algorithm. However, ill-conditioned K and M may cause the numerical instability of the BG algorithm during constructing J' .

(d) The symplectic QR-like algorithm [15] can also be applied to solve the special Hamiltonian eigenvalue problem (1.5). It uses symplectic transformations. Here the Hamiltonian matrix is reduced to a condensed Hamiltonian form $\begin{bmatrix} H_1 & H_3 \\ H_2 & -H_1 \end{bmatrix}$ with H_1 and H_2 being diagonal and H_3 being symmetric tridiagonal, and then the H_3 -block will be made to converge to a quasi-diagonal matrix during the iterative process. The symplectic QR-like algorithm does not really exploit the symmetry properties of JA and JB . Instability can occur when the symplectic Gaussian elimination matrices at some steps have large condition numbers. This phenomenon cannot be avoided because to maintain the Hamiltonian structure only the Gaussian elimination without pivoting is allowed. Furthermore, the symplectic matrices Q in the symplectic QR-like algorithm satisfy $Q^\top JQ = J$, where $J = \Gamma_0\Pi$. The Γ -orthogonal matrices Q in our Γ QR algorithm (to be presented) satisfy $Q\Pi = \Pi Q$ and $Q^\top \Gamma Q = \Gamma'$ with $\Gamma, \Gamma' \in \Gamma_{2n}$.

(e) The Hamiltonian QR-algorithm [17] uses symplectic orthogonal transformations but it is only suitable for a very special Hamiltonian eigenvalue problem such as in (1.1) or (1.5) with $\text{rank}(B)$ being one, or as in (1.5) with $\text{rank}(K)$, or $\text{rank}(M)$ being one.

The main task of this paper is to develop iterative Γ QR algorithms for solving (1.4), while exploiting the inherent structures in \mathcal{H} and Γ for better numerical efficiency, based on (Γ, Γ') -orthogonal transformations with $\Gamma, \Gamma' \in \Gamma_{2n}$ to be defined in Section 2. The transformations preserve the symmetry structures in $\Gamma\mathcal{H}$ and the diagonal structure of Γ . These Γ QR algorithms may be viewed as extensions of the HR algorithm proposed in [18], a pioneering work for solving the eigenvalue problem of an $n \times n$ matrix \mathcal{A} having the property that there exists a so-called *pseudo-orthogonal* matrix H in the sense that $H^\top JH = J'$ for some $J = \text{diag}(\pm 1)$ and $J' = \text{diag}(\pm 1)$ such that $H^{-1}\mathcal{A}H = R$ is upper triangular. The HR algorithm, however, cannot be applied to LREP (1.4) directly as it does not recognize the 2×2 block structure, among others.

Throughout this paper, we assume that \mathcal{H} in (1.1) is nonsingular, and thus 0 is not its eigenvalue.

The rest of this paper is organized as follows. In Section 2, we introduce some basic definitions and state their immediately implied properties. In Section 3, we first give

two kinds of Γ -orthogonal transformations, and then prove existence and uniqueness of the Γ QR factorization and propose an algorithm to compute the factorization for a given matrix G with $G\Pi = -\Pi G$. In Section 4, we present the Π^- -upper Hessenberg reduction/tridiagonalization and prove the implicit Γ -orthogonality theorem of a Π^- -matrix G . In Section 5, we develop Γ QR algorithms for computing all eigenpairs of \mathcal{H} and analyze their convergence with the goal of an efficient implicit multi-shift Γ QR algorithm. Numerical results of the Γ QR algorithm compared to the other existing algorithm are shown in Section 6. Finally, some conclusions are drawn in Section 7.

Notation. $\mathbb{R}^{n \times m}$ is the set of all $n \times m$ complex matrices with real entries, $\mathbb{R}^n = \mathbb{R}^{n \times 1}$, and $\mathbb{R} = \mathbb{R}^1$. We denote by I_n and $\mathbf{0}_{m \times n}$ ($\mathbf{0}_m$) the $n \times n$ identity matrix and $m \times n$ ($m \times m$) zero matrix, respectively, and their subscripts may be dropped if their sizes can be read from the context. Γ_0 and Π_{2n} are reserved as given by (1.2), and often the subscript to Π_{2n} is dropped, too, when no confusion is possible. The j th column of the identity matrix I is e_j whose size will be determined by the context. We shall also adopt MATLAB-like convention to access the entries of vectors and matrices. Let $i : j$ be the set of integers from i to j inclusive. For a vector \mathbf{u} and a matrix X , $\mathbf{u}_{(j)}$ is the j th entry of \mathbf{u} and $X_{(i,j)}$ is the (i, j) th entry of X ; $X_{(\mathbb{I}_1, \mathbb{I}_2)}$ is the submatrix of X consisting of intersections of all rows $i \in \mathbb{I}_1$ and all columns $j \in \mathbb{I}_2$; X^\top is the transpose of X . We denote by $\text{eig}(A)$ the spectrum of matrix A , and $\text{diag}(X, Y)$ is the 2-by-2 block-diagonal matrix with diagonal blocks X and Y .

2. Definitions and preliminaries

In this section, we introduce several kinds of matrix classes and their essential properties. Recall Π_{2n} defined in (1.2).

Definition 2.1. Let $G \in \mathbb{R}^{2n \times 2m}$ with $m \leq n$. G is called a Π^\pm -matrix if

$$G\Pi_{2m} = \pm\Pi_{2n}G, \text{ i.e., } G = \begin{bmatrix} G_1 & G_2 \\ \pm G_2 & \pm G_1 \end{bmatrix} \text{ with } G_1, G_2 \in \mathbb{R}^{n \times m}. \quad (2.1)$$

Denote by $\Pi_{2n \times 2m}^\pm$ the set of all $2n \times 2m$ Π^\pm -matrices, and $\Pi_{2n}^\pm := \Pi_{2n \times 2n}^\pm$ for short.

In this definition and those below, to save space and avoid repetitions, we often pack two statements into one: one for Π^+ -matrix and the other for Π^- -matrix. In the same spirit, in definitions/statements in the rest of this paper, any of them with phrases in parentheses is understood that the phrases can be used to replace the phrases immediately before for another definition/statement.

We say a matrix X , possibly nonsquare, is *upper Hessenberg* if $X_{(i,j)} = 0$ for $i > j + 1$, *upper triangular* if $X_{(i,j)} = 0$ for $i > j$, and *diagonal* if $X_{(i,j)} = 0$ for $i \neq j$. This is consistent with the standard definitions of upper Hessenberg, upper triangular, and diagonal matrices which are usually for square matrices.

A *quasi-upper triangular matrix* means that it is a block upper triangular matrix with diagonal blocks being 1×1 or 2×2 . Similarly, a *quasi-diagonal matrix* means that it is a block diagonal matrix with diagonal blocks being 1×1 or 2×2 .

Definition 2.2. Let $G \in \Pi_{2n \times 2m}^\pm$ as in (2.1).

1. G is Π^\pm -upper Hessenberg if G_1 is upper Hessenberg and G_2 is upper triangular. G is *unreduced Π^\pm -upper Hessenberg* if G_1 is unreduced upper Hessenberg.
2. G is Π^\pm -upper (Π^\pm -quasi-upper) triangular if G_1 is upper (quasi-upper) triangular and G_2 is strictly upper triangular.

Denote by $\mathbb{U}_{2n \times 2m}^\pm$ ($\text{q}\mathbb{U}_{2n \times 2m}^\pm$) the set of all $2n \times 2m$ Π^\pm -upper (Π^\pm -quasi-upper) triangular matrices, and write, for short, $\mathbb{U}_{2n}^\pm := \mathbb{U}_{2n \times 2n}^\pm$ and $\text{q}\mathbb{U}_{2n}^\pm := \text{q}\mathbb{U}_{2n \times 2n}^\pm$.

3. G is Π^\pm -diagonal (Π^\pm -quasi-diagonal) if G_1 is diagonal (quasi-diagonal) and G_2 is diagonal.

Denote by $\mathbb{D}_{2n \times 2m}^\pm$ ($\text{q}\mathbb{D}_{2n \times 2m}^\pm$) the set of all $2n \times 2m$ Π^\pm -diagonal (Π^\pm -quasi-diagonal) matrices, and write, for short, $\mathbb{D}_{2n}^\pm := \mathbb{D}_{2n \times 2n}^\pm$ and $\text{q}\mathbb{D}_{2n}^\pm := \text{q}\mathbb{D}_{2n \times 2n}^\pm$.

Definition 2.3.

1. Let $G \in \Pi_{2n}^+$ as in (2.1). G is Π^+ -symmetric (Π^+ -sym-tridiagonal), if G_1 is symmetric (symmetric tridiagonal) and G_2 is symmetric (diagonal).
2. Let $G \in \Pi_{2n}^-$ as in (2.1). G is Π^- -symmetric (Π^- -sym-tridiagonal) with respect to $\Gamma \in \Gamma_{2n}$ if ΓG is Π^+ -symmetric (Π^+ -sym-tridiagonal).
3. G is *unreduced Π^\pm -sym-tridiagonal* if it is Π^\pm -sym-tridiagonal and G_1 is unreduced.

The following propositions are direct consequences of Definitions 2.1–2.3 and are rather straightforward to verify.

Proposition 2.1.

- (i) $G \in \Pi_{2n \times 2m}^\pm$ if and only if $\Gamma G \in \Pi_{2n \times 2m}^\mp$ and $G\Gamma' \in \Pi_{2n \times 2m}^\mp$ for any $\Gamma \in \Gamma_{2n}$ and $\Gamma' \in \Gamma_{2m}$.
- (ii) The inverse of a Π^\pm -(upper triangular) matrix is still a Π^\pm -(upper triangular) matrix.
- (iii) The product $\tilde{G}G$ of two $2n \times 2n$ matrices \tilde{G} and G in their respective categories belongs to the one as listed in the following tables:

\tilde{G}	G	Π^+	Π^-
Π^+		Π^+	Π^-
Π^-		Π^-	Π^+

\tilde{G}	G	\mathbb{U}^+	\mathbb{U}^-
\mathbb{U}^+		\mathbb{U}^+	\mathbb{U}^-
\mathbb{U}^-		\mathbb{U}^-	\mathbb{U}^+

Proposition 2.2. Let $G \in \mathbf{II}_{2n}^-$. Then G has $2n$ eigenvalues, appearing in pairs $(\lambda, -\lambda)$ for real or purely imaginary eigenvalues λ and in quadruples $(\pm\lambda, \pm\bar{\lambda})$ for complex eigenvalues λ .

Proof. By Definition 2.1, it holds that

$$\det(G - \lambda I) = \det(\mathbf{II}G - \lambda \mathbf{II}) = \det(G\mathbf{II} + \lambda \mathbf{II}) = \det(G + \lambda I) = 0.$$

The assertion follows immediately. \square

Definition 2.4. $Q \in \mathbf{II}_{2n \times 2m}^+$ is Γ -orthogonal with respect to $\Gamma \in \mathbf{\Gamma}_{2n}$ if $\Gamma' := Q^\top \Gamma Q \in \mathbf{\Gamma}_{2m}$. Denote by $\mathbb{O}_{2n \times 2m}^\Gamma$ the set of all $2n \times 2m$ Γ -orthogonal matrices, and $\mathbb{O}_{2n}^\Gamma := \mathbb{O}_{2n \times 2n}^\Gamma$ for short.

Often, for short, we may say $Q \in \mathbf{II}_{2n \times 2m}^+$ is Γ -orthogonal, by which we mean there is $\Gamma \in \mathbf{\Gamma}_{2n}$ that has the requirement of the definition satisfied. Similarly, we may simply say Q is Γ -orthogonal. The same understanding applies to the expression $Q \in \mathbb{O}_{2n \times 2m}^\Gamma$.

Proposition 2.3. Let $Q_i \in \mathbb{O}_{2n}^\Gamma$ with respect to $\Gamma_i \in \mathbf{\Gamma}_{2n}$ for $i = 1, 2$, and suppose $\Gamma_2 = Q_1^\top \Gamma_1 Q_1$.

- (i) $Q_1 Q_2 \in \mathbb{O}_{2n}^\Gamma$ with respect to Γ_1 .
- (ii) Q_i is nonsingular and $Q_i^{-1} = \Gamma_{i+1} Q_i^\top \Gamma_i$, where $\Gamma_3 := Q_2^\top \Gamma_2 Q_2$.
- (iii) If also $Q_i \in \mathbb{U}_{2n}^+$, then $Q_i = \text{diag}(J_i, J_i)$ for some $J_i \in \mathbb{J}_n$.

Proof. Items (i) and (ii) follow from Definition 2.4 directly. For item (iii), $Q_i^{-1} \in \mathbb{U}_{2n}^+$ by Proposition 2.1(ii). On the other hand, by item (ii), $Q_i^{-1} = \Gamma_{i+1} Q_i^\top \Gamma_i$ which is \mathbf{II}^+ -lower triangular. This implies that $Q_i = \text{diag}(J_i, J_i)$ for some $J_i \in \mathbb{J}_n$, completing the proof of item (iii). \square

3. Γ QR factorization

Definition 3.1. $G = QR$ is called a Γ QR factorization of $G \in \mathbf{II}_{2n \times 2m}^-$ with respect to $\Gamma \in \mathbf{\Gamma}_{2n}$ if $R \in \mathbb{U}_{2n \times 2m}^-$ and $Q \in \mathbb{O}_{2n}^\Gamma$ with respect to Γ or if $R \in \mathbb{U}_{2m}^-$ and $Q \in \mathbb{O}_{2n \times 2m}^\Gamma$ with respect to Γ .

The case when $R \in \mathbb{U}_{2m}^-$ and $Q \in \mathbb{O}_{2n \times 2m}^\Gamma$ with respect to Γ in this definition corresponds to the so-called *skinny* QR factorization in numerical linear algebra.

Definition 3.2. Let $M = \begin{bmatrix} M_1 & M_2 \\ -M_2 & -M_1 \end{bmatrix} \in \mathbf{II}_{2n}^-$, and set

$$M_{1i} = (M_1)_{(1:i, 1:i)}, \quad M_{2i} = (M_2)_{(1:i, 1:i)}.$$

$\begin{bmatrix} M_{1i} & M_{2i} \\ -M_{2i} & -M_{1i} \end{bmatrix}$ is called the i th $\mathbf{\Pi}^-$ -leading principal submatrix of M and its determinant is called the i th $\mathbf{\Pi}^-$ -leading principal minor of M .

The next theorem shows that almost every $\mathbf{\Pi}^-$ -matrix $G \in \mathbf{\Pi}_{2n \times 2m}^-$ has a Γ QR factorization with respect to a given $\Gamma \in \mathbf{\Gamma}_{2n}$ and the factorization is unique if it is required that the top-left quarter of the R -factor has positive diagonal entries.

Theorem 3.1. *Suppose that $G \in \mathbf{\Pi}_{2n \times 2m}^- (m \leq n)$ has full column rank and $\Gamma \in \mathbf{\Gamma}_{2n}$.*

- (i) *If $G = QR = \tilde{Q}\tilde{R}$ (with $Q, \tilde{Q} \in \mathbb{O}_{2n \times 2m}^{\mathbf{\Gamma}}$ and $R, \tilde{R} \in \mathbb{U}_{2m}^-$) are two Γ QR factorizations of G with respect to Γ , then*

$$\tilde{Q}^\top \Gamma \tilde{Q} = Q^\top \Gamma Q \in \mathbf{\Gamma}_{2m}$$

and there is a $\mathbf{\Pi}^+$ -diagonal matrix $D = \text{diag}(J, J)$ with $J \in \mathbb{J}_m$ such that $\tilde{Q} = QD$ and $\tilde{R} = DR$. In particular, if the top-left quarters of R and \tilde{R} have positive diagonal entries, then $D = I_{2m}$, $Q = \tilde{Q}$, and $R = \tilde{R}$.

- (ii) *G has a Γ QR factorization with respect to Γ if and only if no $\mathbf{\Pi}^-$ -leading principal minor of $G^\top \Gamma G$ vanishes.*

Proof. We first prove item (i). Let $\Gamma' = Q^\top \Gamma Q$ and $\tilde{\Gamma}' = \tilde{Q}^\top \Gamma \tilde{Q}$. From the assumption we have

$$\Gamma' R = Q^\top \Gamma QR = Q^\top \Gamma \tilde{Q}\tilde{R} \Rightarrow Q^\top \Gamma \tilde{Q} = \Gamma' R \tilde{R}^{-1}.$$

Similarly, $\tilde{Q}^\top \Gamma Q = \tilde{\Gamma}' \tilde{R} R^{-1}$. Therefore

$$\tilde{\Gamma}' \tilde{R} R^{-1} = \tilde{Q}^\top \Gamma Q = (Q^\top \Gamma \tilde{Q})^\top = (\Gamma' R \tilde{R}^{-1})^\top = \tilde{R}^{-\top} R^\top \Gamma'. \tag{3.1}$$

Because $\tilde{\Gamma}' \tilde{R} R^{-1} \in \mathbb{U}_{2m}^-$ and at the same time $\tilde{R}^{-\top} R^\top \Gamma'$ is $\mathbf{\Pi}^-$ -lower triangular, we conclude that $\tilde{R} R^{-1}$ and $\tilde{R}^{-\top} R^\top$ must be diagonal. Set

$$D = \tilde{R} R^{-1} \in \mathbf{\Pi}_{2m}^+ \tag{3.2}$$

which implies $\tilde{R}^{-\top} R^\top = (\tilde{R} R^{-1})^{-\top} = D^{-1}$. Thus, from (3.1) and (3.2), we have $\tilde{\Gamma}' D = \tilde{Q}^\top \Gamma Q$ and $\Gamma' D^{-1} = Q^\top \Gamma \tilde{Q}$. This implies $\Gamma' = D \tilde{\Gamma}' D$, and thus

$$D^2 = I_{2m}, \quad \Gamma' = \tilde{\Gamma}' \in \mathbf{\Gamma}_{2m}.$$

So $D = \text{diag}(J, -J)$ for some $J \in \mathbb{J}_m$ and $\tilde{R} = DR$. Furthermore, since $G = QR = \tilde{Q}\tilde{R}$ has full column rank, it follows that $\tilde{Q} = QD$.

Now if also the top-left quarters of R and \tilde{R} have positive diagonal entries, then $\tilde{R} = DR$ implies $D = I_{2m}$, as expected.

Next we prove item (ii).

Necessity. Let P be the permutation matrix

$$P = [e_1, e_3, \dots, e_{2m-1} \mid e_2, e_4, \dots, e_{2m}] \in \mathbb{R}^{2m \times 2m}. \tag{3.3}$$

Suppose that $G = QR$ is a Γ QR factorization with respect to Γ , and let $\Gamma' = Q^\top \Gamma Q$. Then

$$P^\top G^\top \Gamma G P = (P^\top R^\top P)(P^\top \Gamma' P)(P^\top R P) =: R_{\mathbf{p}}^\top \Gamma'_{\mathbf{p}} R_{\mathbf{p}},$$

where $R_{\mathbf{p}} = P^\top R P$ is upper triangular and $\Gamma'_{\mathbf{p}} = P^\top \Gamma' P$ is diagonal, as in

$$R_{\mathbf{p}} = \begin{bmatrix} R_{11} & \cdots & R_{1m} \\ \vdots & \ddots & \vdots \\ 0 & \cdots & R_{mm} \end{bmatrix}, \quad \Gamma'_{\mathbf{p}} = \begin{bmatrix} \Gamma'_{11} & & 0 \\ & \ddots & \\ 0 & & \Gamma'_{mm} \end{bmatrix} \tag{3.4}$$

with $R_{ij} \in \mathbf{II}_2^-$, $R_{ii} = \begin{bmatrix} d_i & 0 \\ 0 & -d_i \end{bmatrix}$, and $\Gamma'_{ii} \in \mathbf{I}_2$ for $i, j = 1, \dots, m$. Since G has full column rank, it follows that $\det(R_{ii}) \neq 0$ for $i = 1, \dots, m$. Therefore, there is no leading principal minor of $P^\top G^\top \Gamma G P$ of even order vanishes, i.e., no \mathbf{II}^- -leading principal minor of $G^\top \Gamma G$ vanishes.

Sufficiency. Suppose that $G \in \mathbf{II}_{2n \times 2m}^-$ and no \mathbf{II}^- -leading principal minor of $M := G^\top \Gamma G$ vanishes. Then there is an LU factorization of $M_{\mathbf{p}} := P^\top M P$, i.e., $M_{\mathbf{p}} = L_{\mathbf{p}} \widehat{R}_{\mathbf{p}}$ with nonsingular

$$L_{\mathbf{p}} = \begin{bmatrix} I_2 & & & & 0 \\ L_{21} & I_2 & & & \\ \vdots & \ddots & \ddots & & \\ L_{m1} & \cdots & L_{m,m-1} & I_2 \end{bmatrix}, \quad \widehat{R}_{\mathbf{p}} = \begin{bmatrix} \widehat{R}_{11} & \cdots & \widehat{R}_{1m} \\ & \ddots & \vdots \\ 0 & & \widehat{R}_{mm} \end{bmatrix}, \tag{3.5}$$

where $L_{ij} \in \mathbf{II}_2^+$ and $\widehat{R}_{ij} \in \mathbf{II}_2^-$. Decompose $\widehat{R}_{\mathbf{p}}$ as

$$\widehat{R}_{\mathbf{p}} = \begin{bmatrix} \widehat{R}_{11} & & 0 \\ & \ddots & \\ 0 & & \widehat{R}_{mm} \end{bmatrix} \begin{bmatrix} I_2 & R_{12} & \cdots & R_{1m} \\ & \ddots & \ddots & \vdots \\ & & \ddots & R_{m-1,m} \\ & & & I_2 \end{bmatrix} =: \widehat{D}_{\mathbf{p}} R_{\mathbf{p}} \tag{3.6}$$

with $R_{ij} = \widehat{R}_{ii}^{-1} \widehat{R}_{ij} \in \mathbf{II}_2^+$. Then we have

$$M_{\mathbf{p}} = L_{\mathbf{p}} \widehat{R}_{\mathbf{p}} = L_{\mathbf{p}} \widehat{D}_{\mathbf{p}} R_{\mathbf{p}} = R_{\mathbf{p}}^\top \widehat{D}_{\mathbf{p}}^\top L_{\mathbf{p}}^\top = M_{\mathbf{p}}^\top. \tag{3.7}$$

The uniqueness of the LU factorization implies that $L_{\mathbf{p}}^{\top} = R_{\mathbf{p}}$. Since $M_{\mathbf{p}}$ is symmetric, it follows that $\widehat{D}_{\mathbf{p}} = \text{diag}(\{\widehat{R}_{ii}\}_{i=1}^m)$ is symmetric. Because $\widehat{R}_{ii} \in \mathbf{II}_2^{-}$, \widehat{R}_{ii} must be of the form $\widehat{R}_{ii} = \begin{bmatrix} d_i & 0 \\ 0 & -d_i \end{bmatrix}$ for $i = 1, \dots, m$. Write

$$\widehat{R}_{ii} = \begin{bmatrix} \sqrt{|d_i|} & 0 \\ 0 & \sqrt{|d_i|} \end{bmatrix} \begin{bmatrix} \text{sgn}(d_i) & 0 \\ 0 & -\text{sgn}(d_i) \end{bmatrix} \begin{bmatrix} \sqrt{|d_i|} & 0 \\ 0 & \sqrt{|d_i|} \end{bmatrix}$$

and denote

$$D_{\mathbf{p}}^{1/2} = \text{diag}\left(\left\{\begin{bmatrix} \sqrt{|d_i|} & 0 \\ 0 & \sqrt{|d_i|} \end{bmatrix}\right\}_{i=1}^m\right), \quad \Gamma'_{\mathbf{p}} = \text{diag}\left(\left\{\begin{bmatrix} \text{sgn}(d_i) & 0 \\ 0 & -\text{sgn}(d_i) \end{bmatrix}\right\}_{i=1}^m\right). \tag{3.8}$$

From (3.7) and (3.8) we have

$$G^{\top} \Gamma G = P M_{\mathbf{p}} P^{\top} = (P L_{\mathbf{p}} D_{\mathbf{p}}^{1/2} P^{\top})(P \Gamma'_{\mathbf{p}} P^{\top})(P D_{\mathbf{p}}^{1/2} L_{\mathbf{p}}^{\top} P^{\top}) =: R^{\top} \Gamma' R, \tag{3.9}$$

where $R = P D_{\mathbf{p}}^{1/2} L_{\mathbf{p}}^{\top} P^{\top} \in \mathbb{U}_{2m}^{+}$ and $\Gamma' = P \Gamma'_{\mathbf{p}} P^{\top}$. Let

$$Q_{-} := G R^{-1} \Gamma' \in \mathbf{II}_{2n \times 2m}^{+}. \tag{3.10}$$

With the help of (3.9), it can be verified that

$$Q_{-}^{\top} \Gamma Q_{-} = (\Gamma' R^{-\top} G^{\top}) \Gamma (G R^{-1} \Gamma') = \Gamma' R^{-\top} (R^{\top} \Gamma' R) R^{-1} \Gamma' = \Gamma'$$

which says $Q_{-} \in \mathbb{O}_{2n \times 2m}^{\Gamma}$. Therefore

$$G = (G R^{-1} \Gamma') (\Gamma' R) =: Q_{-} R_{-} \quad \text{with} \quad R_{-} \in \mathbb{U}_{2m}^{-} \tag{3.11}$$

to give $G = Q R$, a Γ QR factorization. \square

Our goal in this paper is to develop a structure-preserving QR-like algorithm to compute all eigenvalues of $\mathcal{H} \in \mathbf{II}_{2n}^{-}$. The basic idea is to calculate a sequence of Γ -orthogonal matrices $\{Q_i\}$, based on a Γ QR factorization, such that

$$\mathcal{H}_{i+1} = Q_i^{-1} \mathcal{H}_i Q_i, \quad Q_i^{\top} \Gamma_i Q_i = \Gamma_{i+1} \quad \text{for } i = 1, 2, \dots,$$

where initially $\mathcal{H}_0 = \mathcal{H}$. For this purpose, at first, we introduce two elementary Γ -orthogonal transformations which will be used to zero out a specific entry or entries of a vector. Specifically, given $\Gamma \in \mathbf{\Gamma}_{2n}$ and $\mathbf{u} \in \mathbb{R}^{2n}$, we seek $Q \in \mathbb{O}_{2n}^{\Gamma}$ to zero out some portion of \mathbf{u} . Two different kinds of matrices Q will be used to deal with all possible scenarios that will occur in computing the Γ QR factorizations in Algorithm 3.1 later.

Let $\mathbf{a} \in \mathbb{R}^k$ ($1 \leq k \leq n$), $J \equiv \text{diag}(j_1, \dots, j_k) \in \mathbb{J}_k$. Assume that $\mathbf{a}^\top J \mathbf{a} \neq 0$. Let P_a be a permutation which interchanges row 1 and a row r ($2 \leq r \leq k$) of J such that $\hat{j}_1 \mathbf{a}^\top J \mathbf{a} = \hat{j}_1 \hat{\mathbf{a}}^\top \hat{J} \hat{\mathbf{a}} > 0$, where $\hat{\mathbf{a}} = P_a \mathbf{a}$ and $\hat{J} = P_a J P_a = \text{diag}(\hat{j}_1, \dots, \hat{j}_k)$. A Householder-like transformation is proposed by [18] to zero out the elements of $\hat{\mathbf{a}}_{(2:k)}$ as follows. Let

$$H(\mathbf{a})^{-1} = I - \frac{\hat{j}_1}{\beta} (\hat{\mathbf{a}} - \alpha e_1) (\hat{\mathbf{a}} - \alpha e_1)^\top \hat{J}, \quad \hat{H}(\mathbf{a})^{-1} = H(\mathbf{a})^{-1} P_a, \tag{3.12a}$$

where $\alpha = -\text{sign}(\hat{\mathbf{a}}_{(1)}) \sqrt{\hat{j}_1 \hat{\mathbf{a}}^\top \hat{J} \hat{\mathbf{a}}}$ and $\beta = \alpha[\alpha - \hat{\mathbf{a}}_{(1)}]$. Then it can be verified that

$$\hat{H}(\mathbf{a})^{-1} \mathbf{a} = [H(\mathbf{a})^{-1} P_a] \mathbf{a} = H(\mathbf{a})^{-1} \hat{\mathbf{a}} = \alpha e_1, \quad \hat{H}(\mathbf{a})^\top J \hat{H}(\mathbf{a}) = \hat{J}. \tag{3.12b}$$

Hyp_Householder (hyperbolic Householder) transformation: Suppose $1 \leq \ell < m \leq n$, $\mathbf{u} \in \mathbb{R}^{2n}$ and $\Gamma = \text{diag}(\gamma_1, \dots, \gamma_n, -\gamma_1, \dots, -\gamma_n) \in \mathbf{\Gamma}_{2n}$. There are two cases:

Case 1. $\mathbf{a} \leftarrow \mathbf{u}_{(\ell':m')}$ with $\ell' = n + \ell$ and $m' = n + m$, $J = \text{diag}(\gamma_\ell, \dots, \gamma_m)$;

Case 2. $\mathbf{a} \leftarrow \mathbf{u}_{(\ell:m)}$, $J = \text{diag}(\gamma_\ell, \dots, \gamma_m)$.

Using (3.12) we construct a hyperbolic Householder Γ -orthogonal transformation Q with respect to Γ through its inverse by

$$Q^{-1} = \begin{cases} \mathcal{Q}_h(\ell' : m'; \mathbf{u}), & \text{case 1;} \\ \mathcal{Q}_h(\ell : m; \mathbf{u}), & \text{case 2,} \end{cases} \\ := \text{diag}(I_{\ell-1}, \hat{H}(\mathbf{a})^{-1}, I_{n-m}, I_{\ell-1}, \hat{H}(\mathbf{a})^{-1}, I_{n-m}). \tag{3.13}$$

Then it holds that

$$Q^{-1} \mathbf{u} = \hat{\mathbf{u}} \text{ with } \begin{cases} \hat{\mathbf{u}}_{(\ell'+1:m')} = 0, & \text{case 1;} \\ \hat{\mathbf{u}}_{(\ell+1:m)} = 0, & \text{case 2,} \end{cases} \tag{3.14}$$

and $Q^\top \Gamma Q = \Gamma'$, where $\Gamma' = (\gamma'_1, \dots, \gamma'_n, -\gamma'_1, \dots, -\gamma'_n)$ is given by

$$\begin{cases} \gamma'_s = \gamma_s, & s = 1, \dots, \ell - 1 \text{ and } m + 1, \dots, n, \\ \gamma'_{s+\ell-1} = \hat{j}_s, & s = 1, \dots, m - \ell + 1. \end{cases} \tag{3.15}$$

Hyp_Givens (hyperbolic Givens) transformation: Suppose $1 \leq \ell \leq n$, $\mathbf{u} \in \mathbb{R}^{2n}$ and $\Gamma = \text{diag}(\gamma_1, \dots, \gamma_n, -\gamma_1, \dots, -\gamma_n) \in \mathbf{\Gamma}_{2n}$. Let $\alpha \leftarrow \mathbf{u}_{(\ell)}$, $\beta \leftarrow \mathbf{u}_{(n+\ell)}$. Define

$$\begin{cases} c = \frac{1}{\sqrt{1-r^2}}, s = \frac{r}{\sqrt{1-r^2}} \text{ with } r = \frac{\beta}{\alpha}, \text{ if } |\alpha| > |\beta|, \\ c = \frac{r}{\sqrt{1-r^2}}, s = \frac{1}{\sqrt{1-r^2}} \text{ with } r = \frac{\alpha}{\beta}, \text{ if } |\alpha| < |\beta|. \end{cases} \tag{3.16}$$

Algorithm 3.1 Γ QR factorization.

Input: $G \in \mathbf{II}_{2n \times 2m}^-$, $\Gamma = \text{diag}(J, -J) \in \Gamma_{2n}$ with $J = \text{diag}(\gamma_1, \dots, \gamma_n)$, $n' \leftarrow 2n$;

Output: $Q \in \mathbb{O}_{2n}^{\Gamma}$ with respect to Γ , $\Gamma' = Q^{\top} \Gamma Q \in \mathbb{J}_n$, and $R \in \mathbb{U}_{2m}^-$ such that $G = QR$;

```

1:  $Q \leftarrow I_{2n}$ ,  $\Gamma_{\text{sav}} \leftarrow \Gamma$ ;
2: for  $\ell = 1 : m$  do
3:    $\ell' \leftarrow n + \ell$ ,  $\mathbf{u} \leftarrow G_{(:, \ell)}$ ;
4:   compute Hyp_Householder  $\Gamma$ -orthogonal transformation:  $\tilde{Q}^{-1} = \mathcal{Q}_h(\ell' : n'; \mathbf{u})$  with respect to  $\Gamma$ 
   (by (3.13));
5:    $Q \leftarrow Q\tilde{Q}$ ,  $G \leftarrow \tilde{Q}^{-1}G$ ,  $\Gamma \leftarrow -\Gamma'$  (by (3.15));
6:    $\alpha \leftarrow G_{(\ell, \ell)}$ ,  $\beta \leftarrow G_{(\ell', \ell)}$ ;
7:   compute Hyp_Givens  $\Gamma$ -orthogonal transformation:  $\tilde{Q}^{-1} = \mathcal{Q}_g(\ell; \alpha, \beta)$  with respect to  $\Gamma$  (by (3.17));
8:    $Q \leftarrow Q\tilde{Q}$ ,  $G \leftarrow \tilde{Q}^{-1}G$ ,  $\Gamma \leftarrow \Gamma'$  (by (3.18));
9:    $\mathbf{u} \leftarrow G_{(:, \ell)}$ ;
10:  compute Hyp_Householder  $\Gamma$ -orthogonal transformation:  $\tilde{Q}^{-1} = \mathcal{Q}_h(\ell : n; \mathbf{u})$  with respect to  $\Gamma$  (by
   (3.13));
11:   $Q \leftarrow Q\tilde{Q}$ ,  $G \leftarrow \tilde{Q}^{-1}G$ ,  $\Gamma \leftarrow \Gamma'$  (by (3.18));
12: end for
13: return  $Q \leftarrow Q_{(:, \{1:m, n+1:n+m\})}$ ,  $\Gamma' \leftarrow \Gamma$ ,  $\Gamma \leftarrow \Gamma_{\text{sav}}$ , and  $R = \begin{bmatrix} G_{(1:m, :)} \\ G_{(n+1:n+m, :)} \end{bmatrix}$ .
```

We construct a hyperbolic Givens Γ -orthogonal transformation with respect to Γ through its inverse by

$$Q^{-1} = \mathcal{Q}_g(\ell; \alpha; \beta) = \begin{bmatrix} C & S \\ S & C \end{bmatrix} \in \mathbf{II}_{2n}^+, \tag{3.17}$$

where C is obtained from I_n by resetting $C_{(\ell, \ell)} = c$ and S from $O_{n \times n}$ by resetting $S_{(\ell, \ell)} = -s$. Then we have

$$Q^{-1}\mathbf{u} = \hat{\mathbf{u}} \quad \text{with} \quad \hat{\mathbf{u}}_{(n+\ell)} = 0,$$

and $Q^{\top} \Gamma Q = \Gamma'$, where

$$\begin{cases} \gamma'_{\ell} = \delta \gamma_{\ell}, & \delta = c^2 - s^2 = \pm 1, \\ \gamma'_j = \gamma_j, & j \neq \ell. \end{cases} \tag{3.18}$$

Remark 3.1.

- (i) Utilizing the special structure of \mathbf{II}^- -matrix $G \in \mathbf{II}_{2n \times 2m}^-$, \tilde{Q}^{-1} at lines 4, 7 and 10 of Algorithm 3.1 eliminates the $(n + \ell + 1 : 2n, \ell)$ and $(\ell + 1 : n, \ell)$ or the $(n + \ell, \ell)$ th and $(\ell, n + \ell)$ th or the $(\ell + 1 : n, \ell)$ and $(n + \ell + 1 : 2n, \ell)$ entries of G simultaneously, for $\ell = 1, \dots, m$.
- (ii) Upon exit, Algorithm 3.1 computes $G = QR$, where $Q \in \mathbb{O}_{2n}^{\Gamma}$ is a Γ -orthogonal matrix with respect to Γ and $R \in \mathbb{U}_{2m}^-$. It is worth noting that Γ' is unknown before $G = QR$ is computed but it is unique, according to Theorem 3.1(i).

In the following, we use a small example with $n = 3$ and $m = 2$ by Wilkinson’s diagram to illustrate the elimination process in computing a Γ QR factorization of G .

$$\begin{array}{ccc}
 \left[\begin{array}{cc|cc} \times & \times & \times & \times \\ \times & \times & \times & \times \\ \times & \times & \times & \times \\ \hline \times & \times & \times & \times \\ \times & \times & \times & \times \\ \times & \times & \times & \times \end{array} \right] & \xrightarrow[= \tilde{Q}_1^{-1}]{Q_h(4;6;\mathbf{u})} & \left[\begin{array}{cc|cc} \times & \times & \times & \times \\ \times & \times & 0 & \times \\ \times & \times & 0 & \times \\ \hline \times & \times & \times & \times \\ 0 & \times & \times & \times \\ 0 & \times & \times & \times \end{array} \right] & \xrightarrow[= \tilde{Q}_2^{-1}]{Q_g(1;\alpha,\beta)} & \left[\begin{array}{cc|cc} \times & \times & 0 & \times \\ \times & \times & 0 & \times \\ \times & \times & 0 & \times \\ \hline 0 & \times & \times & \times \\ 0 & \times & \times & \times \\ 0 & \times & \times & \times \end{array} \right] \\
 & & \xrightarrow[= \tilde{Q}_3^{-1}]{Q_h(1;3;\mathbf{u})} & & \xrightarrow[= \tilde{Q}_4^{-1}]{Q_h(5;6;\mathbf{u})} & \\
 & & \left[\begin{array}{cc|cc} \times & \times & 0 & \times \\ 0 & \times & 0 & \times \\ 0 & \times & 0 & \times \\ \hline 0 & \times & \times & \times \\ 0 & \times & 0 & \times \\ 0 & \times & 0 & \times \end{array} \right] & & \left[\begin{array}{cc|cc} \times & \times & 0 & \times \\ 0 & \times & 0 & \times \\ 0 & \times & 0 & 0 \\ \hline 0 & \times & \times & \times \\ 0 & \times & 0 & \times \\ 0 & 0 & 0 & \times \end{array} \right] \\
 & & \xrightarrow[= \tilde{Q}_5^{-1}]{Q_g(2;\alpha,\beta)} & & \xrightarrow[= \tilde{Q}_6^{-1}]{Q_h(2;3;\mathbf{u})} & \\
 & & \left[\begin{array}{cc|cc} \times & \times & 0 & \times \\ 0 & \times & 0 & 0 \\ 0 & \times & 0 & 0 \\ \hline 0 & \times & \times & \times \\ 0 & 0 & 0 & \times \\ 0 & 0 & 0 & \times \end{array} \right] & & \left[\begin{array}{cc|cc} \times & \times & 0 & \times \\ 0 & \times & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \hline 0 & \times & \times & \times \\ 0 & 0 & 0 & \times \\ 0 & 0 & 0 & 0 \end{array} \right]
 \end{array}$$

In general, after m steps we have computed $3m$ Γ -orthogonal matrices $\tilde{Q}_1^{-1}, \dots, \tilde{Q}_{3m}^{-1}$ such that $(\tilde{Q}_{3m}^{-1} \times \dots \times \tilde{Q}_1^{-1})G = R$ is a \mathbf{II}^- -upper triangular.

Remark 3.2. Theorem 3.1(ii) reveals that almost all matrices in $\mathbf{II}_{2n \times 2m}^- (m \leq n)$ have Γ QR factorizations. In practice, for a given $2n \times 2m$ \mathbf{II}^- -matrix G , one way to construct its Γ QR factorization with respect to given $\Gamma \in \Gamma_{2n}$ is through reducing G to a $2n \times 2m$ \mathbf{II}^- -upper triangular matrix by a sequence of Γ -orthogonal transformations: Hyp_Householder Γ -orthogonal transformations and Hyp_Givens Γ -orthogonal transformations. The Hyp_Householder transformation in (3.12a) may not exist if $\hat{\mathbf{a}}^\top J \hat{\mathbf{a}} = 0$. Similarly, the Hyp_Givens transformation in (3.17) may not exist if $|\alpha| = |\beta|$. In [19], it is said that these cases can occur when the matrix is artificially designed. There is clearly a numerical stability issue if $\hat{\mathbf{a}}^\top J \hat{\mathbf{a}} \approx 0$ or $|\alpha| \approx |\beta|$. The danger of severe cancellation can occur and is discussed in [20,21]. If a dangerous cancellation occurs at some ℓ th step of Algorithm 3.1, it is recommended to pre-multiply the current G by a randomly generated Γ -orthogonal \tilde{Q}^{-1} with $\tilde{Q}^\top \Gamma \tilde{Q} = \Gamma'$. Then we set $G \leftarrow \tilde{Q}^{-1}G$, $\Gamma \leftarrow \Gamma'$, and continue performing Algorithm 3.1 from the ℓ th step. It usually can successfully circumvent the cancellation by this [20,21].

4. Implicit Γ -orthogonality theorem

Here and hereafter we suppose that $\mathcal{H} \in \Pi_{2n}^-$ is Π^- -symmetric with respect to $\Gamma \in \Gamma_{2n}$.

Definition 4.1. Given $\mathbf{q}_1 \in \mathbb{R}^{2n}$ with $\mathbf{q}_1^\top \Gamma \mathbf{q}_1 = \pm 1$. For $1 \leq m \leq n$, the m th order Π^+ -Krylov matrix of \mathcal{H} on \mathbf{q}_1 is defined as

$$K_{2m} \equiv K_{2m}(\mathcal{H}, \mathbf{q}_1) := \left[\mathbf{q}_1, \mathcal{H}\mathbf{q}_1, \dots, \mathcal{H}^{m-1}\mathbf{q}_1 \mid \Pi\mathbf{q}_1, \Pi(\mathcal{H}\mathbf{q}_1), \dots, \Pi(\mathcal{H}^{m-1}\mathbf{q}_1) \right] \in \mathbb{R}^{2n \times 2m}. \tag{4.1}$$

Let $\mathcal{K}_{2m} \equiv \mathcal{K}_{2m}(\mathcal{H}, \mathbf{q}_1)$ be the subspace spanned by the columns of K_{2m} .

Theorem 4.1. Let $K_{2m} \equiv K_{2m}(\mathcal{H}, \mathbf{q}_1)$ be the Π^+ -Krylov matrix (4.1), where $m \leq n$. Suppose $\text{rank}(K_{2m}) = 2m$, and let $K_{2m} = Q_{2m}R_{2m}$ (with $Q_{2m} \in \mathbb{O}_{2n \times 2m}^\Gamma$ and $R_{2m} \in \mathbb{U}_{2m}^-$) be a Γ QR factorization with respect to Γ and set $\Gamma' = Q_{2m}^\top \Gamma Q_{2m} \in \Gamma_{2m}$. Then

$$\mathcal{H}Q_{2m} = Q_{2m}T_{2m} + \mathbf{z}_m \mathbf{e}_m^\top - \Pi \mathbf{z}_m \mathbf{e}_{2m}^\top, \tag{4.2a}$$

$$Q_{2m}^\top \Gamma \mathbf{z}_m = Q_{2m}^\top \Gamma (\Pi \mathbf{z}_m) = 0, \tag{4.2b}$$

$$T_{2m} = (\Gamma' Q_{2m}^\top \Gamma) \mathcal{H} Q_{2m}, \tag{4.2c}$$

for some $\mathbf{z}_m \in \mathbb{R}^{2n}$, and $\Gamma' T_{2m}$ is unreduced Π^+ -sym-tridiagonal, i.e., T_{2m} is unreduced Π^- -sym-tridiagonal with respect to Γ' .

Proof. Since $K_{2m} = Q_{2m}R_{2m}$ has full column rank and is the $2n \times 2m$ Π^+ -Krylov matrix by assumption, R_{2m} is Π^+ -upper triangular and nonsingular and so is R_{2m}^{-1} . Using $\mathcal{H}\Pi = -\Pi\mathcal{H}$, we have

$$\begin{aligned} \mathcal{H}K_{2m} &= \mathcal{H} \left[\mathbf{q}_1, \mathcal{H}\mathbf{q}_1, \dots, \mathcal{H}^{m-1}\mathbf{q}_1, \Pi\mathbf{q}_1, \Pi(\mathcal{H}\mathbf{q}_1), \dots, \Pi(\mathcal{H}^{m-1}\mathbf{q}_1) \right] \\ &= K_{2m}C_{2m} + \mathcal{H}^m \mathbf{q}_1 \mathbf{e}_m^\top - \Pi(\mathcal{H}^m \mathbf{q}_1 \mathbf{e}_{2m}^\top), \end{aligned} \tag{4.3}$$

where $C_{2m} = \text{diag}(C_1, -C_1)$ with $C_1 = \begin{bmatrix} \mathbf{0}_{(m-1) \times 1}^\top & 0 \\ I_{m-1} & \mathbf{0}_{(m-1) \times 1} \end{bmatrix}$. Substituting K_{2m} by $Q_{2m}R_{2m}$ into (4.3), we get

$$\begin{aligned} \mathcal{H}Q_{2m} &= Q_{2m} \left[\underbrace{R_{2m}C_{2m}R_{2m}^{-1} + \Gamma' Q_{2m}^\top \Gamma (\mathcal{H}^m \mathbf{q}_1 \mathbf{e}_m^\top - \Pi \mathcal{H}^m \mathbf{q}_1 \mathbf{e}_{2m}^\top) R_{2m}^{-1}}_{=: T_{2m}} \right] \\ &\quad + (I - Q_{2m} \Gamma' Q_{2m}^\top \Gamma) (\mathcal{H}^m \mathbf{q}_1 \mathbf{e}_m^\top - \Pi \mathcal{H}^m \mathbf{q}_1 \mathbf{e}_{2m}^\top) R_{2m}^{-1}. \end{aligned} \tag{4.4}$$

Set $\gamma_{mm} = \mathbf{e}_m^\top R_{2m}^{-1} \mathbf{e}_m = \mathbf{e}_{2m}^\top R_{2m}^{-1} \mathbf{e}_{2m}$ and $\mathbf{z}_m = \gamma_{mm}(I - Q_{2m} \Gamma' Q_{2m}^\top \Gamma) \mathcal{H}^m \mathbf{q}_1$. From (4.4), we have

$$\mathcal{H} Q_{2m} = Q_{2m} T_{2m} + \mathbf{z}_m \mathbf{e}_m^\top - \Pi \mathbf{z}_m \mathbf{e}_{2m}^\top. \tag{4.5}$$

From the fact that $Q_{2m}^\top \Gamma Q_{2m} = \Gamma'$ it follows that

$$Q_{2m}^\top \Gamma \mathbf{z}_m = Q_{2m}^\top \Gamma (\Pi \mathbf{z}_m) = 0. \tag{4.6}$$

Therefore $(\Gamma' Q_{2m}^\top \Gamma) \mathcal{H} Q_{2m} = T_{2m}$ by (4.5) and (4.6). Because C_{2m} in (4.4) is unreduced $\mathbf{\Pi}^-$ -upper Hessenberg, by Proposition 2.1 we know that T_{2m} is unreduced $\mathbf{\Pi}^+$ -upper Hessenberg. Furthermore, since \mathcal{H} is $\mathbf{\Pi}^-$ -symmetric with respect to Γ , $Q_{2m}^\top \Gamma \mathcal{H} Q_{2m}$ is $\mathbf{\Pi}^+$ -sym-tridiagonal and thus T_{2m} is $\mathbf{\Pi}^-$ -sym-tridiagonal with respect to Γ' . This completes the proof. \square

Theorem 4.2. Let $Q_{2m} \in \mathbb{R}^{2n \times 2m}$ ($m \leq n$) be Γ -orthogonal with respect to Γ such that $Q_{2m} \mathbf{e}_1 = \mathbf{q}_1$. Let $\Gamma' = Q_{2m}^\top \Gamma Q_{2m}$. If Q_{2m} satisfies (4.2a) for some unreduced $\mathbf{\Pi}^+$ -sym-tridiagonal, $\Gamma' T_{2m}$ and $\mathbf{z}_m \in \mathbb{R}^{2n}$, then

$$\begin{aligned} K_{2m}(\mathcal{H}, \mathbf{q}_1) &= Q_{2m} \left[\mathbf{e}_1, T_{2m} \mathbf{e}_1, \dots, T_{2m}^{m-1} \mathbf{e}_1, \Pi \mathbf{e}_1, \Pi(T_{2m} \mathbf{e}_1), \dots, \Pi(T_{2m}^{m-1} \mathbf{e}_1) \right] \\ &=: Q_{2m} R_{2m} \end{aligned} \tag{4.7}$$

is a Γ QR factorization of $K_{2m}(\mathcal{H}, \mathbf{q}_1)$ and $\text{rank}(K_{2m}(\mathcal{H}, \mathbf{q}_1)) = 2m$.

Proof. It holds that

$$\mathcal{H} \mathbf{q}_1 = \mathcal{H} Q_{2m} \mathbf{e}_1 = (Q_{2m} T_{2m} + \mathbf{z}_m \mathbf{e}_m^\top - \Pi \mathbf{z}_m \mathbf{e}_{2m}^\top) \mathbf{e}_1 = Q_{2m} T_{2m} \mathbf{e}_1. \tag{4.8}$$

Assume that $\mathcal{H}^{i-1} \mathbf{q}_1 = \mathcal{H}^{i-1} Q_{2m} \mathbf{e}_1 = Q_{2m} T_{2m}^{i-1} \mathbf{e}_1$ holds for $i = 2, \dots, m - 1$. Then

$$\begin{aligned} \mathcal{H}^i \mathbf{q}_1 &= \mathcal{H} Q_{2m} T_{2m}^{i-1} \mathbf{e}_1 \\ &= (Q_{2m} T_{2m} + \mathbf{z}_m \mathbf{e}_m^\top - \Pi \mathbf{z}_m \mathbf{e}_{2m}^\top) T_{2m}^{i-1} \mathbf{e}_1 \\ &= Q_{2m} T_{2m}^i \mathbf{e}_1 + \mathbf{z}_m \mathbf{e}_m^\top T_{2m}^{i-1} \mathbf{e}_1 - \Pi \mathbf{z}_m \mathbf{e}_{2m}^\top T_{2m}^{i-1} \mathbf{e}_1. \end{aligned}$$

It can be verified that $\mathbf{e}_m^\top T_{2m}^{i-1} \mathbf{e}_1 = \mathbf{e}_{2m}^\top T_{2m}^{i-1} \mathbf{e}_1 = 0$. Therefore, we have $\mathcal{H}^i \mathbf{q}_1 = Q_{2m} T_{2m}^i \mathbf{e}_1$ and thus (4.7) holds. Furthermore, R_{2m} in (4.7) is nonsingular and $\mathbf{\Pi}^+$ -upper triangular. Hence, $\text{rank}(K_{2m}(\mathcal{H}, \mathbf{q}_1)) = 2m$. \square

Theorem 4.3 (Implicit Γ -orthogonality theorem). Let $\mathcal{H} \in \mathbf{\Pi}_{2n}^-$ be $\mathbf{\Pi}^-$ -symmetric with respect to Γ and $Q, \tilde{Q} \in \mathbb{R}^{2n \times 2n}$ be two Γ -orthogonal $\mathbf{\Pi}^+$ -matrices with respect to $\Gamma \in \Gamma_{2n}$. Assume $Q \mathbf{e}_1 = \tilde{Q} \mathbf{e}_1$ and let

$$\Gamma' = Q^\top \Gamma Q, \quad \tilde{\Gamma}' = \tilde{Q}^\top \Gamma \tilde{Q}.$$

Algorithm 5.1 The simple Γ QR algorithm.

Input: $\mathcal{H} \in \Pi_{2n}^-$ a Π^- -symmetric matrix with respect to $\Gamma \in \Gamma_{2n}$;
Output: $\Gamma' \mathcal{H} \in \mathbb{qD}_{2n}^+$ (Π^+ -quasi-diagonal).

- 1: $\mathcal{H}_1 \leftarrow \mathcal{H}, \Gamma_1 \leftarrow \Gamma, i = 1$;
 - 2: **repeat**
 - 3: compute the Γ QR factorization with respect to Γ_i : $\mathcal{H}_i = Q_i R_i$;
 - 4: $\Gamma_{i+1} \leftarrow Q_i^\top \Gamma_i Q_i \in \Gamma_{2n}, \mathcal{H}_{i+1} \leftarrow R_i Q_i$;
 - 5: $i \leftarrow i + 1$;
 - 6: **until** convergence $\mathcal{H} \leftarrow \mathcal{H}_i$.
-

If $\mathcal{H}Q = QT_{2n}$ and $\mathcal{H}\tilde{Q} = \tilde{Q}\tilde{T}_{2n}$, where $\Gamma'T_{2n}$ and $\tilde{\Gamma}'\tilde{T}_{2n}$ are unreduced Π^+ -sym-tridiagonal, i.e., T_{2n} and \tilde{T}_{2n} are unreduced Π^- -sym-tridiagonal with respect to Γ' and $\tilde{\Gamma}'$, respectively, then $Q = \tilde{Q}D, \Gamma' = \tilde{\Gamma}'$, and $T_{2n} = D\tilde{T}_{2n}D$ for some $D = \text{diag}(J, J)$ with $J \in \mathbb{J}_n$.

Proof. By Theorem 4.2, it holds that

$$K_{2n}(\mathcal{H}, Qe_1) = QR = \tilde{Q}\tilde{R} = K_{2n}(\mathcal{H}, \tilde{Q}e_1),$$

where R and \tilde{R} are nonsingular and Π^+ -upper triangular. From Theorem 3.1(i), we know that the Γ QR factorization of the nonsingular $K_{2n}(\mathcal{H}, Qe_1)$ is unique modulo some Π^+ -diagonal $D = \text{diag}(J, J)$ with $J \in \mathbb{J}_n$. Thus, $\tilde{Q} = QD, \tilde{R} = DR$, and consequently

$$\begin{aligned} \tilde{\Gamma}' &= \tilde{Q}^\top \Gamma \tilde{Q} = DQ^\top \Gamma QD = D\Gamma'D = \Gamma', \\ \tilde{T}_{2n} &= \tilde{\Gamma}'\tilde{Q}^\top \Gamma \mathcal{H} \tilde{Q} = \Gamma'DQ^\top \Gamma \mathcal{H} QD = D(\Gamma'Q^\top \Gamma)\mathcal{H}QD = DT_{2n}D, \end{aligned}$$

as expected. \square

5. Γ QR algorithms

Based on Γ QR factorizations of Π^- -matrices and inspired by the usual QR algorithm for the standard eigenvalue problem [22], in this section, we will develop structure-preserving Γ QR algorithms for solving the LREP (1.4) of a Π^- -symmetric matrix \mathcal{H} with respect to $\Gamma \in \Gamma_{2n}$. A straightforward extension of the usual QR algorithm is outlined in Algorithm 5.1.

Proposition 5.1. *The following statements hold for Algorithm 5.1.*

- (i) $Q_i^{-1} = \Gamma_{i+1}Q_i^\top \Gamma_i, \mathcal{H}_{i+1} = Q_i^{-1} \mathcal{H}_i Q_i = R_i \mathcal{H}_i R_i^{-1}, \Gamma_{i+1} \mathcal{H}_{i+1} = Q_i^\top (\Gamma_i \mathcal{H}_i) Q_i$.
- (ii) $\mathcal{H}_{i+1} = (Q_1 \cdots Q_i)^{-1} \mathcal{H} (Q_1 \cdots Q_i), \Gamma_{i+1} \mathcal{H}_{i+1} = (Q_1 \cdots Q_i)^\top (\Gamma \mathcal{H}) (Q_1 \cdots Q_i)$.
 Furthermore, \mathcal{H}_i is Π^- -symmetric with respect to Γ_i .
- (iii) $\mathcal{H}_{i+1} = (R_i \cdots R_1) \mathcal{H} (R_i \cdots R_1)^{-1}, \Gamma_{i+1} = (Q_1 \cdots Q_i)^\top \Gamma (Q_1 \cdots Q_i)$.
- (iv) $\mathcal{H}^i = (Q_1 \cdots Q_i)(R_i \cdots R_1)$.

Let the spectral decomposition of \mathcal{H} be

$$\mathcal{H}X = X\Lambda \quad \text{with} \quad \Lambda \in \mathbb{q}\mathbb{D}_{2n}^-, \quad X \in \mathbf{\Pi}_{2n}^+. \tag{5.1a}$$

For P as in (3.3), we have

$$P^\top AP = \text{diag}(A_1, \dots, A_\ell) \quad \text{with} \quad \text{eig}(A_i) = \{\pm\lambda_i\}, \quad \text{or} \quad \text{eig}(A_i) = \{\pm\lambda_i, \pm\bar{\lambda}_i\}. \tag{5.1b}$$

In light of the convergence proof of the HR algorithm in [18], we can also prove the convergence of Algorithm 5.1.

Theorem 5.1. *Given $\Gamma \in \mathbf{\Gamma}_{2n}$, let $\mathcal{H} \in \mathbf{\Pi}_{2n}^-$ be $\mathbf{\Pi}^-$ -symmetric with respect to Γ having the spectral decomposition (5.1). Suppose $|\lambda_1| > \dots > |\lambda_\ell| > 0$ and Algorithm 5.1 is executable for \mathcal{H} in the sense that all Γ QR factorizations at line 3 exist. If the $\mathbf{\Pi}^+$ -LU factorization of $X^{-1} = L_{\mathbf{x}}U_{\mathbf{x}}$ exists, where $L_{\mathbf{x}}^\top, U_{\mathbf{x}} \in \mathbb{q}\mathbb{U}_{2n}^+$ with $L_{\mathbf{x}}$ having 1×1 and/or 2×2 unit diagonal blocks, conforming to the block structure of Λ and if the Γ QR factorization of $X = Q_{\mathbf{x}}R_{\mathbf{x}}$ with respect to Γ exists, then \mathcal{H}_i in Algorithm 5.1 converges to a $\mathbf{\Pi}^-$ -quasi-diagonal matrix with its eigenvalues λ_i emerging in the order of $\lambda_1, \lambda_2, \dots, \lambda_\ell$, as $i \rightarrow \infty$.*

Proof. From the assumption, it follows that $\Lambda^i L_{\mathbf{x}} \Lambda^{-i} = I + E_i$ with $E_i \rightarrow 0$ as $i \rightarrow \infty$. Let $(I + R_{\mathbf{x}}E_i R_{\mathbf{x}}^{-1}) = \tilde{Q}_i \tilde{R}_i$ be the Γ QR factorization with respect to $\Gamma' := Q_{\mathbf{x}}^\top \Gamma Q_{\mathbf{x}}$, and set $\tilde{\Gamma}_{i+1} := \tilde{Q}_i^\top \Gamma' \tilde{Q}_i \in \mathbf{\Gamma}_{2n}$. It holds that $\tilde{Q}_i \rightarrow I_{2n}$ because $E_i \rightarrow 0$.

For i sufficiently large, we have

$$\begin{aligned} \mathcal{H}^i &= X\Lambda^i X^{-1} = X\Lambda^i L_{\mathbf{x}} \Lambda^{-i} \Lambda^i U_{\mathbf{x}} \\ &= X(I + E_i)\Lambda^i U_{\mathbf{x}} \\ &= Q_{\mathbf{x}}(I + R_{\mathbf{x}}E_i R_{\mathbf{x}}^{-1})R_{\mathbf{x}}\Lambda^i U_{\mathbf{x}} \\ &= (Q_{\mathbf{x}}\tilde{Q}_i)\tilde{R}_i R_{\mathbf{x}}\Lambda^i U_{\mathbf{x}} \end{aligned}$$

which gives a Γ QR factorization of \mathcal{H}^i . On the other hand,

$$\mathcal{H}^i = (Q_1 \cdots Q_i)(R_i \cdots R_1)$$

by Proposition 5.1(ii). Now apply the uniqueness of the Γ QR factorization as stated in Theorem 3.1(i) to conclude that there is $D_i = \text{diag}(J_i, J_i)$ with $J_i \in \mathbb{J}_n$ such that

$$(Q_{\mathbf{x}}\tilde{Q}_i)D_i = Q_1 \cdots Q_i, \quad D_i(\tilde{R}_i R_{\mathbf{x}} \Lambda^i U_{\mathbf{x}}) = R_i \cdots R_1,$$

and $\tilde{\Gamma}_{i+1} = \Gamma_{i+1}$. By Proposition 5.1(ii), we have

$$\mathcal{H}_{i+1} = D_i \tilde{Q}_i^{-1} Q_{\mathbf{x}}^{-1} \mathcal{H} Q_{\mathbf{x}} \tilde{Q}_i D_i = D_i \tilde{Q}_i^{-1} R_{\mathbf{x}} \Lambda R_{\mathbf{x}}^{-1} \tilde{Q}_i D_i$$

Algorithm 5.2 Π^- -sym-tridiagonalization.

Input: Π^- -symmetric matrix \mathcal{H} with respect to $\Gamma = \text{diag}(J, -J)$ with $J = \text{diag}(\gamma_1, \dots, \gamma_n) \in \mathbb{J}_n$;

Output: $Q \in \mathbb{O}_{2n}^+$ with respect to Γ , $\Gamma' = Q^\top \Gamma Q \in \Gamma_{2n}$, and $\mathcal{H}' = Q^{-1} \mathcal{H} Q$ is a Π^- -sym-tridiagonal matrix with respect to Γ' .

- 1: $Q \leftarrow I_{2n}$, $\Gamma_{\text{sav}} \leftarrow \Gamma$, $\mathcal{H}_{\text{sav}} \leftarrow \mathcal{H}$, $n' \leftarrow 2n$;
 - 2: **for** $\ell = 1 : n - 1$ **do**
 - 3: $\ell' \leftarrow n + \ell + 1$, $\mathbf{u} \leftarrow G_{(:, \ell)}$;
 - 4: compute Hyp_Householder Γ -orthogonal transformation¹ $\tilde{Q}^{-1} = \mathcal{Q}_h(\ell' : n'; \mathbf{u})$ with respect to Γ (by (3.13));
 - 5: $Q \leftarrow Q \tilde{Q}$, $\mathcal{H} \leftarrow \tilde{Q}^{-1} \mathcal{H} \tilde{Q}$, $\Gamma \leftarrow -\Gamma'$ (by (3.15));
 - 6: $\alpha \leftarrow \mathcal{H}_{(\ell+1, \ell)}$, $\beta \leftarrow \mathcal{H}_{(\ell', \ell)}$;
 - 7: compute Hyp_Givens Γ -orthogonal transformation $\tilde{Q}^{-1} = \mathcal{Q}_g(\ell + 1; \alpha, \beta)$ with respect to Γ (by (3.17));
 - 8: $Q \leftarrow Q \tilde{Q}$, $\mathcal{H} \leftarrow \tilde{Q}^{-1} \mathcal{H} \tilde{Q}$, $\Gamma \leftarrow \Gamma'$ (by (3.18));
 - 9: $\mathbf{u} \leftarrow \mathcal{H}_{(:, \ell)}$;
 - 10: Compute Hyp_Householder Γ -orthogonal transformation $\tilde{Q}^{-1} = \mathcal{Q}_h(\ell + 1 : n; \mathbf{u})$ with respect to Γ (by (3.13));
 - 11: $Q \leftarrow Q \tilde{Q}$, $\mathcal{H} \leftarrow \tilde{Q}^{-1} \mathcal{H} \tilde{Q}$, $\Gamma \leftarrow \Gamma'$ (by (3.18));
 - 12: **end for**
 - 13: **return** $\Gamma' \leftarrow \Gamma$, $\Gamma \leftarrow \Gamma_{\text{sav}}$, $\mathcal{H}' \leftarrow \mathcal{H}$, $\mathcal{H} \leftarrow \mathcal{H}_{\text{sav}}$;
-

¹ We set $\mathcal{Q}_h(\ell : m; \mathbf{u}) = I$ if $\ell = m$.

which converges to a Π^- -quasi-diagonal matrix with its eigenvalues emerging in the order of $\lambda_1, \lambda_2, \dots, \lambda_\ell$, as $i \rightarrow \infty$. \square

In what follows, using Algorithm 5.1 as the basis, we focus on developing an efficient structure-preserving Γ QR algorithm to solve the eigenvalue problem (1.4) for the Π^- -symmetric matrix \mathcal{H} with respect to a given Γ such as Γ_0 in (1.2). To do so, we first reduce \mathcal{H} to its Π^- -sym-tridiagonal form with respect to Γ and then use the two special Γ -orthogonal transformations described in section 3 to implicitly carry out lines 3 and 4 in Algorithm 5.1. The first phase, the Π^- -sym-tridiagonalization, is given in Algorithm 5.2. To illustrate the elimination process in the Π^- -sym-tridiagonalization, we trace actions on a small example with $n = 4$ in Fig. 5.1. In general, after $(n - 1)$ steps in Π^- -sym-tridiagonalization, we have computed $3n - 2$ Γ -orthogonal matrices $\tilde{Q}_1, \dots, \tilde{Q}_{3n-2}$ such that

$$(\tilde{Q}_1 \cdots \tilde{Q}_{3n-2})^{-1} \mathcal{H} (\tilde{Q}_1 \cdots \tilde{Q}_{3n-2}) = \mathcal{H}'$$

is Π^- -sym-tridiagonal with respect to Γ' .

As in the usual QR algorithm, the shift technique should be incorporated to accelerate the convergence of the simple Γ QR algorithm – Algorithm 5.1. By Proposition 2.2, we choose the filtering polynomials $p(x)$ as

$$\begin{cases} p(x) = (x - \lambda)(x + \lambda) & \text{for real or imaginary } \lambda, \\ p(x) = (x - \lambda)(x + \lambda)(x - \bar{\lambda})(x + \bar{\lambda}) & \text{for complex } \lambda \end{cases} \quad (5.2)$$

$$\begin{aligned}
 \mathcal{H} \leftarrow \begin{bmatrix} \times & \times & \times & \times & | & \times & \times & \times & \times \\ \times & \times & \times & \times & | & \times & \times & \times & \times \\ \times & \times & \times & \times & | & \times & \times & \times & \times \\ \times & \times & \times & \times & | & \times & \times & \times & \times \\ \times & \times & \times & \times & | & \times & \times & \times & \times \end{bmatrix}, & \quad \mathcal{H} \leftarrow \tilde{Q}_1^{-1} \mathcal{H} \tilde{Q}_1 = \begin{bmatrix} \times & \times & \times & \times & | & \times & \times & 0 & 0 \\ \times & \times & \times & \times & | & \times & \times & \times & \times \\ \times & \times & \times & \times & | & 0 & \times & \times & \times \\ \times & \times & \times & \times & | & 0 & \times & \times & \times \\ \times & \times & \times & \times & | & 0 & \times & \times & \times \end{bmatrix}, \\
 \tilde{Q}_1^{-1} = \mathcal{Q}_h(6 : 8; \mathbf{u}) & \\
 \\
 \mathcal{H} \leftarrow \tilde{Q}_2^{-1} \mathcal{H} \tilde{Q}_2 = \begin{bmatrix} \times & \times & \times & \times & | & 0 & 0 & 0 & 0 \\ \times & \times & \times & \times & | & 0 & \times & \times & \times \\ \times & \times & \times & \times & | & 0 & \times & \times & \times \\ \times & \times & \times & \times & | & 0 & \times & \times & \times \\ \times & \times & \times & \times & | & 0 & \times & \times & \times \end{bmatrix}, & \quad \mathcal{H} \leftarrow \tilde{Q}_3^{-1} \mathcal{H} \tilde{Q}_3 = \begin{bmatrix} \times & \times & 0 & 0 & | & \times & 0 & 0 & 0 \\ \times & \times & \times & \times & | & \times & \times & \times & \times \\ 0 & \times & \times & \times & | & 0 & \times & \times & \times \\ 0 & \times & \times & \times & | & 0 & \times & \times & \times \\ 0 & \times & \times & \times & | & 0 & \times & \times & \times \end{bmatrix}, \\
 \tilde{Q}_2^{-1} = \mathcal{Q}_g(2 : \alpha, \beta) & \quad \tilde{Q}_3^{-1} = \mathcal{Q}_h(2 : 4; \mathbf{u}) \\
 \\
 \mathcal{H} \leftarrow \tilde{Q}_4^{-1} \mathcal{H} \tilde{Q}_4 = \begin{bmatrix} \times & \times & 0 & 0 & | & \times & 0 & 0 & 0 \\ \times & \times & \times & \times & | & 0 & \times & \times & 0 \\ 0 & \times & \times & \times & | & 0 & \times & \times & \times \\ 0 & \times & \times & \times & | & 0 & 0 & \times & \times \\ \times & 0 & 0 & 0 & | & \times & \times & 0 & 0 \\ 0 & \times & \times & 0 & | & \times & \times & \times & \times \\ 0 & \times & \times & \times & | & 0 & \times & \times & \times \\ 0 & 0 & \times & \times & | & 0 & \times & \times & \times \end{bmatrix}, & \quad \mathcal{H} \leftarrow \tilde{Q}_5^{-1} \mathcal{H} \tilde{Q}_5 = \begin{bmatrix} \times & \times & 0 & 0 & | & \times & 0 & 0 & 0 \\ \times & \times & \times & \times & | & 0 & \times & 0 & 0 \\ 0 & \times & \times & \times & | & 0 & \times & \times & \times \\ 0 & \times & \times & \times & | & 0 & \times & \times & \times \\ \times & 0 & 0 & 0 & | & \times & \times & 0 & 0 \\ 0 & \times & 0 & 0 & | & \times & \times & \times & \times \\ 0 & 0 & \times & \times & | & 0 & \times & \times & \times \\ 0 & 0 & \times & \times & | & 0 & \times & \times & \times \end{bmatrix}, \\
 \tilde{Q}_4^{-1} = \mathcal{Q}_h(7 : 8; \mathbf{u}) & \quad \tilde{Q}_5^{-1} = \mathcal{Q}_g(3 : \alpha, \beta) \\
 \\
 \mathcal{H} \leftarrow \tilde{Q}_6^{-1} \mathcal{H} \tilde{Q}_6 = \begin{bmatrix} \times & \times & 0 & 0 & | & \times & 0 & 0 & 0 \\ \times & \times & \times & 0 & | & 0 & \times & 0 & 0 \\ 0 & \times & \times & \times & | & 0 & 0 & \times & \times \\ 0 & 0 & \times & \times & | & 0 & 0 & \times & \times \\ \times & 0 & 0 & 0 & | & \times & \times & 0 & 0 \\ 0 & \times & 0 & 0 & | & \times & \times & \times & 0 \\ 0 & 0 & \times & \times & | & 0 & \times & \times & \times \\ 0 & 0 & \times & \times & | & 0 & 0 & \times & \times \end{bmatrix}, & \quad \mathcal{H} \leftarrow \tilde{Q}_7^{-1} \mathcal{H} \tilde{Q}_7 = \begin{bmatrix} \times & \times & 0 & 0 & | & \times & 0 & 0 & 0 \\ \times & \times & \times & 0 & | & 0 & \times & 0 & 0 \\ 0 & \times & \times & \times & | & 0 & \times & \times & 0 \\ 0 & 0 & \times & \times & | & 0 & 0 & \times & \times \\ \times & 0 & 0 & 0 & | & \times & \times & 0 & 0 \\ 0 & \times & 0 & 0 & | & \times & \times & \times & 0 \\ 0 & 0 & \times & \times & | & 0 & \times & \times & \times \\ 0 & 0 & 0 & \times & | & 0 & 0 & \times & \times \end{bmatrix}. \\
 \tilde{Q}_6^{-1} = \mathcal{Q}_h(3 : 4; \mathbf{u}) & \quad \tilde{Q}_7^{-1} = \mathcal{Q}_g(4 : \alpha, \beta)
 \end{aligned}$$

Fig. 5.1. The Π^- -sym-tridiagonalization for $n = 4$.

to ensure $p(\mathcal{H}) \in \Pi_{2n}^+$. On the other hand, from Theorem 4.3, because of the uniqueness of the Π^- -sym-tridiagonalization of \mathcal{H} , the Γ QR factorization can be performed without explicitly computing the Γ QR factorization of $p(\mathcal{H})$. It only needs to construct a Γ -orthogonal transformation Q to reduce the first column of $p(\mathcal{H})$ to a vector parallel to \mathbf{e}_1 . We outline the implicit multi-shift Γ QR algorithm in Algorithm 5.3.

Remark 5.1.

- (i) In Algorithm 5.3, lines 11–13 can be executed in two substeps with $p_1(x)$ and $p_2(x)$, respectively, where

$$p_1(x) = (x - \lambda_1)(x + \lambda_1), \quad p_2(x) = (x - \lambda_2)(x + \lambda_2)$$

for real or purely imaginary λ_1 and λ_2 , and

$$p_1(x) = (x - \lambda_1)(x - \bar{\lambda}_1), \quad p_2(x) = (x + \lambda_1)(x + \bar{\lambda}_1)$$

for complex λ_1 . Doing so enables that all computations are done in the real arithmetics.

Algorithm 5.3 Implicit multi-shift Γ QR algorithm.

Input: Π^- -symmetric matrix \mathcal{H} with respect to $\Gamma = \text{diag}(J, -J)$ with $J = \text{diag}(\gamma_1, \dots, \gamma_n) \in \mathbb{J}_n$, and tolerance ϵ ;

Output: $Q \in \mathbb{O}_{2n}^+$ with respect to Γ , $\Gamma' = Q^\top \Gamma Q \in \Gamma_{2n}$, $\Lambda = Q^{-1} \mathcal{H} Q \in \mathbb{q}\mathbb{D}_{2n}^-$;

```

1:  $\Gamma_{\text{sav}} \leftarrow \Gamma$ ,  $\mathcal{H}_{\text{sav}} \leftarrow \mathcal{H}$ ,  $Q \leftarrow I_{2n}$ ,  $\Lambda_i \leftarrow \emptyset$  ( $i = 1, 2$ );
2: while  $n > 2$  do
3:   Use Algorithm 5.2 to perform  $\Pi^-$ -sym-tridiagonalization:  $\mathcal{H} \leftarrow \tilde{Q}^{-1} \mathcal{H} \tilde{Q}$ ,  $Q \leftarrow Q \tilde{Q}$ ,  $\Gamma \leftarrow \Gamma'$  ( $\Gamma'$  is
   an output of Algorithm 5.2);
4:   if  $|\mathcal{H}_{(n,n-1)}| < \epsilon(|\mathcal{H}_{(n-1,n-1)}| + |\mathcal{H}_{(n,n)}|)$  then
5:      $\Lambda_1 \leftarrow \text{diag}(\mathcal{H}_{(n,n)}, \Lambda_1)$ ,  $\Lambda_2 \leftarrow \text{diag}(\mathcal{H}_{(2n,n)}, \Lambda_2)$ ,
      $\mathbb{I} = [1, \dots, n-1, n+1, \dots, 2n-1]$ ,  $\mathcal{H} \leftarrow \mathcal{H}_{(\mathbb{I}, \mathbb{I})}$ ,  $\Gamma \leftarrow \Gamma_{(\mathbb{I}, \mathbb{I})}$ ,  $n \leftarrow n-1$ ;
6:   else
7:     if  $|\mathcal{H}_{(n-1,n-2)}| < \epsilon(|\mathcal{H}_{(n-2,n-2)}| + |\mathcal{H}_{(n-1,n-1)}|)$  then
8:        $\Lambda_1 \leftarrow \text{diag}(\mathcal{H}_{([n-1,n],[n-1,n])}, \Lambda_1)$ ,  $\Lambda_2 \leftarrow \text{diag}(\mathcal{H}_{([2n-1,2n],[n-1,n])}, \Lambda_2)$ ,  $\mathbb{I} = [1, \dots, n-2, n+1, \dots, 2n-2]$ ,  $\mathcal{H} \leftarrow \mathcal{H}_{(\mathbb{I}, \mathbb{I})}$ ,  $\Gamma \leftarrow \Gamma_{(\mathbb{I}, \mathbb{I})}$ ,  $n \leftarrow n-2$ ;
9:     else
10:       $\mathbb{I} = [n-1, n, 2n-1, 2n]$ ,  $H_4 = \mathcal{H}_{(\mathbb{I}, \mathbb{I})}$ , and compute  $\text{eig}(H_4) = \{\pm\lambda_1, \pm\lambda_2\}$ ;
11:       $\mathbf{h} = p(\mathcal{H})\mathbf{e}_1$ , where  $p(x)$  is as given in (5.2) (see also Remark 5.1(i)).
12:      construct the  $\Gamma$ -orthogonal transformation  $Q_1$  such that  $Q_1^{-1}\mathbf{h} = \mathbf{h}\mathbf{e}_1$ ;
13:       $\mathcal{H} \leftarrow Q_1^{-1} \mathcal{H} Q_1$ ,  $Q \leftarrow Q Q_1$ ,  $\Gamma \leftarrow \Gamma'$ ;
14:    end if
15:  end if
16: end while
17:  $\Lambda := \begin{bmatrix} \Lambda_1 & \Lambda_2 \\ -\Lambda_2 & -\Lambda_1 \end{bmatrix} \in \mathbb{q}\mathbb{D}_{2n}^-$ ,  $\Gamma' \leftarrow \Gamma$ ,  $\Gamma \leftarrow \Gamma_{\text{sav}}$ ,  $\mathcal{H} \leftarrow \mathcal{H}_{\text{sav}}$ .

```

Table 5.1
The flop counts of the Γ QR algorithm and the PQR algorithm.

Methods	Phase	Flop
Γ QR	i Π^- -sym-tridiagonalization on \mathcal{H} by Algorithm 5.2	$8n^3$
	ii one step of implicit double-shift Γ QR iteration (Algorithm 5.3)	$120n$
PQR	i Hessenberg-triangular reduction by Householder transformation on $JKJM$ in (1.5)	$11n^3$
	ii one step of implicit double-shift PQR iteration [23]	$35n^2$

(ii) There are many other structure-preserving approaches as discussed in Section 1. Based on the characteristic analysis of these algorithms, we will compare the performance of the Γ QR algorithm with that of the PQR algorithm [16] in our numerical studies. The flop counts of the implicit multi-shift Γ QR algorithm and the PQR algorithm for a Π^- -symmetric matrix \mathcal{H} with respect to Γ are summarized in Table 5.1. In each phase, the Γ QR algorithm consumes less than the PQR algorithm, especially in each iterative step in Phase ii. This is because the PQR algorithm cannot take advantage of the symmetric structures in JA, JB of (1.4b) but has to treat them like an n -by- n nonsymmetric matrix.

6. Numerical experiments

To test the efficiency of the Γ QR algorithm, we borrow K and M in the numerical example of [5] for the sodium dimer Na_2 with order $n = 1862$. They are symmetric positive definite. We then recover the Casida’s eigenvalue problem as in (1.1) by $A = \frac{1}{2}(K + M) - 4.88I_n$ and $B = \frac{1}{2}(K - M)$ with an excitation energy 4.88, and reset

Table 6.1
The CPU time by Γ QR and PQR.

Methods	Phase	Time (s)
Γ QR	i $\mathbf{\Pi}^-$ -sym-tridiagonalization of \mathcal{H} with Q accumulated	326.05
	ii Implicit Γ QR algorithm (Algorithm 5.3)	399.23
PQR ²	i Hessenberg-triangular reduction on KM	643.02
	ii Implicit PQR algorithm	2078.09

² jupiter.math.nctu.edu.tw/~wwlin/code/PQZ.zip.

$K = A - B, M = A + B$. In Table 6.1, we list the CPU time by the Γ QR algorithm and the PQR algorithm for the computation of eigenvalues of $\mathcal{H} = \begin{bmatrix} A & B \\ -B & -A \end{bmatrix}$ and KM , respectively.

All numerical computations are carried out by MATLAB Version 2014b, on a MacBook Pro with a 2.8 GHz Intel Core i7 processor and 8GB RAM, with the unit machine roundoff $u = 2^{-53} = 1.11 \times 10^{-16}$.

Table 6.1 shows that the PQR algorithm takes about 3.6 times as much the CPU time as the Γ QR algorithm does. The Γ QR algorithm is much cheaper than the PQR algorithm, as expected from Table 5.1.

To demonstrate accuracies in computed approximations, we calculate the normalized residual norms for the j th approximate eigenpair (μ_j, \mathbf{z}_j) :

$$r(\mu_j) = \frac{\|\mathcal{H}\mathbf{z}_j - \mu_j\mathbf{z}_j\|_1}{(\|\mathcal{H}\|_1 + |\mu_j|)\|\mathbf{z}_j\|_1}.$$

The approximate eigenpair (μ_j, \mathbf{z}_j) is computed, as follows, by step (a) or, by step (a) followed by step (b) for more accurate approximate eigenpairs:

- (a) Apply the inverse iteration with the computed eigenvalues $\mu_j^{(0)}$ (by Algorithm 5.3) as the shifts to the $\mathbf{\Pi}^-$ -sym-tridiagonal matrix (the output of Algorithm 5.2) to compute an approximate eigenpairs $(\tilde{\mu}_j, \tilde{\mathbf{z}}_j)$ of the $\mathbf{\Pi}^-$ -sym-tridiagonal matrix, and finally use $(\tilde{\mu}_j, \tilde{Q}\tilde{\mathbf{z}}_j)$ as approximate eigenpairs of the original \mathcal{H} , where \tilde{Q} is an output of Algorithm 5.2.
- (b) Further apply the inverse iteration on $(\tilde{\mu}_j, \tilde{Q}\tilde{\mathbf{z}}_j)$ from item (a) to the original $\mathbf{\Pi}^-$ -symmetric \mathcal{H} to get more accurate approximate eigenpair (μ_j, \mathbf{z}_j) of the original \mathcal{H} .

In principle, at step (a), the eigenvectors to the $\mathbf{\Pi}^-$ -sym-tridiagonal matrix (the output of Algorithm 5.2) can be read off from the accumulated Q -matrix within Algorithm 5.3. But the columns of the Q -matrix may provide poor approximations due to the fact that the Γ -orthogonal transformations used in the algorithm are not orthogonal. There are a large number of them, resulting possibly large errors in the accumulated Q -matrix. Fortunately, because of the extremely simple structure in the $\mathbf{\Pi}^-$ -sym-tridiagonal matrix, the inverse iterations are very cheap and at the same time eigenvalues $\mu_j^{(0)}$ are improved,

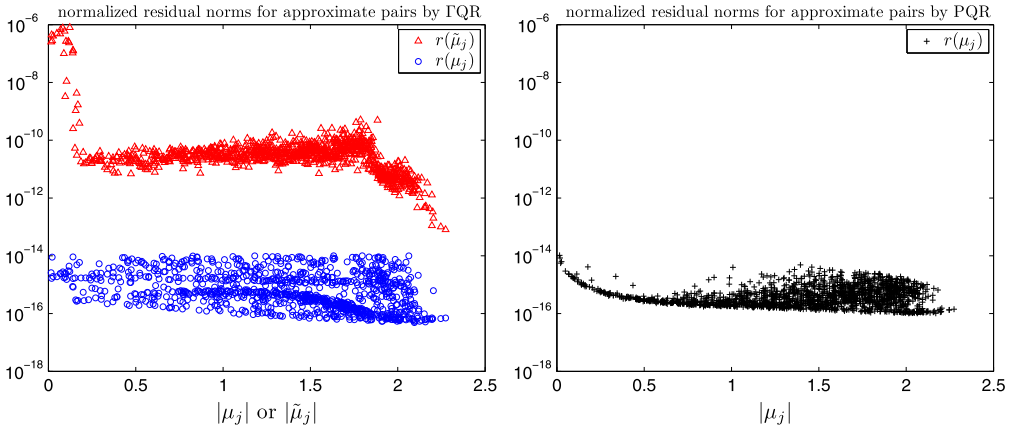


Fig. 6.1. Normalize residual norms for approximate eigenpairs by Γ QR (left) and by PQR (right). The approximate eigenpairs by Γ QR with step (a) are decent, although not as good as the ones with step (b) which is expensive and those by PQR which is also much more expensive than Γ QR excluding step (b).

too. However, the inverse iterations in step (b) can be expensive and thus should be only performed when the accuracy of the approximate eigenpairs from step (a) is not adequate.

On the other hand, the approximate eigenpairs of the PQR algorithm are computed, currently in our code, by applying the inverse iteration with the computed eigenvalues as the shift to the upper Hessenberg form of $(JK)(JM)$, and then they are transformed back to find approximate eigenpairs of $(JK)(JM)$ first and finally approximate eigenpairs (μ_j, z_j) of \mathcal{H} in the way as described in the paragraph after (1.5).

The dominant step for the computation of eigenpairs by the Γ QR algorithm is the LU factorization of the matrix $\mathcal{H} - \mu_j I$ for the inverse iteration if step (b) above is performed. Hopefully, in most applications, approximate eigenpairs from step (a) are accurate enough.

In general, the Hyp_Householder and Hyp_Givens transformations are not orthogonal matrices which may lead to loss of accuracy during the reduction/iteration process in the Γ QR algorithm. However, the Hyp_Householder and Hyp_Givens transformations are Γ -orthogonal, which are strongly structure-preserving for \mathbf{II}^- -symmetric matrix with respect to Γ , and the entry magnitudes of the reduced \mathbf{II}^- -symmetric matrix somehow achieve some balanced state. This is the reason why the Γ QR algorithm still keeps good accuracy.

In Fig. 6.1, we plot, in the left figure for Γ QR, the normalized residual norms $r(\tilde{\mu}_j)$ for $(\tilde{\mu}_j, \tilde{Q}\tilde{z}_j)$ obtained at the end of step (a) above and $r(\mu_j)$ for (μ_j, z_j) obtained at the end of step (b), and, in the right figure for PQR, the normalized residual norms $r(\mu_j)$. What we can see is that, as far as normalized residual norms are concerned, the approximation eigenpairs by Γ QR at the end of step (a) are still inferior to the ones at the end of step (b) and the ones by PQR, but as we commented above step (b) is very expensive, especially when a large number of eigenpairs are needed and PQR is much

more expensive than Γ QR excluding step (b). On the other hand, we argue that the normalized residual norms for Γ QR with step (a) are still very decent and likely good enough for most applications.

7. Conclusions

In this paper, we developed an efficient implicit multi-shift Γ QR algorithm for solving the linear response eigenvalue problem (LREP) in (1.1) structurally. This algorithm relies on two basic Γ -orthogonal transformations, which preserve $\mathbf{\Pi}^-$ -symmetric structure of \mathcal{H} with respect to given Γ throughout the whole computation. Thus the computed eigenvalues and eigenvectors are guaranteed to appear pairwise as in $\{(\lambda, \mathbf{x}), (-\lambda, \mathbf{\Pi}\mathbf{x})\}$ for a real or purely imaginary eigenvalue λ and in $\{(\lambda, \mathbf{x}), (-\lambda, \mathbf{\Pi}\mathbf{x}), (\bar{\lambda}, \bar{\mathbf{x}}), (-\bar{\lambda}, \mathbf{\Pi}\bar{\mathbf{x}})\}$ for a true complex eigenvalue λ . Note that, these structures will be lost if the Γ -orthogonality is not preserved, as in the HR algorithm [18] and the usual QR algorithm. We accelerate the convergence of the Γ QR algorithm by using the double-shift technique based on the implicit Γ -orthogonality theorem. The final algorithm can be found in Algorithm 5.3.

We presented a brief comparison of our Γ QR algorithm with the block structure-preserving periodic QR algorithm – the PQR algorithm [16]. Our algorithm costs much less than the PQR algorithm in the flop counts, and also the numerical experiment shows that the Γ QR algorithm can compute eigenpairs at a fractional CPU time by PQR.

In summary, the Γ QR algorithm is an efficient structure-preserving algorithm for solving the $\mathbf{\Pi}^-$ -symmetric eigenvalue problem compared with the other existing algorithms. But our current implementation is not sophisticated enough to incorporate many useful ideas developed in the past for the QR algorithm, most notably aggressive early deflations [24,25]. We think some of these ideas with modifications should naturally apply and plan to pursue them elsewhere.

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